Semiclassical Approach To Systems Of Identical Particles

Diplomarbeit

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1 Introduction

During the last century regarding the history of physics, quantum mechanics has become an invaluable theory in describing fundamental properties of physical reality. All former theories, subsumed by the notion of classical physics, have turned out to fail as a sufficient description of microscopic systems. In contrast to that, quantum mechanics in its present form, as developed around 1930, has been extraordinarily successful in the correct reproduction of experimental results that elude classical explanations.

Since the quantum theory requires a mathematical framework incomparably more complex than classical mechanics, there is only a handful of simple quantum systems that can be solved exactly. Nonetheless, there has been developed a variety of powerful methods to obtain approximations of quantum properties like the spectrum of energies. Among them are for example perturbation theory for the description of a slightly perturbed but otherwise solvable system, or the Born-Oppenheimer approximation that decouples systems composed of very light and very heavy particles, like the electrons and nuclei in a molecule. Other methods to mention are mean-field approaches that are reducing systems of many particles into single particle systems with effective mean-field potentials. Also computer-based numerical calculations have become an important tool since the last decades.

Among all possible ways to simplify and gain access to quantum systems is the approach of semiclassical approximation, which is the basic concept the present work is built on. Semiclassical approximations thereby respect the most fundamental quantum features like interference and superpositions, while they are only based on dynamical properties of the classical analogue of the actual quantum system under investigation. This opens the door to gain intuitive pictures of quantum mechanical systems by relating them to the classical perceptible world, thus the pool of experience in connection to classical dynamics can be used to build up an intuition of quantum mechanical concepts. In this sense the semiclassical approach builds a bridge that allows one to get a better understanding how the perceptible classical world arises from the quantum nature it inherits in its core. Related to that is the special applicability to mesoscopic systems, which form the transition region between the macroscopic and the microscopic world and are defined by quantum wavelengths much smaller than the characteristic system length scales. One might think that in this sense semiclassics constitute a step back in the correct description of physical reality.

But indeed the contrary is the case. There is a variety of quantum systems that are especially accessible by semiclassical approximations. Above all those are systems whose classical analogue obey highly chaotic dynamics and elude other analytical methods. One of the central features of semiclassics is the ability to provide analytical results even in such systems whereas numerical computer simulations always depend on specific parameters and therefore are not an adequate tool to make analytical statements in closed form.
While semiclassics meanwhile has grown up to a well developed field in the context of single particle systems, it still lacks in a well sophisticated methodology applicable to many body systems. One reason for this may be the often used argument that it was pointless to put effort into investigations in this direction because interacting many body systems are too complicated to treat them even in the classical analogue. But one point to hold against this is the knowledge of quantum manifestations of chaos in single particle systems that can be understood semiclassically without explicitly solving the dynamics of the particular classical system. Thus the argument of too complex classical dynamics is not relevant and there is no point in preventing oneself from expanding the powerful tools to systems of many particles. The special feature of many body quantum systems one has to treat carefully is thereby the concept of indistinguishability of particles of the same kind. Second, as can be observed throughout the field of condensed matter physics, when dealing with systems of large particle numbers, one of the most important objects to gain knowledge of is the average behaviour of the quantum density of states, while in many applications, the exact energy level fluctuations are negligible. In single particle systems this average part can be related semiclassically to few fundamental system properties like the volume and the surface of a cavity without the exact knowledge of the classical orbital dynamics. Therefore one can also be hopeful in searching for semiclassical expressions for the smooth part of the density of states in general interacting systems of many identical particles. These two points eventually provide the main subjects to be investigated in the present work.

In the first part of the work we will introduce the general concepts of systems of many identical particles in comparison to single particle systems. The implication of particle exchange symmetry in classical systems on the one hand and quantum mechanical systems on the other hand will be discussed with a special emphasis on the concept of indistinguishability in quantum mechanics. The second section of this chapter shall serve as an introduction to the general concept of the semiclassical approximation in quantum single particle systems. This will lead to the theory of periodic orbits and the theory of short path propagations for an average description, where both together give an asymptotic description of the spectrum of a quantum system.

The second part will incorporate the special concepts inherent to quantum many

body systems into the semiclassical periodic orbit theory. The derivation of a correspondingly modified version of the existing Gutzwiller formula for single particle systems, which is central in the field of semiclassics, will be followed. One main difference will be the inclusion of open orbits which can eventually be related back to periodic orbits. An alternative equivalent description in a reduced phase space will be given, where we put special emphasis on the possibility of constructing such a reduced phase space in the context of many particles. In this description we will find again periodic orbits as the crucial quantities. In order to give an argument of confirmation for the semiclassical approach, we shall relate some general configurations of many body systems to the corresponding single particle systems that are equivalent by means of semiclassical periodic orbit theory with and without exchange symmetry respectively. We will see that these equivalences are also inherent to the particular pairs of many body and single particle systems in a quantum mechanical description. Building on the periodic orbit theory for identical particles the subsequent section treats the issue of statistical analysis of chaotic many body spectra. The classical sum rule of Hannay and Ozorio de Almeida is usually used to obtain universal properties of chaotic quantum spectra by the virtue of semiclassical analysis. In order to obtain similar results in many body systems in an equally rigorous manner the sum rule must be modified. This modification is then also applicable to general discrete symmetries in quantum systems. Exploiting the new sum rule, we will attempt an application to a specific universal statistical property of systems that undergo a transition from time-reversal symmetry to broken time-reversal symmetry. An apparent many body transition catastrophe in the sense of infinitely fast transition in the limit of large particle numbers is discussed. Thereby we will gain clarity that in order to solve the question of a possible catastrophe, an accurate analysis of the smooth part of the many body density of states is indispensable.

In the last chapter we derive a semiclassical approximation to the smooth part of the density of states similar to the Weyl expansion for single particle systems. First we will recognise that, although often supposed and suggested in literature, the Thomas-Fermi-like description by available phase space volume equivalent to a strict zero-length orbit description is not sufficient. In particular, the wrong reproduction of the behaviour around the many body ground state in fermionic systems will become evident.
In order to clarify the reasons for this failure we give an argument of cancellation of energy levels using a convolution formula by Weidenmüller for the exact many body density of states in terms of single particle densities utilisable in systems without particle-particle interaction.
After recognising that an accurate description needs a much more complete analysis, we will relate the full incorporation of exchange symmetry to the propagation over short distances in a Weyl-like manner. For this purpose we address the special features of the geometrical structure of the phase space of many body

systems. The introduction of the notion of cluster zones as vicinities of invariant manifolds under particle exchange will help us to organise the corresponding analysis. General analytical calculations regarding those manifolds will provide potentially useful tools for the future incorporation of particle-particle interactions.
After that, the case of non-interacting particles will be addressed explicitly. The corresponding results will turn out to accurately describe the behaviour of the many body density of states at all energies, especially around and below the many body ground state energy.
Finally we will draw a comparison to the average behaviour of unrestricted and restricted partition number functions known in number theory. The possibility of mutual facilitation of the analysis in the two fields is regarded briefly.
Closing, the general concept of introducing modifications due to short range interactions will be discussed in the last section.

2 Preliminary Concepts

2.1 Systems Of Identical Particles

2.1.1 Exchange Symmetry In Classical Systems

The subject of the present work is the semiclassical treatment of quantum systems of identical particles. Therefore one first should compare the concept of many identical particles in a quantum system with the corresponding classical system. In order to get a basic understanding it is important to point out their similarities and differences. For an introduction to the subject see, for example [26, 7].
First let us consider a classical system of N identical particles moving in D spatial dimensions. Every possible state of the system is then described by (ND) coordinates

$$\mathbf{q} = (\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_N) \qquad \mathbf{q}_i = \left(q_i^{(1)}, \ldots, q_i^{(D)}\right) \tag{2.1}$$

and conjugated momenta

$$\mathbf{p} = (\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_N) \qquad \mathbf{p}_i = \left(p_i^{(1)}, \ldots, p_i^{(D)}\right). \tag{2.2}$$

The concept of identity between particles in a classical system leaves the feature of symmetry with respect to exchanging all properties of any two of the considered particles. In a *Hamiltonian* description of the system this means the invariance of the *classical Hamiltonian* under permutations of the particle labels

$$H(\mathbf{q}, \mathbf{p}) = H(P\mathbf{q}, P\mathbf{p}) \tag{2.3}$$

where the permutation matrix P is a representation of any element of the *symmetric group* $\sigma \in S_N$,

$$\begin{aligned} P\mathbf{q} &= P(\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_N) = \left(\mathbf{q}_{\sigma(1)}, \mathbf{q}_{\sigma(2)}, \ldots, \mathbf{q}_{\sigma(N)}\right), \\ P\mathbf{p} &= P(\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_N) = \left(\mathbf{p}_{\sigma(1)}, \mathbf{p}_{\sigma(2)}, \ldots, \mathbf{p}_{\sigma(N)}\right). \end{aligned} \tag{2.4}$$

This implies that all solutions of *Hamilton's equations* yield again solutions after applying the permutation operations. In order to keep an easy notation the

following considers only one dimension, but holds for each dimension separately. Let $(\mathbf{q}, \mathbf{p})(t)$ be a solution of *Hamilton's equations*

$$\begin{aligned} \dot{p}_i &= -\frac{\partial H}{\partial q_i} \\ \dot{q}_i &= \frac{\partial H}{\partial p_i}. \end{aligned} \tag{2.5}$$

Then $(\mathbf{q}', \mathbf{p}')(t) = (P\mathbf{q}, P\mathbf{p})(t)$ is also a solution:

$$\begin{aligned} \dot{p}'_i &= P_{ij}\dot{p}_j = -P_{ij}\frac{\partial H}{\partial q_j} = -\frac{\partial H}{\partial q_{\sigma(i)}} = -\frac{\partial H}{\partial (P\mathbf{q})_i} = \\ &= -\frac{\partial H\,(P\mathbf{q}, P\mathbf{p})}{\partial (P\mathbf{q})_i} = -\frac{\partial H}{\partial q_i}\,(P\mathbf{q}, P\mathbf{p}) = -\frac{\partial H}{\partial q_i}\,(\mathbf{q}', \mathbf{p}') \end{aligned} \tag{2.6}$$

and similarly

$$\dot{q}'_i = \frac{\partial H}{\partial p_i}\,(\mathbf{q}', \mathbf{p}') \tag{2.7}$$

where H abbreviates $H(\mathbf{q}, \mathbf{p})$. Consider the special case of solutions that run after some time T through an arbitrarily permuted version of the initial phase space point $(\mathbf{q}_0, \mathbf{p}_0) = (\mathbf{q}, \mathbf{p})(t = 0)$

$$(\mathbf{q}, \mathbf{p})(T) = (P\mathbf{q}_0, P\mathbf{p}_0). \tag{2.8}$$

Then the final phase space point (2.8) is at the same time the initial point of the permuted version of the orbit. This means that the continuation of the orbit along time successively runs through all phase space points that are related to $(\mathbf{q}_0, \mathbf{p}_0)$ by powers P^n of P . Due to the finiteness of the symmetric group this eventually includes the identity, which means such an orbit always is periodic. This fact will become important later on.
Any classical system of N particles in D dimensions is completely equivalent to a system of one particle in ND spatial dimensions. If the canonical coordinates and momenta $\mathbf{q}, \mathbf{p}$ are just the Cartesian positions and kinetic momenta and m denotes the isotropic mass of each particle, the Hamiltonian has the form

$$H\,(\mathbf{q}, \mathbf{p}) = \frac{\mathbf{p}^2}{2m} + V\,(\mathbf{q}) = \frac{\mathbf{p}^2}{2m} + \sum_{i=1}^{N} V_{\mathrm{SP}}\,(\mathbf{q}_i) + V_{\mathrm{int}}\,(\mathbf{q})\,. \tag{2.9}$$

Therefore the multidimensional quasi particle also has (isotropic) mass m and the potential $V(\mathbf{q})$ it's moving in is subject to the discrete spatial symmetry according to the point transformations $\mathbf{q} \to P\mathbf{q}$.

2.1.2 Quantum Mechanical Many Body Systems

General Concept

In the standard formulation of quantum mechanics (see, for example [26]) any state of a given system is described by an element $|\psi\rangle$ of a *Hilbert space* $\mathscr{H}$ over the complex numbers $\mathbb{C}$ using the standard Dirac bracket notation. Observable quantities are described by *self adjoint* or *Hermitian* linear operators $\hat{O}$ acting on that Hilbert space. States that have a definite value respective one specific observable are the *eigenvectors* or *eigenstates* of that operator. For example states of definite coordinate q are written

$$\hat{Q}|q\rangle = q|q\rangle \tag{2.10}$$

The scalar product of $|\psi\rangle$ and variable coordinate states is the *wave function*

$$\psi(\mathbf{q}) = \langle \mathbf{q}|\psi\rangle \tag{2.11}$$

which also describes all properties of a given state. Its standard interpretation is that of a probability amplitude to find the system at the coordinate $\mathbf{q}$.
In the non-relativistic case, dynamics are given by *Schrödinger's equation* for the time dependent wave function

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{q},t) = \hat{H}\psi(\mathbf{q},t) \tag{2.12}$$

where the *Hamiltonian* $\hat{H}$ is the observable corresponding to the classical *Hamilton function* H . When $\hat{H}$ is time independent the stationary Schrödinger equation together with the time evolution of the Eigenstates give the systems dynamics

$$\begin{aligned} \hat{H}|\psi\rangle &= E|\psi\rangle \\ |\psi(t)\rangle &= \exp\left(-\frac{i}{\hbar}\,E\,t\right)|\psi(0)\rangle. \end{aligned} \tag{2.13}$$

Moving from a single particle system to a many body system, one has to increase the degrees of freedom. This is done by expanding the Hilbert space $\mathscr{H}$. The new Hilbert space is constructed as *tensor product* of the old one with the Hilbert space corresponding to the new degrees of freedom. A many body system of N identical particles is then described by the tensor product of N single particle (SP) Hilbert spaces

$$\mathscr{H} = \mathscr{H}_{\mathrm{SP}} \otimes \mathscr{H}_{\mathrm{SP}} \otimes \cdots \otimes \mathscr{H}_{\mathrm{SP}}. \tag{2.14}$$

A possible basis in terms of single particle bases is given by product states:

$$\mathscr{B} = \Big\{\ |\phi_1\rangle \otimes \cdots \otimes |\phi_N\rangle \quad \Big|\quad |\phi_i\rangle \in \mathscr{B}_{\mathrm{SP}}\ \ \forall\, i = 1,\ldots,N\ \Big\}. \tag{2.15}$$

Exchange Symmetry

Dealing with identical particles in quantum mechanics one has to address two different aspects of identity. First, quite analogue to classical mechanics, the dynamics of the system have to be symmetric under the exchange of particle labels. So let us for a moment address this first point.

Like (almost) every transformation of quantum states the exchange of particles is represented by a unitary linear operator $\hat{P}$.

$$\hat{P}^\dagger \hat{P} = 1 \tag{2.16}$$

Due to its linearity, $\hat{P}$ is completely defined by its action on all vectors of a specific basis. Most simply this is done in a basis of product states:

$$\hat{P}|\psi\rangle = \hat{P}\big(|\phi_1\rangle \otimes \cdots \otimes |\phi_N\rangle\big) = |\phi_{\sigma(1)}\rangle \otimes \cdots \otimes |\phi_{\sigma(N)}\rangle \tag{2.17}$$

where $\hat{P}$ is uniquely assigned to a permutation of particle indexes so that $1, \ldots, N \mapsto \sigma(1), \ldots, \sigma(N)$ which in turn uniquely maps to an element of the symmetric group $\sigma \in S_N$ and therefore to a permutation matrix P

$$P\mathbf{v} = P(v_1, \ldots, v_N) = (v_{\sigma(1)}, \ldots, v_{\sigma(N)}). \tag{2.18}$$

For reasons of simplicity the operator, permutation, group element and matrix shall from now on all be referred to as permutations with the implicit understanding of bijective mapping among them.
The symmetry under permutations is reflected by its commutation with the Hamiltonian

$$\left[\hat{P}, \hat{H}\right] = 0. \tag{2.19}$$

So that the permutation of a solution is again a solution:

$$\hat{H}\left(\hat{P}|\psi(t)\rangle\right) = \hat{P}\hat{H}|\psi(t)\rangle = \hat{P}\left(i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle\right) = i\hbar\frac{\partial}{\partial t}\left(\hat{P}|\psi(t)\rangle\right) \tag{2.20}$$

or in the stationary form:

$$\hat{H}\left(\hat{P}|\psi\rangle\right) = \hat{P}\hat{H}|\psi\rangle = \hat{P}E|\psi\rangle = E\left(\hat{P}|\psi\rangle\right). \tag{2.21}$$

So far the quantum mechanical description of a system of N particles in D dimensions also is equivalent to the system of a single particle in (ND) dimensions. In the case of a single particle Hamiltonian of the form

$$\hat{H} = \hat{T} + \hat{V} = \frac{1}{2m}\hat{\mathbf{P}}^2 + V(\hat{\mathbf{Q}}) \tag{2.22}$$

with isotropic particle mass m, momentum operator $\hat{\mathbf{P}}$ (not to be confused with the permutation $\hat{P}$)and potential V, the corresponding multidimensional quasi particle also has isotropic mass m and feels a potential that is symmetric under the spatial symmetry according to the point transformation $\mathbf{q} \to P\mathbf{q}$.
But as mentioned above, there is a second effect of identity.

Indistinguishability

Besides the exchange symmetry, there is the concept of indistinguishability in quantum mechanics that completely misses a classical analogue. This concept reflects the fact that identical quantum particles do not only share same properties and therefore behave exactly the same way, but they really can not be distinguished in the sense that one is not able to mark a single one of them and follow its own dynamics. Even asking after the state of one of them without asking after all of them at the same time is just not possible. This oddity looses its peculiarity when regarding quantum theories as effective representations of quantum field theories, where states of more than one particle correspond to higher excitations of one sole field, so that there is just one single physical quantity giving rise to the observation of many particles of the same kind.
According to the *Spin-Statistic Theorem* the physical states of the system have to be *symmetric* respectively *antisymmetric* under exchange of two particles depending on whether the particles are *bosons* or *fermions*. That is they have integer or half-integer spin respectively.

$$\begin{aligned} \hat{P}_2|\psi_\pm\rangle &= \pm|\psi_\pm\rangle & P_2 &: \text{ transposition} \\ \hat{P}|\psi_\pm\rangle &= (\pm 1)^P\,|\psi_\pm\rangle & (-1)^P &\equiv \operatorname{sgn}\sigma \end{aligned} \tag{2.23}$$

where $+$ refers to bosons and $-$ refers to fermions.
Hence for a correct physical description one needs to restrict the full Hilbert space $\mathscr{H}$ to the subspaces $\mathscr{H}_\pm$ of states $|\psi_\pm\rangle$ with correct symmetry. This can be achieved by introducing the projection operators $\hat{\mathbb{1}}_\pm$ that are projecting any state in Hilbert space onto the subspaces $\mathscr{H}_\pm$. If $\{|\phi_\pm^{(n)}\rangle\}$ are orthonormal sets spanning these subspaces the projectors can be written

$$\begin{aligned} & \hat{\mathbb{1}}_\pm = \sum_n |\phi_\pm^{(n)}\rangle\langle\phi_\pm^{(n)}| \\ \Rightarrow \qquad & \hat{\mathbb{1}}_\pm^\dagger = \hat{\mathbb{1}}_\pm. \end{aligned} \tag{2.24}$$

These sets of symmetric basis vectors can be expressed in terms of *Slater determinants* or *permanents* of single particle basis vectors.

$$|\phi_\pm\rangle = \frac{1}{\sqrt{N!}} \sum_P (\pm 1)^P \hat{P}\big(|\varphi_1\rangle \otimes \cdots \otimes |\varphi_N\rangle\big) \tag{2.25}$$

where $|\varphi_i\rangle$ are N distinct orthonormal single particle basis vectors. Note that in the bosonic case there are also basis vectors when some of the single particle vectors are the same. Then the scaling factor has to be modified:

$$\frac{1}{\sqrt{N!}} \to \frac{1}{\sqrt{N!\, N_1!\, N_2! \cdots N_d!}} \tag{2.26}$$

for d distinct single particle vectors with multiplicities N_i.

The action of the projectors on product states is

$$\begin{aligned} \hat{\mathbb{1}}_\pm \, |\phi_1, \ldots, \phi_N\rangle &= \frac{1}{N!} \sum_P (\pm 1)^P \, \hat{P} \, |\phi_1, \ldots, \phi_N\rangle \\ &= \frac{1}{N!} \sum_P (\pm 1)^P \, |\phi_{\sigma(1)}, \ldots, \phi_{\sigma(N)}\rangle, \end{aligned} \tag{2.27}$$

or after Hermitian conjugation

$$\begin{aligned} \langle \phi_1, \ldots, \phi_N| \, \hat{\mathbb{1}}_\pm &= \frac{1}{N!} \sum_P (\pm 1)^P \, \langle \phi_1, \ldots, \phi_N| \, \hat{P} \\ &= \frac{1}{N!} \sum_P (\pm 1)^P \, \langle \phi_{\sigma(1)}, \ldots, \phi_{\sigma(N)}|, \end{aligned} \tag{2.28}$$

using (2.24) and

$$\sum_P (\pm 1)^P \hat{P}^\dagger = \sum_P (\pm 1)^P \hat{P}^{-1} = \sum_{P^{-1}} (\pm 1)^{P^{-1}} \hat{P}^{-1} = \sum_P (\pm 1)^P \hat{P}. \tag{2.29}$$

Note that (2.27) and (2.28) also hold in case of equality of some $|\phi_i\rangle$. This means the matrix elements of $\hat{\mathbb{1}}_\pm$ in coordinate basis are

$$\langle \mathbf{q}'_1, \ldots, \mathbf{q}'_N | \hat{\mathbb{1}}_\pm | \mathbf{q}_1, \ldots, \mathbf{q}_N \rangle = \frac{1}{N!} \sum_P (\pm 1)^P \Delta_{1,\sigma(1)} \cdots \Delta_{N,\sigma(N)} = \frac{1}{N!} \det_\pm \Delta, \tag{2.30}$$

where

$$\Delta_{ij} = \delta^{(D)}(\mathbf{q}'_i - \mathbf{q}_j). \tag{2.31}$$

Here $\det_\pm \Delta$ denotes the permanent $(+)$ respectively determinant $(-)$ of the matrix Δ. The projectors themselves commute with the Hamiltonian which can be easily seen using again product states

$$\begin{aligned} \langle \chi_1, \ldots, \chi_N| \, \hat{H} \, \hat{\mathbb{1}}_\pm \, |\phi_1, \ldots, \phi_N\rangle &= \frac{1}{N!} \sum_P (\pm 1)^P \, \langle \chi_1, \ldots, \chi_N| \, \hat{H} \, \hat{P} \, |\phi_1, \ldots, \phi_N\rangle \\ &= \frac{1}{N!} \sum_P (\pm 1)^P \, \langle \chi_1, \ldots, \chi_N| \, \hat{P} \, \hat{H} \, |\phi_1, \ldots, \phi_N\rangle \\ &= \langle \chi_1, \ldots, \chi_N| \, \hat{\mathbb{1}}_\pm \, \hat{H} \, |\phi_1, \ldots, \phi_N\rangle \\ \Rightarrow \qquad \left[\hat{H} \, , \, \hat{\mathbb{1}}_\pm\right] &= 0. \end{aligned} \tag{2.32}$$

This implies that symmetric (respectively antisymmetric) states keep their symmetry under time evolution.

One should also note that any two symmetric and antisymmetric states are orthogonal to each other, which also simply can be seen using Slater determinants or corresponding permanents:

$$\begin{aligned}\langle\chi_+|\phi_-\rangle &= \frac{1}{N!}\sum_{P_1\,,P_2}(-1)^{P_1}\,\langle\chi_1,\ldots,\chi_N|\,\hat{P}_1\,\hat{P}_2\,|\phi_1,\ldots,\phi_N\rangle \\ &= \frac{1}{N!}\sum_{P'}\langle\chi_1,\ldots,\chi_N|\,\hat{P}'\,|\phi_1,\ldots,\phi_N\rangle\;\sum_{P_1}(-1)^{P_1}=0,\end{aligned} \tag{2.33}$$

with the definition $\hat{P}_2=\hat{P}_1^{-1}\,\hat{P}'$ using the fact that for $N>1$ the number of even permutations equals the number of odd permutations. Since every (anti-)symmetric state can be written as a sum of Slater determinants or permanents this implies the orthogonality of fermionic and bosonic subspaces

$$\begin{aligned}&\mathscr{H}_+\;\perp\;\mathscr{H}_- \\ \Leftrightarrow\quad &\hat{\mathbb{1}}_\pm\,\hat{\mathbb{1}}_\mp=0 \\ \Rightarrow\quad &\left[\hat{\mathbb{1}}_\pm\,,\;\hat{\mathbb{1}}_\mp\right]=0.\end{aligned} \tag{2.34}$$

Knowing that every projection operator is idempotent $\hat{\mathbb{1}}_\pm=\hat{\mathbb{1}}_\pm^2$ and hence only has eigenvalues 0 and 1 the commutation relations (2.32) and (2.34) imply that a common eigenbasis of $\hat{H}$, $\hat{\mathbb{1}}_+$ and $\hat{\mathbb{1}}_-$ can be found so that it is divided into Eigenstates of $\hat{H}$ spanning $\mathscr{H}_+$, $\mathscr{H}_-$ and the rest of Hilbert space $\mathscr{H}\setminus(\mathscr{H}_+\oplus\mathscr{H}_-)$. All of the three lying orthogonal to each other:

$$\mathscr{H}\setminus(\mathscr{H}_+\oplus\mathscr{H}_-)\;\perp\;\mathscr{H}_+\;\perp\;\mathscr{H}_-\;\perp\;\mathscr{H}\setminus(\mathscr{H}_+\oplus\mathscr{H}_-)\,. \tag{2.35}$$

This means the energy spectrum of a physical system of bosons or fermions is part of the full set of eigenvalues of the Hamiltonian. I will refer to this part as the *symmetry projected spectrum*. Whereas the full set of eigenvalues will be referred to as the *unsymmetrized spectrum*

2.2 The Semiclassical Density Of States

2.2.1 Periodic Orbit Theory

Green's Function And Propagator

Often when investigating quantum systems obeying Schrödinger's equation

$$\hat{H}|\psi\rangle=E|\psi\rangle \tag{2.36}$$

the most interesting part of its solution will be the spectrum of eigenenergies since it contains valuable information about the behaviour of the system itself and as part of a larger system for example in a thermodynamical equilibrium.

The set of Eigenvalues $\{E_n\}$ of a quantum system can be expressed in form of the *density of states* [26]

$$\rho(E) = \sum_n \delta(E - E_n), \tag{2.37}$$

where δ denotes the Dirac delta distribution. Solving Schrödinger's equation is equivalent to finding Green's function G obeying the differential equation

$$\left(E - \hat{H}\right) G(\mathbf{q}', \mathbf{q}, E) = \delta(\mathbf{q}' - \mathbf{q}). \tag{2.38}$$

For closed systems with a discrete spectrum, $G(E)$ is a meromorphic function in the complex E plane with all poles along the real energy axis. It can be written in terms of the eigenfunctions and eigenenergies as

$$G(\mathbf{q}', \mathbf{q}, E) = \langle \mathbf{q}' | \left(E - \hat{H}\right)^{-1} |\mathbf{q}\rangle = \sum_n \psi_n^*(\mathbf{q})\, \psi_n(\mathbf{q}') \frac{1}{E - E_n} \tag{2.39}$$

with the complete orthonormal set $\{|\psi_n\rangle\}$ of eigenstates of $\hat{H}$. Then the density of states can be obtained by

$$\rho(E) = -\frac{1}{\pi} \Im \left[\operatorname{tr} \hat{G}(E + i\epsilon)\right] \text{ in the limit } \epsilon \to 0^+, \tag{2.40}$$

where the trace is performed as integral in coordinate space

$$\operatorname{tr} G(E + i\epsilon) = \int \mathrm{d}^D q\, G(\mathbf{q}, \mathbf{q}, E + i\epsilon). \tag{2.41}$$

Instead of finding the Green's function in energy domain, one can solve the corresponding equation in time domain. Then one has to find the propagator K which is the position representation of the *time evolution operator* $\hat{U}$

$$K(\mathbf{q}', \mathbf{q}; t', t) = \langle \mathbf{q}' | \hat{U}(t', t) | \mathbf{q} \rangle. \tag{2.42}$$

$\hat{U}$ describes the time evolution of an arbitrary state by

$$|\psi(t')\rangle = \hat{U}(t', t)\, |\psi(t)\rangle. \tag{2.43}$$

In the general case of explicitly time dependent systems $\partial \hat{H}/\partial t \neq 0$ it can formally be written as

$$\hat{U}(t', t) = T \exp\left[-\frac{i}{\hbar} \int_t^{t'} \mathrm{d}t'' \hat{H}(t'')\right], \tag{2.44}$$

with the *time ordered exponential* T exp defined as series of time ordered powers.

Throughout the rest of the work we will regard explicitly time independent systems only where $\hat{U}$ reduces to an usual exponential

$$\hat{U}(t',t) \equiv \hat{U}(t'-t) = \exp\left[-\frac{i}{\hbar}\hat{H}(t'-t)\right] \tag{2.45}$$

and the time dependence reduces to a dependence on the evolution time difference $t'-t$.

The relation between Green's function and the time dependent propagator is by virtue of Laplace transform

$$G(\mathbf{q}',\mathbf{q},E+i\epsilon) = \frac{1}{i\hbar}\int_0^\infty \mathrm{d}t\, e^{\frac{i}{\hbar}(E+i\epsilon)t}\, K(\mathbf{q}',\mathbf{q};t) = \mathscr{L}_t\{K(\mathbf{q}',\mathbf{q};t)\}\left(-\frac{i}{\hbar}(E+i\epsilon)\right). \tag{2.46}$$

The use of a small positive imaginary part in the energy corresponds to the expression via positive times $t' > t$ in the propagator.
$G(E+i\epsilon)$ is accordingly called the *retarded* Green's function whereas one could also use the *advanced* Green's function by choosing a negative imaginary part in the energy and using the half sided Laplace transform for negative times.

As we see now that with the knowledge of $K(\mathbf{q}',\mathbf{q},t)$ one has all the information about the system, we can especially express the density of states as

$$\rho(E) = \frac{1}{\pi\hbar}\,\Re\left[\int_0^\infty \mathrm{d}t\, e^{\frac{i}{\hbar}(E+i\epsilon)t}\int \mathrm{d}^D q\, K(\mathbf{q},\mathbf{q},t)\right] \tag{2.47}$$

Since in complex quantum systems it is in general neither possible to exactly solve for the Green's function nor the propagator, the above formalism seems kind of pointless. To see its advantage one needs to recognise that it is possible to give an approximation to the propagator in terms of properties of the underlying classical system. Mention is being made here of the semiclassical approximation.

Semiclassical Approximation

In this section we will see that the propagator and therefore the Green's function and the density of states can be expressed in terms of classical properties as sums over classical allowed orbits. The derivations below can be followed in literature [9, 19] but we will go into some detail from time to time because later it will allow us to incorporate particle exchange symmetry. On this basis it will

be easier to understand the upcoming special features.

Already in 1928 [29], Van Vleck realised that in the case of a free particle, the propagator can be expressed in terms of simple classical quantities. The free propagator can be solved exactly and reads

$$K_0(\mathbf{q}', \mathbf{q}; t) = \left(\frac{m}{2\pi\hbar i t}\right)^{\frac{D}{2}} \exp\left[\frac{i}{\hbar}\frac{m}{2t}(\mathbf{q}' - \mathbf{q})^2\right]. \tag{2.48}$$

The exponent in (2.48) equals $i/\hbar$ times *Hamilton's principal function* $W_0(\mathbf{q}', \mathbf{q}; t)$ for a free particle. In general Hamilton's principal function is defined as

$$W(\mathbf{q}', \mathbf{q}; t' - t) = \int_t^{t'} \mathrm{d}t''\, L(\mathbf{q}'', \dot{\mathbf{q}}''; t''), \tag{2.49}$$

where $L(\mathbf{q}, \dot{\mathbf{q}}; t)$ is the *Lagrange function*. Under the time integral on the right hand side of (2.49), $\mathbf{q}(t)$ is a solution of the classical equations of motion with definite starting point $\mathbf{q}$, end point $\mathbf{q}'$ and transit time t. After *Hamilton's principle* the solutions are exactly those paths under which the integral in (2.49) is stationary. If there is more than one solution, W has to be indexed for all possible orbits.

In the free case, there is always just one solution going straight from $\mathbf{q}$ to $\mathbf{q}'$ and Hamilton's principal function reads

$$W_0(\mathbf{q}', \mathbf{q}, t) = \frac{m}{2t}(\mathbf{q}' - \mathbf{q})^2. \tag{2.50}$$

Furthermore, Van Vleck realised that one can express the prefactor in (2.48) in terms of the second derivatives of W_0.

$$\left(\frac{m}{t}\right)^D = \left|-\frac{\partial^2 W_0}{\partial q_i \partial q_j'}\right| \equiv |C_0(\mathbf{q}', \mathbf{q}; t)|, \tag{2.51}$$

denoting the absolute value of the determinant of the matrix using the indexes i, j. Therefore the free propagator in D dimensions can be expressed in terms of W_0 as

$$K_0(\mathbf{q}', \mathbf{q}; t) = (2\pi\hbar i)^{-\frac{D}{2}} \sqrt{|C_0(\mathbf{q}', \mathbf{q}; t)|}\, \exp\left[\frac{i}{\hbar} W_0(\mathbf{q}', \mathbf{q}, t)\right]. \tag{2.52}$$

Based on that, Van Vleck introduced his propagator K_{VV} as the generalisation $W_0 \to W$ for systems with potential

$$K_{\mathrm{VV}}(\mathbf{q}', \mathbf{q}; t) = (2\pi\hbar i)^{-\frac{D}{2}} \sqrt{|C(\mathbf{q}', \mathbf{q}; t)|}\, \exp\left[\frac{i}{\hbar} W(\mathbf{q}', \mathbf{q}, t)\right] \tag{2.53}$$

with the usual principal function (2.49) including a potential V in the Lagrangian L.

Inspired by Van Vleck's propagator for the free particle, Gutzwiller [9] derived a semiclassical approximation to the propagator for general Hamiltonians based on a path integral representation of K :

$$K_{\mathrm{scl}}(\mathbf{q}', \mathbf{q}; t) = \sum_{\gamma} (2\pi\hbar i)^{-\frac{D}{2}} \sqrt{|C_\gamma(\mathbf{q}', \mathbf{q}; t)|} \, \exp\left[\frac{i}{\hbar} W_\gamma(\mathbf{q}', \mathbf{q}, t) - i\frac{\pi}{2}\kappa_\gamma\right], \tag{2.54}$$

where γ indexes all classical allowed trajectories running from $\mathbf{q}$ to $\mathbf{q}'$ in time t , W_γ denotes their principal functions and C_γ the determinant of second derivatives of W_γ similar to the free case. κ_γ is the number of conjugated points along the trajectory γ (points for which C_γ becomes singular; poles of higher order are thereby counted repeatedly).

Derivation Of The Semiclassical Propagator

Expressing K as a *Feynman path integral* is based on dividing the evolution time t into $n+1$ small time steps $\Delta t = t/(n+1)$. By inserting complete sets of position states after every time step

$$\int \mathrm{d}^D q_i |\mathbf{q}_i\rangle\langle\mathbf{q}_i| = \mathbb{1} \qquad i = 1, \ldots, n \tag{2.55}$$

one gets an n-fold integral over a product of $n+1$ short time propagators

$$\begin{aligned} K(\mathbf{q}', \mathbf{q}; t) &= \langle\mathbf{q}'|\hat{U}(t)|\mathbf{q}\rangle \\ &= \langle\mathbf{q}'|\, \hat{U}(\Delta t) \int \mathrm{d}^D q_n |\mathbf{q}_n\rangle\langle\mathbf{q}_n|\, \hat{U}(\Delta t) \, \cdots \\ &\quad \cdots \hat{U}(\Delta t) \int \mathrm{d}^D q_1 |\mathbf{q}_1\rangle\langle\mathbf{q}_1|\, \hat{U}(\Delta t)\, |\mathbf{q}\rangle \\ &= \left[\prod_{i=1}^{n} \int \mathrm{d}^D q_i\right] \prod_{i=1}^{n+1} K(\mathbf{q}_i, \mathbf{q}_{i-1}; \Delta t), \end{aligned} \tag{2.56}$$

where $\mathbf{q}_{n+1} = \mathbf{q}'$ and $\mathbf{q}_0 = \mathbf{q}$. The *path integral* is obtained in the *continuous limit* $n \to \infty, \Delta t \to 0$. The sense of this lies in the asymptotic behaviour of the intermediate short time propagators, which become Van Vleck propagators in this limit. This can be derived by additionally inserting full sets of momentum states

$$\frac{1}{(2\pi\hbar)^D} \int \mathrm{d}^D p_i |\mathbf{p}_i\rangle\langle\mathbf{p}_i| = \mathbb{1} \qquad i = 1, \ldots, n \tag{2.57}$$

after each time step. Then the continuous limit allows to write intermediate propagators as

$$\begin{aligned} K(\mathbf{q}_i, \mathbf{q}_{i-1}; \Delta t) &= \frac{1}{(2\pi\hbar)^D} \int \mathrm{d}^D p_i \, \langle \mathbf{q}_i | \, e^{-\frac{i}{\hbar}\hat{H}(\hat{\mathbf{Q}},\hat{\mathbf{P}})\Delta t} \, |\mathbf{p}_i\rangle\langle \mathbf{p}_i | \mathbf{q}_{i-1}\rangle \\ &= \frac{1}{(2\pi\hbar)^D} \int \mathrm{d}^D p_i \, \exp\left[-\frac{i}{\hbar}\Delta t \left(H(\mathbf{q}_i, \mathbf{p}_i) - \frac{\mathbf{q}_i - \mathbf{q}_{i-1}}{\Delta t}\mathbf{p}_i \right)\right]. \end{aligned} \tag{2.58}$$

After completing the square in $\mathbf{p}_i$ and solving the complete Fresnel integral, (2.58) gives then Van Vleck's propagator expressed as a path integral over all paths in *phase space*

$$K(\mathbf{q}', \mathbf{q}; t) = \int\limits_{\mathbf{q}(0)=\mathbf{q}}^{\mathbf{q}(t)=\mathbf{q}'} \mathscr{D}\mathbf{q} \int \frac{\mathscr{D}\mathbf{p}}{2\pi\hbar} \, \exp\left[\frac{i}{\hbar} S[\mathbf{q}, \mathbf{p}]\right], \tag{2.59}$$

with the canonical action

$$S[\mathbf{q}, \mathbf{p}] = \int\limits_0^t \mathrm{d}t'' \big(\dot{\mathbf{q}}(t'')\mathbf{p}(t'') - H(\mathbf{q}(t''), \mathbf{p}(t'')) \big). \tag{2.60}$$

By solving all momentum integrals one ends up with a path integral in *position space* of an infinite product of Van Vleck propagators

$$K(\mathbf{q}', \mathbf{q}; t) = \int\limits_{\mathbf{q}(0)=\mathbf{q}}^{\mathbf{q}(t)=\mathbf{q}'} \mathscr{D}\mathbf{q} \, \lim_{n\to\infty} \prod_{i=1}^{n} K_{VV}\left(\mathbf{q}\left(\frac{i}{n}t\right), \mathbf{q}\left(\frac{i-1}{n}t\right) ; \frac{t}{n} \right). \tag{2.61}$$

The semiclassical approximation (2.54) is then obtained by a stationary phase-quantum mechanical many body systems approximation of the path integral assuming $\hbar$ to be small compared to the involved actions. This is possible as a stationary phase approximation of a multidimensional integral at once with $n \to \infty$ for some special cases only as done by Gutzwiller. The other way is to successively perform stationary phase approximations at every intermediate step as shown by Berry and Mount [3]. The latter works in the general case of arbitrary dimension and potential.

The condition of stationary phase means vanishing variations of the phase function which is Hamilton's principal function. The points of stationary phase in path space are thus exactly the classical allowed paths according to Hamilton's principle.

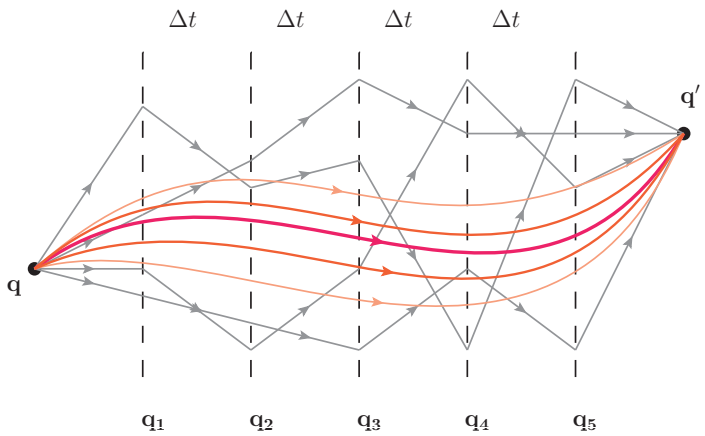


Figure 2.1: Illustration of a path integral in coordinate space. Shown are some possible classically forbidden paths for a division of transit time into five steps (grey). In the limit of infinitely many steps those will interfere rather destructively. The curves in red tones illustrate a classical allowed path and some exemplary slightly deviated paths of its vicinity in path space. Those are interfering constructively.

The emerging semiclassical propagator sums over classical trajectories only. To get an intuitive picture one could say that in the path integral (2.61) classical paths and their vicinities in infinitely-dimensional path space give the main contributions as their phases interfere constructively whereas others cancel each other due to rapid oscillation of the integrand. Figure 2.1 illustrates this.

The Semiclassical Green's Function And Density Of States

In order to arrive at a semiclassical expression for the Green's function one has again to perform an approximation of stationary phase. The according stationarity condition in the Fourier integral leads to a sum over classical orbits of definite energy E instead of given transit time t . The semiclassical Green's function is

$$G_{\mathrm{scl}}(\mathbf{q}',\mathbf{q};E) = 2\pi \sum_{\gamma} (2\pi\hbar i)^{-\frac{D+1}{2}} \, \Delta_{\gamma}^{\frac{1}{2}}(\mathbf{q}',\mathbf{q};E) \, \exp\left[\frac{i}{\hbar} S_{\gamma}(\mathbf{q}',\mathbf{q};E) - i\frac{\pi}{2}\nu_{\gamma}\right], \tag{2.62}$$

where S_γ denotes the classical action along the orbit γ

$$S_{\gamma}(\mathbf{q}',\mathbf{q};E) = W_{\gamma}(\mathbf{q}',\mathbf{q};t(E)) + E\,t(E) = \int_{\gamma} \mathrm{d}\mathbf{q}\cdot\mathbf{p}, \tag{2.63}$$

and the phase shift includes the number of conjugated points and an additional phase if the transit time increases with the energy

$$\nu_\gamma = \kappa_\gamma + \theta\left(\frac{\partial t}{\partial E}\right). \tag{2.64}$$

The prefactor is the square root of the determinant of second derivatives of S with respect to the coordinates and the energy

$$\Delta_\gamma^{\frac{1}{2}}(\mathbf{q}', \mathbf{q}; E) = \left| \det \begin{pmatrix} \dfrac{\partial^2 S_\gamma}{\partial q_i \partial q_j'} & \dfrac{\partial^2 S_\gamma}{\partial q_i \partial E} \\ \dfrac{\partial^2 S_\gamma}{\partial E \partial q_j'} & \dfrac{\partial^2 S_\gamma}{\partial E^2} \end{pmatrix} \right|^{\frac{1}{2}} \qquad i, j = 1, \ldots, D. \tag{2.65}$$

The last step before arriving at a semiclassical density of states is to perform the trace in (2.40) in coordinate space. Thereby a third and last stationary phase approximation has to be done. The stationarity condition yields the restriction to periodic orbits only:

$$\begin{aligned} 0 &= \frac{\partial S(\mathbf{q}, \mathbf{q}; E)}{\partial q_i} \\ &= \left[\frac{\partial S(\mathbf{q}', \mathbf{q}; E)}{\partial q_i} + \frac{\partial S(\mathbf{q}', \mathbf{q}; E)}{\partial q_i'}\right]_{\mathbf{q}'=\mathbf{q}} \\ &= -p_i(0) + p_i(t) \\ &\Rightarrow \mathbf{p}(t) = \mathbf{p}(0). \end{aligned} \tag{2.66}$$

For the purpose of integration one better uses local coordinates $\mathbf{q} = (q_\parallel, \mathbf{q}_\perp)$ parallel and perpendicular to the orbit. The component parallel to the orbit comes with vanishing derivatives. Thus the integral along the orbit has to be evaluated by foot. We separate the dependence on $q_\parallel$ in the prefactor

$$\Delta_\gamma^{\frac{1}{2}} = \left| \frac{\partial^2 S}{\partial q_{\perp,i}\, \partial q'_{\perp,j}} \right|^{\frac{1}{2}} \frac{1}{|\dot{\mathbf{q}}|} \qquad i, j = 1, \ldots, D-1. \tag{2.67}$$

The integral along the orbits then yields its *primitive period*

$$T_{\mathrm{ppo},\gamma} = \int\limits_\gamma \mathrm{d}q_\parallel \frac{1}{|\dot{\mathbf{q}}|} = \int\limits_\gamma \mathrm{d}q_\parallel \frac{\mathrm{d}t}{\mathrm{d}q_\parallel} = \int\limits_\gamma \mathrm{d}t, \tag{2.68}$$

which is the transit time of a single traversal. For the integration of perpendicular coordinates under the assumption of isolated periodic orbits the according stationary phase approximation gives a prefactor that combines with the remaining prefactor to a fraction of determinants that can be simplified to a prefactor

only depending on stability properties of the periodic orbit.

Before writing the final result it is important that in the process above one misses contributions from direct propagation from a point to itself without the detour of an extended orbit. These contributions are usually referred to as *0-length orbits*. Those give only contributions smoothly varying with the energy and will become important later. For now, the other part of the density of states $\rho_{scl}(E)$, called the *oscillatory part* $\tilde{\rho}_{scl}(E)$ is

$$\tilde{\rho}_{\mathrm{scl}}(E) = \frac{1}{\pi\hbar}\sum_{\gamma}\frac{T_{\mathrm{ppo},\gamma}}{\left|\det\left(\tilde{\mathbb{M}}_{\gamma}-1\right)\right|^{\frac{1}{2}}}\cos\left[\frac{1}{\hbar}S_{\gamma}(E)-\frac{\pi}{2}\sigma_{\gamma}\right], \tag{2.69}$$

where γ indexes all periodic orbits of the system including repetitions. $\tilde{\mathbb{M}}_{\gamma}$ is called the *stability matrix* of the orbit γ and describes the evolution of small deviations of the trajectory over one period.

2.2.2 Weyl Expansion

As we have seen in the Gutzwiller formula (2.69) the periodic orbit contribution to the density of states is oscillatory in the energy. Every orbit gives a function of energy that is locally oscillating with a frequency of

$$\frac{1}{\hbar}S'_{\gamma}(E) = \frac{1}{\hbar}T_{\gamma}(E). \tag{2.70}$$

In the formal semiclassical limit $\hbar \to 0$ this frequency becomes infinitely large, thus we can consider the oscillations in $\tilde{\rho}_{\mathrm{scl}}(E)$ to be very fast with rather constant frequency over some periods. This means a local average $\langle\ldots\rangle_E$ over some small energy window around E would become asymptotically zero.

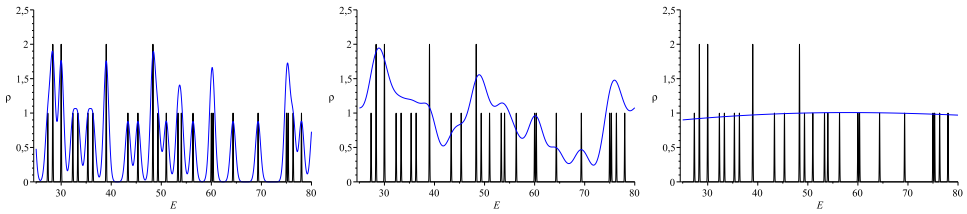
$$\langle\tilde{\rho}_{\mathrm{scl}}(E)\rangle_E \approx 0 \tag{2.71}$$

Of course this can not be true for the full density of states as is illustrated in figure (2.2) for a two dimensional billiard.
So we know that what is missing in the Gutzwiller trace formula is the average or *smooth part* of the density of states $\bar{\rho}$ [19].

$$\rho_{\mathrm{scl}}(E) = \bar{\rho}_{\mathrm{scl}}(E) + \tilde{\rho}_{\mathrm{scl}}(E) \tag{2.72}$$

As mentioned at the end of section 2.2.1 the smooth part corresponds to short path contributions that are not caught by periodic orbits in the analysis of the trace of the propagator.

To illustrate this absence let us briefly consider a free particle in D dimensions.



(a) small variance (b) medium variance (c) large variance

Figure 2.2: successive steps in smoothing the quantum mechanical density of states of a two dimensional billiard by virtue of convolution with a Gaussian of increasing variance.

In this case there are no periodic orbits at all, but still the free propagator (2.48) is non-zero for the propagation from some coordinate $\mathbf{q}$ to itself,

$$K_0(\mathbf{q},\mathbf{q};t) = \left(\frac{m}{2\pi\hbar i t}\right)^{\frac{D}{2}}. \tag{2.73}$$

Thus, through expression (2.47) we get a non-zero contribution to $\rho(E)$. Since (2.73) shows a fast decay in time $\propto 1/t^{(D/2)}$ we can speak of a short time contribution. After the Fourier transform in (2.47) this will result in a function that has only very slowly oscillating modes in energy domain. So we see that indeed the missing part in the periodic orbit sum is a smoothly varying function.

Despite the existence of a formalism to obtain the smooth part in systems with smooth potentials $V(\mathbf{q})$ [19] we will restrict ourselves to billiard systems which are of special interest in the context of semiclassics, since they often offer easy access to a systematic specification of periodic orbits.

A D-dimensional billiard is defined by zero potential inside some D-dimensional region $\Omega \subset \mathbb{R}^D$ and an infinite potential barrier outside

$$V(\mathbf{q}) = \begin{cases} 0 & \mathbf{q} \in \Omega \\ \infty & \mathbf{q} \notin \Omega \end{cases} \tag{2.74}$$

Let us deduce $\bar{\rho}(E)$ for a two-dimensional billiard. Since we are interested in short time contributions to the propagator, we assume local free propagation (see figure 2.3). The trace in coordinate space restricted to Ω and adjacent Fourier transformation yield

$$\int \mathrm{d}^2 q \; K_0(\mathbf{q},\mathbf{q};t) = \left(\frac{m}{2\pi\hbar i t}\right) A \tag{2.75}$$

$$\bar{\rho}_{\mathrm{v}}(E) = \frac{A}{4\pi}\left(\frac{2m}{\hbar^2}\right)\theta(E) = \bar{\rho}_{\mathrm{TF}}(E). \tag{2.76}$$

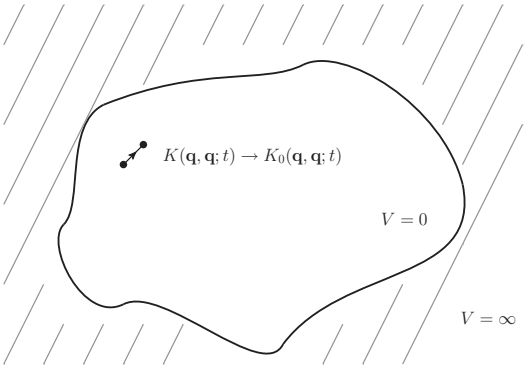


Figure 2.3: local free propagation in the interior of a billiard in the limit of short time propagation.

A denotes the area of the billiard's interior Ω and θ is the Heaviside step function. Indeed we see a smoothly varying behaviour in E. $\bar{\rho}_{\mathrm{v}}(E)$ is often called the *volume Weyl term* and equals the *Thomas-Fermi approximation* (see also example [19]), which in general for arbitrary dimension and potential V reads

$$\bar{\rho}_{\mathrm{TF}}(E) = \left(\frac{m}{2\pi\hbar^2}\right)^{\frac{D}{2}} \int \mathrm{d}^D q \, \frac{[E-V(\mathbf{q})]^{\frac{D}{2}-1}}{\Gamma(D/2)} \theta(E-V(\mathbf{q})). \tag{2.77}$$

$\bar{\rho}_{\mathrm{v}}(E)$ is the first term of the *Weyl expansion* in orders of $\hbar$. Higher order terms arise due to the modification of the free propagator near the boundary $\partial\Omega$ of the billiard. Since the wave function has to fulfil Dirichlet boundary conditions

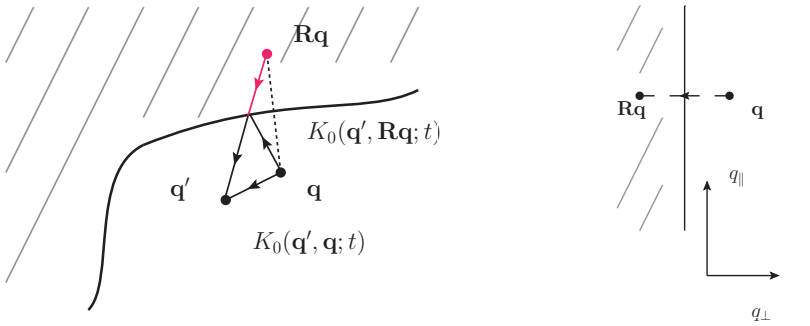
$$\psi(\mathbf{q}) = 0 \quad \forall \mathbf{q} \in \partial\Omega, \tag{2.78}$$

the propagator has to be adjusted appropriately (see figure 2.4). In other words, wave propagation is affected by wave reflection on the boundary. For the second term in the Weyl expansion we assume the boundary as locally flat (fig. 2.4b) and modify the free propagator by the propagator with the final point $\mathbf{q}' = R\mathbf{q}$ reflected with respect to $\partial\Omega$. The corresponding trace yields a complete Fresnel integral

$$\int_{\partial\Omega} \mathrm{d}q_{\parallel} \int_0^{\infty} \mathrm{d}q_{\perp} \, \left(\frac{m}{2\pi i\hbar\, t}\right) \exp\left(\frac{i}{\hbar}\frac{m}{2t}|2q_{\perp}|^2\right) \tag{2.79}$$

which is converging fast with the upper limit of the perpendicular integration, since $\hbar$ is assumed to be small in the semiclassical limit. Therefore we can simply send the upper limit of $q_{\perp} \to \infty$ not caring about what happens deep inside the interior of the billiard far away from the boundary. Fourier transformation yields the second term in the Weyl expansion

$$\bar{\rho}_{\mathrm{p}}(E) = -\frac{L}{8\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} E^{-\frac{1}{2}}\theta(E), \tag{2.80}$$



(a) shaped boundary (b) flat boundary

Figure 2.4: wave reflection on a flat boundary. Dirichlet boundary condition is maintained by modifying the propagator by a term with one point reflected with respect to the boundary.

which is often called the *perimeter Weyl term*, since it is proportional to the perimeter L of the billiard. Notice that in a system with flat wall, there is also no periodic orbit at all, thus we can be sure not to count any contribution to the propagation redundantly.

There is also a third term in the Weyl expansion associated with the curvature of $\partial\Omega$. Taking corners into account separately, the Weyl expansion for a $2D$ billiard reads [19].

$$\bar{\rho}(E) = \frac{A}{4\pi}\left(\frac{2m}{\hbar^2}\right)\theta(E) \; - \; \frac{L}{8\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} E^{-\frac{1}{2}}\theta(E) + \tag{2.81}$$

$$+ \; \frac{1}{12\pi}\int_{\partial\Omega} \frac{\mathrm{d}l}{R_{\mathbf{q}}}\,\delta(E) \; + \; \sum_i \frac{\pi^2 - \alpha_i^2}{24\pi\alpha_i}\,\delta(E), \tag{2.82}$$

where the third term is an integral along the boundary over the inverse of local curvature radii $R_{\mathbf{q}}$. The fourth term is a sum over all corners i with opening angles α_i. In the absence of corners and a simply connected billiard interior Ω (2.81) simplifies to

$$\bar{\rho}(E) = \frac{A}{4\pi}\left(\frac{2m}{\hbar^2}\right)\theta(E) \; - \; \frac{L}{8\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} E^{-\frac{1}{2}}\theta(E) \; + \; \frac{1}{6}\delta(E) \tag{2.83}$$

We see that the several terms are of successively increasing order in $\hbar$ and decreasing order in E. So that higher terms in the Weyl expansion mainly affect the low energy regime. For high energies the description through the volume term is sufficient.

One should mention that there is also a generalised form of Weyl expansion similar to (2.83) derived by Balian and Bloch for arbitrary D-dimensional curved

manifolds which can even be applied to a curvature description by means of inner geometry expressed through Riemann curvature [1].

3 Periodic Orbit Theory For Identical Particles

3.1 Symmetry Projected Trace Formula

3.1.1 From Periodic To Exchange Orbits

In this section we will sketch the usual derivation of a semiclassical trace formula as followed in section 2.2.1. But this time we want to incorporate Fermi-Dirac or Bose-Einstein statistics for many body systems, and see how this affects the derivation. The following approach has been presented by Weidenmüller in 1993 [31]. There is also another approach that uses dynamics in a reduced phase space that will be presented in the next section.

Remind how we get the full unsymmetrized quantum mechanical spectrum via Green's function (see section 2.2.1):

$$\rho(E) = -\frac{1}{\pi}\Im\left(\operatorname{tr}\hat{G}(E+i\epsilon)\right) \text{ in the limit } \epsilon \to 0^+ \tag{3.1}$$

where

$$\hat{G}(E+i\epsilon) = \sum_n \frac{|\psi_n\rangle\langle\psi_n|}{E-E_n+i\epsilon} \tag{3.2}$$

with the full set $\{|\psi_n\rangle\}$ of eigenstates of $\hat{H}$.

For the symmetrized spectrum we take $\{|\psi_n\rangle\}$ as the common eigenbasis of $\hat{H}$ and $\hat{\mathbb{1}}_\pm$ so that the set consists of two subsets. One lying in the subspace of symmetric states and the other one being orthogonal to it (see section (2.1.2)). $+$ refers to bosonic symmetry and $-$ to fermions.

We insert the projector inside the trace in order to get rid of all states without the wanted symmetry

$$\rho_\pm(E) = -\frac{1}{\pi}\Im\left(\operatorname{tr}\left(\hat{G}(E+i\epsilon)\hat{\mathbb{1}}_\pm\right)\right) \tag{3.3}$$

As in the last section we can introduce the semiclassical approximation for the Green's function in coordinate space

$$\langle \mathbf{q}'|\hat{G}(E)|\mathbf{q}\rangle \approx G_{\mathrm{scl}}(\mathbf{q}', \mathbf{q}; E) \tag{3.4}$$

Without symmetrisation we had to perform the trace as spatial integral $\int \mathrm{d}^{DN}q$ of $G_{\mathrm{scl}}(\mathbf{q}, \mathbf{q}; E)$, which containts all orbits travelling from coordinates $\mathbf{q}$ back to themselves with given energy E . The according stationary phase approximation yielded the condition of equal initial and final momentum $\mathbf{p}' = \mathbf{p}$ hence leaving only periodic orbits in the sum (see equation (2.66)).

Taking symmetrisation into account by applying the projector in coordinate space yields

$$\mathrm{tr}(\hat{G}\hat{\mathbb{1}}_{\pm}) = \frac{1}{N!}\int \mathrm{d}^{ND}q \sum_{\sigma\in S_N} (\pm 1)^{\sigma} G(P\mathbf{q}, \mathbf{q}; E) \tag{3.5}$$

When introducing again the semiclassical Green's function and doing a stationary phase approximation, the stationarity condition is

$$\begin{aligned} 0 &= \frac{\partial S(P\mathbf{q}, \mathbf{q}; E)}{\partial q_i} \\ &= \left[\frac{\partial S(\mathbf{q}', \mathbf{q}; E)}{\partial q_i} + \frac{\partial S(\mathbf{q}', \mathbf{q}; E)}{\partial q'_k}\frac{\partial (P\mathbf{q})_k}{\partial q_i}\right]_{\mathbf{q}'=P\mathbf{q}} \\ &= -p_i(0) + p_k(0)P_{ki} \\ &= -p_i(0) + \left(P^{-1}\mathbf{p}\right)_i \\ &\Rightarrow \mathbf{p}(t) = P\mathbf{p}(0) \end{aligned} \tag{3.6}$$

which means the sum over orbits is now restricted to all kinds of orbits that connect an initial phase space point with an arbitrary permuted version of it as a final phase space point. Note that the identity as a special permutation yields the normal periodic orbits. All others shall be referred to as *exchange orbits* form now on.

Because of the symmetry of the system, every exchange orbit is part of a periodic orbit (see also section 2.1.1). Let $\xi(t)$ be the trajectory of a partial orbit starting at the phase space point ξ_0 at time $t = 0$ and ending at $P\xi_0$ at time $t = t_0$. Following the trajectory again for the time t_0 is done by regarding $P\xi_0$ as new initial condition at $t = 0$. The solution of the equations of motion is now just the permuted version $P\xi(t)$ with final point $P^2\xi_0$. As the multiple repetition of every permutation yields identity for a smallest number n of repetitions

$$P^n = \mathbb{1} \qquad \hat{P}^n = \hat{\mathbb{1}}, \tag{3.7}$$

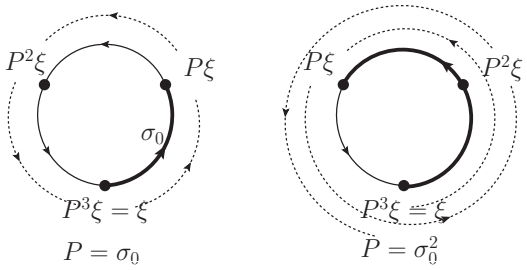


Figure 3.1: some example of orbits related to specific choices of the permution.

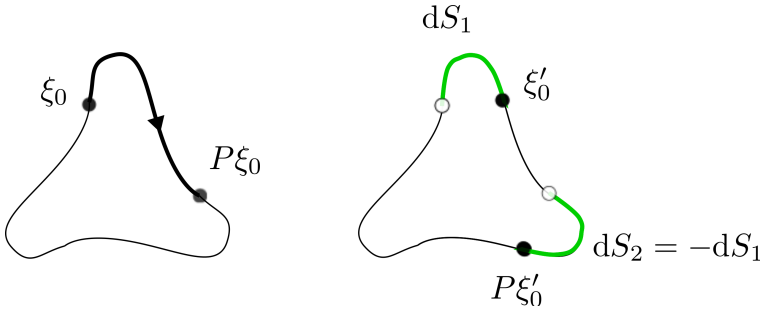


Figure 3.2: The classical action along exchange orbits is invariant under time shift.

every exchange orbit eventually closes itself after n repetitions and hence is part of a *full periodic orbit* which in general is the m-th repetition of a primitive periodic orbit (see figure 3.1).

Again we use local coordinates $\mathbf{q} = (q_\parallel, \mathbf{q}_\perp)$ in the vicinity of that primitive periodic orbit and separate the dependence on $q_\parallel$ in the prefactor of the semiclassical Green's function (2.67). Notice that also for exchange orbits the classical action is independent of the parallel component even though initial and final points of the according line integral are not equal and change with variation of $q_\parallel$:

$$\begin{aligned}\frac{\mathrm{d}S(P\mathbf{q},\mathbf{q};E)}{\mathrm{d}q_\parallel} &= \frac{\mathrm{d}}{\mathrm{d}q_\parallel}\int\limits_{\gamma:\mathbf{q}\to P\mathbf{q}} \mathrm{d}\mathbf{q}\cdot p \\ &= \mathbf{p}(t)\cdot\frac{\mathrm{d}\mathbf{q}(t)}{\mathrm{d}q_\parallel} - \mathbf{p}(0)\cdot\frac{\mathrm{d}\mathbf{q}(0)}{\mathrm{d}q_\parallel} \\ &= (P\mathbf{p})\cdot(P\hat{\mathbf{q}}) - \mathbf{p}\cdot\hat{\mathbf{q}} \\ &= 0 \end{aligned} \tag{3.8}$$

This is illustrated in figure 3.2. Integrating over $q_\parallel$ gives again the primitive period T_{ppo} of the full periodic orbit while integrating over $\mathbf{q}_\perp$ yields a final

prefactor of

$$\left|\det\left({}_P\tilde{\mathbb{M}}^{\frac{m}{n}} - \mathbb{1}\right)\right|^{-\frac{1}{2}} \tag{3.9}$$

with the stability matrix ${}_P\tilde{\mathbb{M}}^{\frac{m}{n}}$ being the area preserving map of perpendicular phase space deviations at an initial point ξ_0 onto the perpendicular deviations at the final point $P\xi_0$ in linearised motion. The perpendicular coordinates must be defined in such a way, that the same vector $\mathbf{q}'_\perp = \mathbf{q}_\perp$ at the final and initial point means that the phase space deviation at the final point is the permutation of the deviation at the initial point. In other words, the basis of deviations at $P\xi_0$ should be the transformation of the basis at ξ_0 by virtue of the permutation P. This rule is worked out in the appendix A. Notice that also ${}_P\tilde{\mathbb{M}}^{\frac{m}{n}}$ is independent on the starting point along the orbit.

The exponent indicates that the n-th repetition of the exchange orbit has the usual stability matrix of the m-th repetition of the according primitive periodic orbit

$$\left({}_P\tilde{\mathbb{M}}^{\frac{m}{n}}\right)^n = \left(\tilde{\mathbb{M}}_{\text{ppo}}\right)^m \tag{3.10}$$

m and n are fully determined by the actual orbit and its related permutation and therefore are only kept to keep in mind this relation. Note: the partial stability matrix cannot be constructed uniquely by taking the root of the full stability matrix with sole knowledge of m and n because it is not clear which branch to take for the root. Therefore the subscript P cannot be dropped and the matrix should be seen as a stand-alone object.

With all that the trace formula for the symmetry projected density of states in given by

$$\tilde{\rho}_{\text{scl},\pm} = \frac{1}{\pi\hbar N!}\sum_{\sigma\in S_f}(\pm 1)^\sigma \sum_{\gamma,\xi\to P\xi} \frac{T_{\text{ppo},\gamma}}{\left|\det\left({}_P\tilde{\mathbb{M}}_\gamma^{\frac{m}{n}} - \mathbb{1}\right)\right|^{\frac{1}{2}}} \cos\left(\frac{1}{\hbar}S_\gamma(E) - \frac{\pi}{2}\mu_\gamma\right), \tag{3.11}$$

where γ refers to all exchange orbits (or periodic in the case $\sigma = 1$) of energy E. $T_{\text{ppo},\gamma}$ represents the period of the full primitive periodic orbit related to γ. Note that γ is allowed to contain multiple traversals of the related full primitive periodic orbit.

3.1.2 A Formulation In Reduced Phase Space

Interestingly, Jonathan M. Robbins [23] 1988 developed a form of trace formula for systems with discrete spatial symmetries working in a symmetry reduced system. This formula gives a Gutzwiller type semiclassical approximation of the

symmetry projected spectrum. The projection is according to any irreducible representation of the group of discrete spatial transformations under which the system is symmetric. The projected density of states is given in terms of classical periodic orbits in a reduced phase space weighted with the group characters of the representation. Before the application to the special case of particle exchange symmetry, let us see how it works in general.

Trace Formula For Discrete Symmetries

Let G be the group of point transformations $g \in G$ under which the system under consideration is symmetric. The Hilbert space may be restricted to a subspace that is invariant under the symmetry. The states in that subspace then transform according to an irreducible representation α of G with characters $\chi_\alpha(g)$ and dimension d_α. The classical dynamics can be expressed in a symmetry reduced phase space instead of the full phase space.
Therefore the phase space is divided into a net of primitive cells according to the symmetry. One is free to pick one of them. Then all pairs of points lying on the boundary of that primitive cell that are related by symmetry are identified topologically. The dynamics in the reduced phase space are inherited from the original phase space. The full dynamics are then obtained by the reduced ones together with an additional ignorable discrete coordinate $g(t)$ which is just the group element relating a point $\xi^{(\mathrm{sr})}(t)$ in reduced phase space to the point in full phase space $\xi(t) = g\left(\xi^{(\mathrm{sr})}(t)\right)$. So for a trajectory $\xi(t)$ starting in the considered primitive cell its value is just the identity in the beginning and changes every time the trajectory moves from one primitive cell into another.

With this construction, the oscillatory part of the semiclassical density of states for the invariant subspace according to the irreducible representation α reads

$$\tilde{\rho}_\alpha^{(\mathrm{sr})}(E) = \frac{d_\alpha}{\pi\hbar} \sum_\gamma \frac{T_\gamma^{(\mathrm{sr})}}{|K_\gamma|} \sum_{r=1}^{\infty} \chi_\alpha(g_\gamma^r) \frac{\cos\left(r\frac{1}{\hbar}S_\gamma^{(\mathrm{sr})} - r\frac{\pi}{2}\mu_\gamma^{(\mathrm{sr})}\right)}{\left|\det\left(\left(\tilde{\mathbb{M}}_\gamma^{(\mathrm{sr})}\right)^r - \mathbb{1}\right)\right|^{1/2}}. \tag{3.12}$$

Here, all quantities marked with (sr) denote the corresponding standard classical properties of the orbit γ but all obtained in the reduced phase space. $T^{(\mathrm{sr})}$ here denotes the primitive period in reduced phase space. $|K_\gamma|$ is the order of the subgroup of G under which the orbit γ remains unaffected. For the vast majority of periodic orbits this subgroup only contains identity because only orbits completely lying on the boundary of the primitive cell can be invariant under some symmetry transformation. So we feel free to drop this factor in most cases.

It is worth to hold on for a moment and notice how the definition of stability matrix $\tilde{\mathbb{M}}_\gamma^{(\mathrm{sr})}$ on the basis of reduced phase space dynamics is related to the

standard definition $\tilde{\mathbb{M}}_\gamma$ in full phase space. Let us consider a point in the primitive cell $\xi(0)$ and a slight deviation $\delta\xi(0)$ perpendicular to $\dot{\xi}(0)$ and within the energy surface. When following the trajectories of this point $\xi(t)$ and its slightly perturbed counterpart $\xi'(t) = (\xi + \delta\xi)(t) \equiv \xi(t) + \delta\xi(t)$ we assume the deviation to be small enough that both, $\xi(t)$ and $\xi'(t)$ lie in the same primitive cell (in the end we need infinitesimal deviations only). Thus the evolution of deviation $\delta\xi(t)$ in full phase space and reduced phase space are related by the same symmetry transformation as are the respective versions of the unperturbed point $\xi(t)$

$$\begin{aligned}\xi(t) &= g\left(\xi^{(\mathrm{sr})}(t)\right)\\ \xi'(t) &= g\left(\xi'^{(\mathrm{sr})}(t)\right) = \xi(t) + g\left(\delta\xi^{(\mathrm{sr})}(t)\right).\end{aligned}$$

In the definition of the stability matrix in reduced phase space we need derivatives of $\delta\xi^{(sr)}$

$$\tilde{\mathbb{M}}^{(\mathrm{sr})}_{ij} = \frac{\partial\, \delta\xi_i^{(\mathrm{sr})}(T^{(\mathrm{sr})})}{\partial\, \delta\xi_j(0)}. \tag{3.13}$$

So for reasons of compatibility the stability matrix of the corresponding unfolded orbit in full phase space which is not periodic in general has to be defined through

$$\tilde{\mathbb{M}}_{ij} = \frac{\partial\, (g^{-1}(\delta\xi))_i(T^{(\mathrm{sr})})}{\partial\, (\delta\xi)_j(0)}. \tag{3.14}$$

This means the deviation after time $T^{(\mathrm{sr})}$ has to be measured in a basis that is the transformation of the basis used for the original deviation. Note that normally in periodic orbit theory one does not have open orbits. The question of relation between these local coordinate systems for deviations only emerges in the context of discrete symmetries and therefore had to be extra addressed.

We immediately see that in the case of identical particles the symmetry reduced stability matrix used here is exactly the branch of root we had to take of the full periodic orbit stability matrix in the Weidenmüller trace formula (3.11).

$$\left(\tilde{\mathbb{M}}^{(\mathrm{sr})}\right)^r = {}_P\tilde{\mathbb{M}}^{\frac{m}{n}} \tag{3.15}$$

Also let me briefly comment on the Maslov index μ in (3.12) in the case of particle exchange symmetry. Let us discuss the case of *unstable periodic* orbits at first. Then one can define the Maslov index as a winding number of a quantity $C(t)$ in complex plane (see for example the appendix in [19]) that is related to the number of windings of the unstable manifold around the trajectory during one period T. As the unstable manifold itself remains invariant under time evolution, the winding number (and therefore μ) is an integer. Using the same definition of $C(t)$ for an unfolded unstable orbit connecting a point $\xi(0)$ and its

symmetry transformation $\xi(T) = g(\xi(0))$, the cut through the unstable manifold at $t = T$ is the permuted version of the cut through the unstable manifold at $t = 0$. Due to this, the permutation matrix appears in $C(t)$ as a factor of squared determinant $(\det P)^2$, which is simply unity and therefore $C(T)$ is a real multiple of $C(0)$ just as for a periodic orbit. Meaning that the corresponding winding number is integer. Thus the Maslov index for an exchange orbit γ - which is then equal to the standard Maslov index obtained in reduced phase space - is also an additive integer. So that the n-th repetition of γ has got an index of $n\mu$.
Contrary to that, for stable isolated orbits, Maslov indexes are in general not additive [19]. Nonetheless we will write the according indexes as multiples silently assuming that all isolated periodic orbits in a considered system are either unstable or stable with the additional property of additive indexes.

Reduced Phase Space For Exchange Symmetry

All we need now to be fully able to use (3.12) for identical particles is to formulate a reduced phase space for exchange symmetry. This can be done by introducing unique ordering of particle coordinates $\mathbf{q}_i$. Thereby only one specific spatial component $q_i^{(d)}$ has to be ordered. One choice of primitive cell $(d = 1)$ then reads

$$\mathscr{P}^{(sr)} = \left\{ (\mathbf{q}, \mathbf{p}) \in \mathbb{R}^{2ND} \;\middle|\; q_1^{(1)} \leq q_2^{(1)} \leq \ldots \leq q_N^{(1)} \right\}. \tag{3.16}$$

Its boundary or surface is given by equality of any two particles in this specific component

$$\mathcal{S} = \left\{ (\mathbf{q}, \mathbf{p}) \in \mathbb{R}^{2ND} \;\middle|\; (\exists i \neq j) \; \left(q_i^{(1)} = q_j^{(1)} \right) \right\} = \bigcup_{i \leq j} \mathcal{S}_{ij}, \tag{3.17}$$

where the whole surface is made out of hyperplanes

$$\mathcal{S}_{ij} = \left\{ (\mathbf{q}, \mathbf{p}) \in \mathbb{R}^{2ND} \;\middle|\; q_i^{(1)} = q_j^{(1)} \right\}. \tag{3.18}$$

When the unfolded trajectory passes through such an hyperplane $\mathcal{S}_{ij}$ the primitive cell it enters is mapped back to $\mathscr{P}^{(\mathrm{sr})}$ by exchange of the particles i and j

$$\begin{aligned} (\ldots, \mathbf{q}_i, \ldots, \mathbf{q}_j, \ldots) &\mapsto (\ldots, \mathbf{q}_j, \ldots, \mathbf{q}_i, \ldots) \\ (\ldots, \mathbf{p}_i, \ldots, \mathbf{p}_j, \ldots) &\mapsto (\ldots, \mathbf{p}_j, \ldots, \mathbf{p}_i, \ldots) \,. \end{aligned}$$

The full phase space can be reobtained by applying all possible permutations $\sigma \in S_N$ to $\mathscr{P}^{(\mathrm{sr})}$

$$\mathscr{P} = \mathbb{R}^{2ND} = \bigcup_{\sigma \in S_N} \sigma \left(\mathscr{P}^{(\mathrm{sr})} \right). \tag{3.19}$$

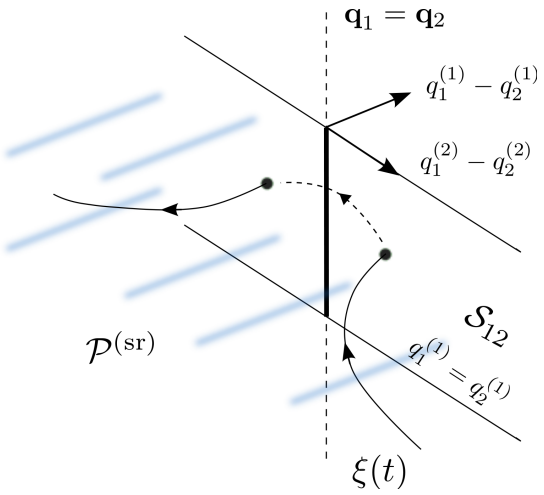


Figure 3.3: Reduced phase space of a many body system. A trajectory passing through the boundary is mapped to a topologically identified point on the surface in order to keep it inside the reduced phasespace (light blue).

Figure 3.3 illustrates an example of reduced phase space, where some of the coordinates and the momenta are projected in order to give a effective three dimensional illustration.

Intersections And Boundary Multiplets

When passing the intersection $\mathcal{S}_\cap$ of more than one hyperplanes the according exchanges could be applied one after another. By mapping back to the reduced phase space through the first exchange operation, the direction of motion also changes. Thus the next penetrated surface has to be determined according to the new time derivative $\dot{\xi}$. Or for a more systematic treatment of this case, let us subsume all particle indexes whose $q^{(1)}$ components are equal in $\mathcal{S}_\cap$.

$$\mathcal{S}_\cap = \mathcal{S}_{I_1} \cap \mathcal{S}_{I_2} \cap \cdots \cap \mathcal{S}_{I_n} \tag{3.20}$$

with ordered sets of indexes

$$\begin{aligned} I_a &= \{i_{a,1}, i_{a,2}, \ldots, i_{a,m_a}\} \qquad\qquad a = 1, \ldots, n \\ i_{a,1} &< i_{a,2} < \cdots < i_{a,m_a} \\ (i_a \in I_a) &< (i_b \in I_b) \quad \forall \quad a < b, \end{aligned}$$

so that

$$\mathcal{S}_{I_a} = \left\{ \xi \in \mathbb{R}^{2ND} \;\middle|\; q_{i_{a,1}}^{(1)} = q_{i_{a,2}}^{(1)} = \cdots = q_{i_{a,m_a}}^{(1)} \right\}. \tag{3.21}$$

Right before the penetration of $\mathcal{S}_\cap$ the phase space point inside $\mathscr{P}^{(sr)}$ has the ordering

$$\begin{aligned} & q^{(1)}_{i_{1,1}} < q^{(1)}_{i_{1,2}} < \cdots < q^{(1)}_{i_{1,m_1}} \\ < \quad & q^{(1)}_{i_{2,1}} < q^{(1)}_{i_{2,2}} < \cdots < q^{(1)}_{i_{2,m_2}} \\ & \vdots \\ < \quad & q^{(1)}_{i_{n,1}} < q^{(1)}_{i_{n,2}} < \cdots < q^{(1)}_{i_{n,m_n}} . \end{aligned} \tag{3.22}$$

As the trajectory is supposed to pierce every hyperplane $\mathcal{S}_{ij}$ involved, the time derivatives have to be ordered

$$\dot{q}^{(1)}_i > \dot{q}^{(1)}_j \qquad \text{for} \qquad i < j \,! \tag{3.23}$$

So right before passing through $\mathcal{S}_\cap$ the velocities of each index set I_a are ordered inverse to (3.22) and therefore the ordering of coordinates $q'^{(1)}_i$ right after the penetration also is inverted set-wise. The ordering between the sets remains the same since the according components are supposed not to become equal at the time of penetration.

$$\dot{q}^{(1)}_{i_{a,1}} > \dot{q}^{(1)}_{i_{a,2}} > \cdots > \dot{q}^{(1)}_{i_{a,m_a}} \qquad \forall a \tag{3.24}$$

$$q'^{(1)}_{i_{a,1}} > q'^{(1)}_{i_{1,2}} > \cdots > q'^{(1)}_{i_{a,m_a}} \qquad \forall a \tag{3.25}$$

$$q'^{(1)}_{i_{a,r}} < q'^{(1)}_{i_{b,s}} \qquad (\forall a < b)\ (\forall r, s) \tag{3.26}$$

This tells us uniquely how points lying on intersections of hyperplanes on the boundary have to be identified which is important to know since those boundary points do not only appear in pairs related by symmetry in general. Instead they occur as Boundary Multiplets. This contradicts the claim in [23] that this situation does not exist.

In order to support this statement and to illustrate the above construction we will first show an easy example for particle exchange symmetry. Then we shall show an even easier example of symmetry for which the manifestation of symmetry related pairs also does not hold.

First, consider a system of three free particles in two dimensions with coordinates

$$(x_1, y_1, x_2, y_2, x_3, y_3) \,. \tag{3.27}$$

Momenta may be ignored for simplicity. At time $t_<$ in the primitive cell $\mathscr{P}^{(\mathrm{sr})}$ forming the reduced phase space the coordinates are ordered

$$x_1(t_<) < x_2(t_<) < x_3(t_<) \,, \tag{3.28}$$

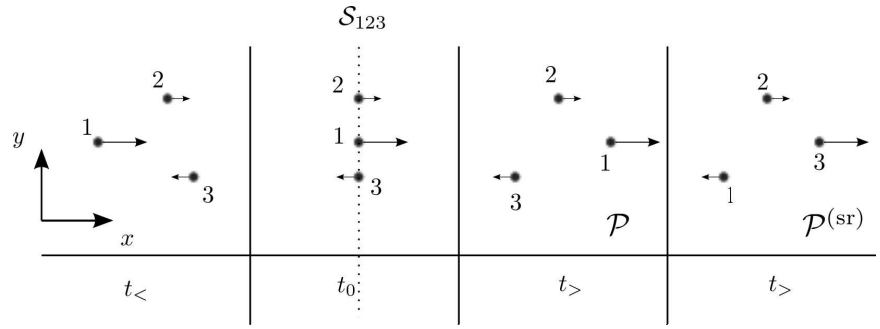


Figure 3.4: A system of three identical particles in two dimensions right before, at and after the penetration of the boundary of the reduced phase space. The last step maps the system from full phase space back into the reduced phase space. Numbers denote particle indexes.

at time $t_0 > t_<$ the trajectory shall penetrate the boundary at the intersection $\mathcal{S}_{123}$

$$x_1(t_0) = x_2(t_0) = x_3(t_0), \tag{3.29}$$

and at time $t_> > t_0$ the unfolded trajectory lies outside $\mathscr{P}^{(\mathrm{sr})}$

$$x_1(t_>) > x_2(t_>) > x_3(t_>)\,. \tag{3.30}$$

It then has to be mapped back into $\mathscr{P}^{(\mathrm{sr})}$ by inverting the sequence of all three particles. That is by virtue of the permutation σ

$$\begin{aligned} &(\mathbf{x},\mathbf{y}) \mapsto \left(\mathbf{x}^{(\mathrm{sr})},\mathbf{y}^{(\mathrm{sr})}\right) = (\sigma(\mathbf{x}),\sigma(\mathbf{y})) \\ \text{with} \qquad &\sigma = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix} \end{aligned} \tag{3.31}$$

in standard notation of permutations.
So by this unique mapping of surface points, the trajectory $\xi^{(\mathrm{sr})}(t)$ stays in $\mathscr{P}^{(\mathrm{sr})}$ for all times. Figure 3.4 illustrates this situation Due to the additional degrees of freedom $\mathbf{y}$ (and momenta) there are in general $3! - 2 = 4$ additional distinct permutations of the surface point $\xi(t_0)$ also lying on the boundary. But all of these would immediately evolve out of $\mathscr{P}^{(\mathrm{sr})}$ again. Hence by mapping the pairs of symmetry related boundary points that correspond to the inversion of index sets we can maintain well defined reduced dynamics in the reduced phase space.

Speaking of the reduced phase space as a continuous topological space in its own right all six related points are identical and dynamics in that point have to be defined by the correct map of the dynamics in full phase space back into the reduced one. This means Robbins formula (3.12) can be used despite failure of

the argument of pair manifestation of boundary points!

In order to show that the existence of boundary multiplets is not inherent to the special case of exchange symmetry I shall show another example in appendix B. It will also serve to illustrate what was the false conclusion in the pair argument in [23]. Closing, one should stress that this is not supposed to affect the formalism of Robbins significantly which in its beauty has served many as the approach to semiclassics with discrete symmetries.

3.1.3 Equivalence Of Many Body And Single Particle Pictures

In this section let us mainly consider systems of many fermions moving on a line. These systems have some special properties that are setting them apart from higher dimensional ones. It is worth restricting ourselves to such systems for a moment since we will see that on the one hand, they can easily be mapped onto single particle systems in a quantum mechanical description. On the other hand, the semiclassical description of this effective single particle system will also turn out to be equivalent to the semiclassical treatment of the many body system. So this simple example shows that the symmetry projected trace formula indeed gives the correct semiclassical description and that there is no additional loss when incorporating symmetry. In a sense, this means the semiclassical approximation of a many body system is just as good as semiclassics work with single particle systems.

In one dimensional systems a fundamental domain in coordinate space can be given by

$$\mathscr{F} := \left\{ \mathbf{q} \in \mathbb{R}^N \middle| q_1 \leq q_2 \leq \cdots \leq q_N \right\} \tag{3.32}$$

Its boundaries are given by the equations $q_i = q_j$ and the full domain can be reobtained by applying all possible permutations $\sigma \in S_N$ to the fundamental domain

$$\mathbb{R}^N = \bigcup_{\sigma \in S_N} \sigma\left(\mathscr{F}\right) \tag{3.33}$$

The fundamental domain often is referred to as reduced coordinate space and can be regarded as the coordinate part of the reduced phase space $\mathscr{P}^{(\mathrm{sr})}$ introduced in section 3.1.2. Topological identification of boundary points in this context is not needed.

Quantum Mechanical Equivalence

For fermions the restriction to antisymmetric states yields the condition of vanishing wave function all along the boundary

$$\psi\left(\mathbf{q}\right) = 0 \qquad (\forall \mathbf{q})(\exists i \neq j)(q_i = q_j). \tag{3.34}$$

As a Dirichlet boundary condition this condition is sufficient to determine the eigenfunctions in $\mathscr{F}$ together with some single particle condition at finite (for a hard confined system) or infinite distance (for free or smoothly confined fermions). The condition can be thought of as hard wall or in other words an infinite potential barrier.
The wave functions in the other parts of the full domain are then obtained by

$$\psi\left(P\,\mathbf{q}\right) = (-1)^P\,\psi\left(\mathbf{q}\right). \tag{3.35}$$

One has to stress that this is a feature of one dimensional systems only because there, no additional condition besides (3.34) is induced to the wave function within the fundamental domain. In contrast to that, the corresponding Dirichlet condition for dimensions larger than one are not given along the whole boundaries ($q_i^{(1)} = q_j^{(1)}$) of the fundamental domain, but instead only on lower dimensional manifolds ($\mathbf{q}_i = \mathbf{q}_j$) embedded in those. On the rest of the boundary the symmetry condition (3.35) can not be expressed as a Dirichlet boundary condition.

It is worth to note that one could topologically identify points along the boundary of $\mathscr{F}$ that are related by symmetry and thereby create a fundamental domain with complex topology. We will call this object the *wrapped fundamental domain*. The problem in the fermionic case then would be the need of an additional condition of sign inversion $\psi\left(\mathbf{q}\right) \to -\psi\left(\mathbf{q}\right)$ respective the direction perpendicular to the boundary. This condition seems quite peculiar and so far the author has not found a treatment of it in the literature.

Note also that in the bosonic case this additional condition would not be needed. There, one would just have to solve the Schrödinger equation on the wrapped fundamental domain for a continuous wave function. Also the symmetry induced Neumann condition on the sub-manifolds ($\mathbf{q}_i = \mathbf{q}_j$) would be automatically implied by the topology in their vicinities.

So an equivalence of quantum mechanical many body systems with simple multidimensional single particle systems defined on (possibly wrapped) fundamental domains seems to be easily findable for one dimensional systems with fermionic statistics on the one hand and higher dimensional systems with bosonic statistics on the other hand.

Semiclassical Equivalence

Now that we know of the equivalence of many body and single particle quantum systems we can test both perspectives in the semiclassical approximation.

For a $D = 1$ system of fermions we use Robbins formula in reduced phase space (3.12). The latter being the Cartesian product of the fundamental domain of

the above section $\mathscr{F}$ with $\mathbb{R}^{2N}$ for momenta together with the identification of symmetry related boundary points.

$$(\ldots, q_i, \ldots, q_j, \ldots, p_i, \ldots, p_j, \ldots) \leftrightarrow (\ldots, q_j, \ldots, q_i, \ldots, p_j, \ldots, p_i, \ldots)\,.$$

When a classical trajectory passes $\mathcal{S}_{ij}$ the according momenta are switched. This process is exactly what happens when a single (ND)-dimensional particle is reflected on a hard wall defined by the boundary $\mathcal{S}_{ij}$. So we easily see the equivalence of dynamics in reduced phase space on the one hand and the fundamental domain with hard walls along the boundaries on the other hand. The only difference is that in reduced phase space, due to topological identification, the trajectory is moving continuously whereas a proper hard wall reflection is an immediate jump from one phase space point to another.

Working with Robbins formula, by passing a boundary $\mathcal{S}_{ij}$ the ignorable coordinate $g(t) = \sigma$ gets multiplied by a transposition (in cycle notation)

$$(ij) = \begin{pmatrix} \cdots & i & \cdots & j & \cdots \\ \cdots & j & \cdots & i & \cdots \end{pmatrix}, \tag{3.36}$$

so that the group character $\chi_-(g) = \mathrm{sgn}(\sigma)$ for the fermionic representation gets multiplied by $(-1) = \mathrm{sgn}\,((ij))$.

Working with the Gutzwiller formula in the fundamental domain with infinite potential barriers along the boundaries, every reflection on a hard wall $\mathcal{S}_{ij}$ gives an additional phase shift of $e^{-i\pi} = (-1)$. The essential here is the fact that phase shifts for exchange come in as Maslov phases in the single particle picture whereas in the many body picture they are incorporated as the group characters of the ignorable coordinate. There, due to the smoothness of the trajectory, no extra Maslov phase is accumulated. So we get the same result for the oscillating part of the density of states $\tilde{\rho}(E)$ in both pictures.

One should shortly comment on in-plane orbits and corner reflections. The factor of $1/|K_\gamma|$ in (3.12) is nontrivial only for orbits that lie in a hyperplane $\mathcal{S}_{ij}$. This corresponds to orbits along the hard wall in the single particle picture. For these, Gutzwiller's periodic orbit sum has to be modified by the same factor because in its derivation the Gaussian integral perpendicular to the orbit only has to be performed for those coordinates lying inside the fundamental domain. For a more detailed discussion on that we refer the reader to the appendix of [23]. For simultaneous reflection on some hard walls, the total phase shift is $-\pi$ times the number of hard walls involved. So for the reflection on $\mathcal{S}_{i_1,\ldots,i_n}$ the number of involved hard walls is

$$\binom{n}{2} = \frac{1}{2}n(n-1), \tag{3.37}$$

yielding a factor of $e^{-i\pi\frac{1}{2}n(n-1)} = (-1)^{\frac{1}{2}n(n-1)}$.

As discussed in section 3.1.2 in the many body picture the according permutation is the inversion

$$\sigma = \begin{pmatrix} i_1 & \cdots & i_n \\ i_n & \cdots & i_1 \end{pmatrix}, \tag{3.38}$$

which can be written as successive transposition of neighbouring indexes. This yields the total number of transpositions

$$\sum_{i=1}^{n-1} i = \frac{1}{2}n(n-1), \tag{3.39}$$

resulting in a character factor of $\mathrm{sgn}(\sigma) = (-1)^{\frac{1}{2}n(n-1)}$. So all cases are contained in the equivalence of both pictures.

For the higher dimensional bosonic case all group characters are just unity

$$\chi_+(g(t)) = 1 \tag{3.40}$$

and thus the corresponding symmetry projected periodic orbit sum is exactly the same as the normal Gutzwiller trace in the wrapped fundamental domain. No hard wall reflections do appear in this case. There are no additional phase shifts. So also in this case the equivalence of both pictures is evident.

3.2 Spectral Statistics

3.2.1 A Classical Sum Rule For Systems With Discrete Symmetry

The key of a semiclassical access to universal behaviour are classical sum rules based on ergodic behaviour of the underlying classical system. The sum rule most cited and used in this context is a sum rule originally found by Hannay and Ozorio de Almeida in 1984 [12]. It allows to use the semiclassical trace formula in terms of periodic orbits to obtain several universal properties of chaotic ergodic systems. We shall refer to it in abbreviated form as the HOdA sum rule. For educational reasons, as with the trace formula itself, we want to follow the derivation of the usual form first. Then we introduce a discrete symmetry and point out how modifications arise. As the HOdA sum rule is much easier to be understood for area-preserving maps than for flows, the reader is invited to first have a brief look on that implementation in appendix B.

HOdA Sum Rule For Flows

The derivation of the sum rule for flows below is basically following Hannay [12]. In this subsection we use $\mathbf{x}$ as variable for a point in the $2n$-dimensional phase space $\mathscr{P}$. For the sake of simplicity we consider the phase space as euclidean with coordinates and canonical momenta both measured in units of square root of action

$$[q_i] = [p_i] = [x_i] = [\sqrt{\hbar}]. \tag{3.41}$$

Actually, one would have to consider $\mathscr{P}$ as symplectic with rather complicated mathematical description. But the simple description turns out to be sufficient. Let us consider a conservative system $H = E = const.$ with the flow

$$\begin{aligned} \Phi : \quad \mathbb{R} \times \mathscr{P} &\to \mathscr{P} \\ (t, \mathbf{x}) &\mapsto \Phi_t(\mathbf{x}) \end{aligned} \tag{3.42}$$

Since we are interested in properties of classical orbits at constant energy, the whole analysis is restricted to the energy shell

$$\mathscr{E} := \{\, \mathbf{x} \in \mathscr{P} \mid H(\mathbf{x}) = E \,\}. \tag{3.43}$$

Therefore we introduce the Liouville measure μ for integrations on $\mathscr{E}$ instead of the usual Lebesgue measure. The Liouville measure of a piece $A \subset \mathscr{E}$ of energy shell ($(2n-1)$-dimensional) is defined to remain constant during time evolution.

$$\frac{\mathrm{d}}{\mathrm{d}t} \int\limits_{\Phi_t(A)} \mathrm{d}^{2n-1}\mu = 0 \tag{3.44}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \int\limits_{\Phi_t(V)} \mathrm{d}^{2n}x = 0, \tag{3.45}$$

although the Lebesgue measure of a piece $V \subset \mathscr{P}$ of phase space ($2n$-dimensional) remains constant. Also the difference in energy $\mathrm{d}E$ is a constant of motion. Therefore the infinitesimal Liouville measure $\mathrm{d}\mu$ can be implicitly defined by

$$\mathrm{d}^{2n-1}\mu \, \mathrm{d}E = \mathrm{d}^{2n}x \tag{3.46}$$

For reasons of simplicity we drop the subscript $^{2n-1}$ and simply write $\mathrm{d}\mu$. If we write the phase space volume element as product of the euclidean area on the energy shell $\mathrm{d}a$ and the euclidean length $\mathrm{d}x_\perp$ perpendicular to $\mathscr{E}$, which are both just the usual Lebesgue measures, one finds

$$\begin{aligned} \mathrm{d}V = \mathrm{d}^{2n}x = \mathrm{d}a \, \mathrm{d}x_\perp = \mathrm{d}a \frac{\mathrm{d}E}{|\nabla H|} \\ \mathrm{d}\mu = \frac{1}{|\nabla H|} \mathrm{d}a \end{aligned} \tag{3.47}$$

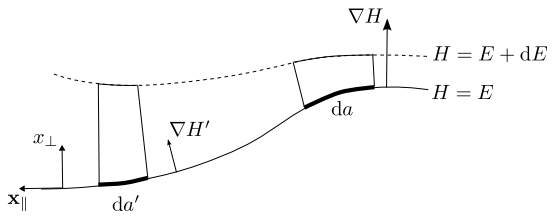


Figure 3.5: The Liouville measure of a piece of energy-shell remains constant under evolution whereas the the euclidean volume does not.

Note that the Liouville measure of $\mathscr{E}$ in total is (besides constants) the Thomas-Fermi-Approximation of the smooth part of density of states for the corresponding quantum mechanical system

$$M := \int\limits_{H=E} \mathrm{d}\mu = \int \mathrm{d}\mu \int \mathrm{d}E\ \delta(E-H) = \int \mathrm{d}^{2n}x\ \delta(E-H) = \frac{\mathrm{d}\Omega(E)}{\mathrm{d}E} = (2\pi\hbar)^n \bar{\rho} \tag{3.48}$$

Figure (3.5) illustrates the concept of liouville measure. Define a delta function on $\mathscr{E}$ corresponding to the Liouville measure:

$$\delta_\mu(\mathbf{x}-\mathbf{x}_0) = 0 \quad \forall\, \mathbf{x} \neq \mathbf{x}_0 \int\limits_{H=E} \mathrm{d}\mu\ \delta_\mu(\mathbf{x}-\mathbf{x}_0) = 1 \tag{3.49}$$

with $\mathbf{x}_0$ lying in $\mathscr{E}$ of course. Note that δ_μ itself as a function of differences of phase space points implicitly always depends on $\mathbf{x}$. Not only on the function argument $\mathbf{x}-\mathbf{x}_0$. Thus the subscript μ can be understood as a function parameter where the unique mapping between μ and $\mathbf{x}$ is always assumed implicitly. On $\mathscr{E}$:

$$\delta_\mu^{(2n-1)}(\mathbf{x}-\mathbf{x}_0) = |\nabla H|(\mathbf{x})\ \delta^{(2n-1)}(\mathbf{x}_\parallel - \mathbf{x}_{0\parallel}) \tag{3.50}$$

where $(x_\perp, \mathbf{x}_\parallel)$ are phase space coordinates perpendicular respectively parallel to $\mathscr{E}$ at the point $\mathbf{x}$

$$\delta_\mu^{(2n-1)}(\mathbf{x}-\mathbf{x}_0)\ \delta^{(1)}(H(\mathbf{x})-E) = \delta^{(2n)}(\mathbf{x}-\mathbf{x}_0) \tag{3.51}$$

With these preliminaries we can now formulate the *ergodic hypothesis* for hard chaotic Hamiltonian systems.

Ergodic hypothesis (EH):
The phase space average over $\mathscr{E}$ by means of Liouville measure equals average over all times of a time evolving phase space point for almost all starting points on $\mathscr{E}$.

Define phase space average as

$$\langle f(\mathbf{x})\rangle_\mu := M^{-1} \int\limits_{H=E} \mathrm{d}\mu\, f(\mathbf{x}). \tag{3.52}$$

Define time average as

$$\langle f(\mathbf{x}(t))\rangle_t := \lim_{T\to\infty} \frac{1}{2T} \fint_{-T}^{T} \mathrm{d}t f(\mathbf{x}(t)) \tag{3.53}$$

with some phase space trajectory $\mathbf{x}(t)$ starting from $\mathbf{x}_0 = \mathbf{x}(0)$. $\fint$ here means there is a small time interval around $t = 0$ that is excluded from the integral.

The EH then can be written in the form

$$\langle f(\mathbf{x})\rangle_\mu = \langle f(\mathbf{x}(t))\rangle_t \quad (\forall \mathbf{x}_0)(\nexists T \in \mathbb{R}^+)(\mathbf{x}(T) = \mathbf{x}_0) \tag{3.54}$$

This equivalence also holds approximately for points on periodic orbits with primitive period greater than some time $T_{\min}$ as long as the function $f(\mathbf{x})$ and the systems properties don't vary to strongly in directions perpendicular to the orbit over the scale of

$$\Delta q_\perp^{n-1} \Delta p_\perp^{n-1} = (2\pi\hbar)^{n-1} \frac{T_{\mathrm{H}}}{T_{\min}} \tag{3.55}$$

The Heisenberg-time T_{H} is roughly the time a non-periodic chaotic trajectory needs to visit every Planck's cell about once. So the above relation basically means the mean spacing in between the track of a periodic orbit should be less than the characteristic sizes of the system itself and the function to be averaged over. We now write the EH for a smoothed delta function:

$$\langle \delta_{\mu,\epsilon}(\mathbf{y} - \mathbf{x})\rangle_\mu = \langle \delta_{\mu,\epsilon}(\mathbf{y} - \mathbf{x}(t))\rangle_t \tag{3.56}$$

with smoothing parameter ϵ.

$$\begin{gathered} \lim_{\epsilon\to 0} \delta_{\mu,\epsilon} = \delta_\mu \\ \int \mathrm{d}\mu\, \delta_{\mu,\epsilon}(\mathbf{x} - \mathbf{x}_0) = 1 \qquad \forall \epsilon \geq 0 \end{gathered} \tag{3.57}$$

Equation (3.56) exactly holds for unperiodic orbits and asymptotically for periodic ones with primitive period greater than some minimal time $T_{\min}(\epsilon)$. Since the Liouville integral over $\delta_{\mu,\epsilon}(\dots)$ equals unity, the left hand side of (3.56) equals M^{-1}

$$\langle \delta_{\mu,\epsilon}(\mathbf{y} - \mathbf{x})\rangle_\mu = M^{-1}. \tag{3.58}$$

So in this case, the EH means available phase space gets filled up uniformly by means of the Liouville measure. This statement holding for unperiodic motion on the one hand and longtime primitive periodic motion on the other hand.

$$\langle \delta_{\mu,\epsilon}(\mathbf{y} - \mathbf{x}(t)) \rangle_t \approx M^{-1} \quad (\forall \mathbf{y}, \mathbf{x}_0 \in \mathscr{E})(\nexists T < T_{\min}(\epsilon))(\mathbf{x}(T) = \mathbf{x}_0) \tag{3.59}$$

In order to get a sum over periodic orbits one is free to choose

$$\mathbf{y} \to \mathbf{x}_0. \tag{3.60}$$

Integrating the resulting relation over $\mathbf{x}_0$ by means of the Liouville-measure $\mathrm{d}\mu_0$ and interchanging time and phase space integrations then yields

$$\left\langle \int \mathrm{d}\mu_0 \; \delta_{\mu,\epsilon}(\mathbf{x}_0 - \mathbf{x}(t, \mathbf{x}_0)) \right\rangle_t = 1 \tag{3.61}$$

Note that since in a fully chaotic system there is only a finite number of periodic orbits with primitive period less than the critical time $T_{\min}(\epsilon)$ their measure on $\mathscr{E}$ is zero. Thus the related points $\mathbf{x}_0$ don't have to be excluded from the integral. At least as long as the integrand remains finite at these points. In this sense it is important to keep a small but finite smearing parameter ϵ.

Only periodic orbits account for the μ_0 integral. And, due to smearing, their vicinity. Thus we write the δ function as a sum over all primitive periodic orbits j and separately perform the integral in local coordinates for the contribution of each orbit j and its repetitions. The calculation for a specific orbit now follows in general and without explicitly indexing everything with j.
We use local canonical coordinates

$$H, T, \mathbf{Q}, \mathbf{P} \tag{3.62}$$

H : energy as coordinate perpendicular to $\mathscr{E}$
T : transit time as coordinate along the orbit
$\mathbf{Q}, \mathbf{P}$: remaining phase space coordinates perpendicular to $\dot{\mathbf{x}}$ and ∇H

Every canonical transformation is preserving phase space volume. Thus we see

$$\mathrm{d}^{2n}x = \mathrm{d}H \; \mathrm{d}T \; \mathrm{d}^{n-1}Q \; \mathrm{d}^{n-1}P \overset{(3.46)}{=} \mathrm{d}H \; \mathrm{d}\mu \tag{3.63}$$

$$\mathrm{d}\mu = \mathrm{d}T \; \mathrm{d}Q \; \mathrm{d}P \tag{3.64}$$

leaving the dimension of the differentials for simplicity.

For $\mathbf{x}_0$ on $\mathscr{E}$:

$$\begin{aligned} \delta_\epsilon(\mathbf{x} - \mathbf{x}_0) &= \delta(H - E) \; \delta_\epsilon(T - T_0, \mathbf{Q} - \mathbf{Q}_0, \mathbf{P} - \mathbf{P}_0) \\ &= \delta(H - E) \, \delta_{\mu,\epsilon}(\mathbf{x} - \mathbf{x}_0) \end{aligned} \tag{3.65}$$

$$\Rightarrow \qquad \delta_{\mu,\epsilon}(\mathbf{x} - \mathbf{x}_0) = \delta_\epsilon(T - T_0, \mathbf{Q} - \mathbf{Q}_0, \mathbf{P} - \mathbf{P}_0) \tag{3.66}$$

where δ_ϵ denotes a delta function that is sharp in the H and T direction but smoothed with ϵ in the other directions on $\mathscr{E}$.
One special problem arising with flows in contrast to maps is that the on-shell δ_μ-function not only peaks for isolated points according to periodic orbits but for the whole one dimensional manifold of points along the orbit. We will see how time averaging eventually helps us to get rid of that.
Regarding the evolution of time coordinate T we set some offset T_0 for the initial value:

$$\mathbf{x}_0 \leftrightarrow (T_0, \mathbf{Q}_0, \mathbf{P}_0) \qquad T(\mathbf{x}_0) = T_0 \in [0, \tau_j[\tag{3.67}$$

$$T(\mathbf{x}(t, \mathbf{x}_0)) = T(\mathbf{x}_t) = T_t = T_0 + t - m\,\tau_j \qquad \text{so that} \qquad T(\mathbf{x}_t) \in [0, \tau_j[\tag{3.68}$$

τ_j : primitive period of the orbit j
m : counter of repetitions after time t

The delta function peaks for all possible repetitions. So they all should be taken into account:

$$\delta_{\mu,\epsilon}(\mathbf{x}_0 - \mathbf{x}_t) = \delta_\epsilon((\mathbf{Q}, \mathbf{P})_0 - (\mathbf{Q}, \mathbf{P})_t) \sum_{m \in Z} \delta(T_0 - T_0 - t + m\,\tau_j) \tag{3.69}$$

After integrating over local variables we get

$$\begin{aligned} &\int_0^{\tau_j} \mathrm{d}T_0 \int \mathrm{d}Q\mathrm{d}P\; \delta_\epsilon((\mathbf{Q}, \mathbf{P})_0 - (\mathbf{Q}, \mathbf{P})_t) \sum_{m \in Z} \delta(m\,\tau_j - t) \\ &\quad = \tau_j \sum_{m \in Z} \delta(m\,\tau_j - t) \int \mathrm{d}Q\mathrm{d}P\; \delta_\epsilon((\mathbf{Q}, \mathbf{P})_0 - (\mathbf{Q}, \mathbf{P})_t) \end{aligned} \tag{3.70}$$

When performing the time average $\langle \dots \rangle_t$, in $\fint_{-T}^{T} \mathrm{d}t$ the delta-function picks out all repetitions that satisfy

$$0 < |t| = |m\,\tau_j| < T \tag{3.71}$$

So we see now that the time average solved the problem of delta-function-like divergence all along the orbit. For each repetition m, perform the $(\mathbf{Q}, \mathbf{P})_0$-integral by transforming the delta-function:

$$\delta_\epsilon\left((\mathbf{Q}, \mathbf{P})_0 - (\mathbf{j}\mathbf{Q}, \mathbf{P})_{m\,\tau_j}\right) \approx \left|\det\left(\frac{\partial\left[(\mathbf{Q}, \mathbf{P})_0 - (\mathbf{Q}, \mathbf{P})_{m\,\tau_j}\right]}{\partial\left[(\mathbf{Q}, \mathbf{P})_0\right]}\right)\right|^{-1} \delta_\epsilon\left((\mathbf{Q}, \mathbf{P})_0\right) \tag{3.72}$$

thus the $(\mathbf{Q}, \mathbf{P})_0$-integration returns the determinant prefactor which is just the squared stability prefactor of the orbit appearing in the Gutzwiller trace formula (2.69)

$$A_{j,m}^2 = \left|\det\left(\mathbb{1} - \tilde{\mathbb{M}}_j^m\right)\right|^{-1}. \tag{3.73}$$

This corresponds to the fact that the difference between a small deviation and its time evolved deviation grows more rapidly with $|(\mathbf{Q},\mathbf{P})|$ for more unstable orbits. Thus, the more unstable it is, the faster the peak falls of with respect to $(\mathbf{Q},\mathbf{P})$ and the smaller its contribution. Sloppy speaking one could say an orbits contribution is its blurred returning probability which is of course small if its unstable. Note that for $\epsilon \to 0$ the transformation (3.72) would work perfectly well. But in our case, this implies a new condition. That is to demand the width of the delta peak to be small enough to allow the assumption of linearised motion within the according vicinity of the orbit.

All together the sum rule in the end reads

$$\lim_{T\to\infty}\frac{1}{2T}\sum_{|m\,\tau_j|<T}\frac{\tau_j}{\left|\det\left(\mathbb{1}-\tilde{\mathbb{M}}_j^m\right)\right|}=1. \tag{3.74}$$

Or by restricting the time average (3.53) to a large time interval $t\in]T,T+\Delta T[$:

$$\lim_{\Delta T\to\infty}\frac{1}{\Delta T}\sum_{T<T_\gamma<T+\Delta T}^{\gamma}\frac{T_{\mathrm{ppo},\gamma}}{\left|\det\left(\mathbb{1}-\tilde{\mathbb{M}}_\gamma\right)\right|}=1, \tag{3.75}$$

where γ indexes periodic orbits including repetitions. To allow the restriction to a finite time interval in the EH, ΔT has to be sufficiently large to let unperiodic motion fill up the energy shell uniformly after that time. This is meant in the sense that the interspace in between the orbits track (3.55) becomes smaller than the system's typical scale in phase space. As in the semiclassical limit this should be much bigger than a Planck's cell, this time will be much smaller than the Heisenberg time

$$\Delta T_{\min}\ll T_{\mathrm{H}} \tag{3.76}$$

In many applications one actually needs to evaluate sums with additional functions of time in the summands. Then under the condition that the total time is much larger than the time interval

$$\Delta T_{\min}<\Delta T\ll T \tag{3.77}$$

one can just evaluate the function for the average time:

$$\lim_{T\to\infty}\frac{1}{\Delta T}\sum_{T<T_\gamma<T+\Delta T}^{\gamma}\frac{T_{\mathrm{ppo},\gamma}\,f(T_\gamma)}{\left|\det\left(\mathbb{1}-\tilde{\mathbb{M}}_\gamma\right)\right|}=f(T) \tag{3.78}$$

For long times, the sum is clearly dominated by primitive periodic orbits with $T_\gamma = T_{\mathrm{ppo},\gamma}$, because they are much more in number and similar in stability

than repeated orbits with $T_\gamma = rT_{\mathrm{ppo},\gamma}$, $r = 2, \ldots$. Hence we can also take a function of primitive periods $T_{\mathrm{ppo},\gamma}$ into the sum and evaluate it for the total time T. This yields the HOdA sum rule in its general form

$$\lim_{T\to\infty} \frac{1}{\Delta T} \sum_{\substack{\gamma \\ T<T_\gamma<T+\Delta T}} \frac{f_1(T_{\mathrm{ppo},\gamma})\, f_2(T_\gamma)}{\left|\det\left(\mathbb{1} - \tilde{\mathbb{M}}_\gamma\right)\right|} = \frac{f_1(T)\, f_2(T)}{T} \tag{3.79}$$

In both forms the limit has to be understood in the sense that the equations become asymptotically valid.

Before we go over to a modified sum rule in the presence of discrete symmetries I want to close this section with a short intuitive interpretation of the sum rule. We can interpret the smeared delta function

$$\delta_{\mu,\epsilon}(\mathbf{x}_0 - \mathbf{x}(t, \mathbf{x}_0)) \tag{3.80}$$

as classical *recurrence probability* of $\mathbf{x}_0$ after time t if we understand the starting point $\mathbf{x}$ to be subject to some uncertainty where $\delta_{\mu,\epsilon}(\mathbf{x} - \mathbf{x}_0)$ is then understood as probability density distribution. The average over all times gives then the probability density to return after arbitrary time. At this stage, the EH comes in. It states that recurrence after random time is equally probable for all points on $\mathscr{E}$ because for long times there should be no preferred region to stay in for the trajectory. So the overall recurrence probability on $\mathscr{E}$ after random time is just unity. This is exactly the statement of equation (3.61).
On the other hand the recurrence of phase space points $\mathbf{x}_0$ is obviously described by periodic orbits. For each periodic orbit, all points on it have a recurrence probability given by the stability prefactors (3.69). And since longer primitive periods correspond to greater influence on a energy shell average it is not surprising that each orbit's contribution is weighted with T_{ppo}.

Modified HOdA Sum Rule For Flows

Now we introduce a discrete symmetry with respect to point transformations according to a finite symmetry group G. Our goal is to give a sum rule similar to the HOdA sum rule but not over periodic orbits but counting symmetry related orbits $j : \mathbf{x} \mapsto g(\mathbf{x})$ with respect to one specific symmetry transformation $g \in G$ exclusively. The normal HOdA sum rule is then included as the case $g = 1_G$.
In order to arrive there, instead of taking $\mathbf{y} \to \mathbf{x}_0$ in (3.59), we set

$$\mathbf{y} \to g(\mathbf{x}_0). \tag{3.81}$$

To the corresponding energy shell integral in

$$\left\langle \int \mathrm{d}\mu_0\; \delta_{\mu,\epsilon}(g(\mathbf{x}_0) - \mathbf{x}(t, \mathbf{x}_0)) \right\rangle_t = 1. \tag{3.82}$$

Now instead of periodic orbits, only symmetry related orbits $j : \mathbf{x} \mapsto g(\mathbf{x})$ and their vicinity will contribute. Since in finite groups every group element has a power that is identity, these orbits always are parts of periodic orbits. Let l_j be the smallest such power of g and k_j denote the repetition number of the corresponding (in general not primitive) periodic orbit. So the transit time for $\mathbf{x} \mapsto g(\mathbf{x})$ is just the fraction k_j/l_j of the primitive period τ_j of the full periodic orbit.

We go again to local coordinates of the corresponding periodic orbit and define the action of g on the local coordinates as $g(T)$ and $g(\mathbf{Q}, \mathbf{P})$ by virtue of the action on $\mathbf{x}$ and the mapping between normal phase space coordinates and local ones:

$$g\,(\,\mathbf{x}(T, \mathbf{Q}, \mathbf{P})\,) = \mathbf{x}\,(\,g(T), g(\mathbf{Q}, \mathbf{P})\,) \tag{3.83}$$

The transformation of the time coordinate is

$$g(T) = T + \frac{k_j}{l_j}\tau_j \mod \tau_j \tag{3.84}$$

$$T(t) = T_t = T_0 + t \mod \tau_j \tag{3.85}$$

The time dependent part of $\delta_{\mu,\epsilon}(g(\mathbf{x}_0) - \mathbf{x}_t)$ is

$$\delta(g(T_0) - T_t) = \sum_{m \in Z} \delta(T_0 + \frac{k_j}{l_j}\tau_j - T_0 - t + m\,\tau_j). \tag{3.86}$$

So again we are independent on the local time coordinate T_0 and the corresponding integral gives the primitive period of the full periodic orbit

$$\int_0^{\tau_j} \mathrm{d}T_0 = \tau_j. \tag{3.87}$$

The time average over the sum of deltas yields a sum of all orbits with transit times

$$t = \left(m + \frac{k_j}{l_j}\right)\tau_j = m^{(\mathrm{sr})}\tau_j^{(\mathrm{sr})} \qquad t \in [-T, T]\,,\; m \in \mathbb{Z} \tag{3.88}$$

where $\tau_j^{(\mathrm{sr})}$ and $m^{(\mathrm{sr})}$ denote the primitive period respectively repetition number in reduced phase space. Note that $m^{(\mathrm{sr})}$ here takes only values giving an unfolded orbit with the relating group element g.

What remains to be done is the integral of perpendicular coordinates. In the definition of perpendicular coordinates along the orbit one is free to choose any basis as long as it yields canonical variables. So we are able to choose the bases

at points related by symmetry to be related by the same symmetry. This is again exactly the definition we used in section (3.1). Then

$$\mathbf{g} \equiv \frac{\partial[g(\mathbf{Q},\mathbf{P})]}{\partial[(\mathbf{Q},\mathbf{P})]} = \mathbb{1}. \tag{3.89}$$

Then the corresponding delta-function transforms according to

$$\begin{aligned} &\delta_\epsilon \left(g((\mathbf{Q},\mathbf{P})_0) - (\mathbf{Q},\mathbf{P})_{m^{(\mathrm{sr})}\,\tau_j^{(\mathrm{sr})}} \right) \approx \\ &\quad \approx \left| \det \left(\frac{\partial \left[(\mathbf{Q},\mathbf{P})_0 - (\mathbf{Q},\mathbf{P})_{m^{(\mathrm{sr})}\,\tau_j^{(\mathrm{sr})}} \right]}{\partial \left[(\mathbf{Q},\mathbf{P})_0 \right]} \right) \right|^{-1} \delta_\epsilon \left((\mathbf{Q},\mathbf{P})_0 \right). \end{aligned} \tag{3.90}$$

So this time after $(\mathbf{Q},\mathbf{P})_0$-integration we get the squared determinant prefactor appearing in the trace formula by Robbins in reduced phase space (3.12)

$$\int \mathrm{d}Q\mathrm{d}P\, \delta_\epsilon \left(g((\mathbf{Q},\mathbf{P})_0) - (\mathbf{Q},\mathbf{P})_{m^{(\mathrm{sr})}\,\tau_j^{(\mathrm{sr})}} \right) = \left| \det \left(\mathbb{1} - \tilde{\mathbb{M}}^{(\mathrm{sr})} \right) \right|^{-1} \tag{3.91}$$

which is of course again the same as the prefactor appearing in Weidenmüller's trace (3.11) in the case of particle exchange symmetry.
We recognise that the primitive period τ_j is the primitive period in reduced phase space $\tau_j^{(\mathrm{sr})}$ multiplied by the number n_j of symmetry transformations that map the orbit j onto itself. In other words, for any point $\mathbf{x}$ on j there are exactly n_j transformations of it $g(\mathbf{x})\,,\ g \in G$ that lie also on j. Furthermore, generically there are $|G|$ different transformations of that point. Hence the periodic orbit j comes as a multiplet of $|G|/n_j$ different orbits related by symmetry that are not counted in reduced phase space. So in order to give a sum rule in terms of reduced phase space dynamics we have to multiply each summand by this number. All in all we get

$$\lim_{T\to\infty} \frac{1}{2T} \sum_{\substack{j:\, \mathbf{x}\mapsto g(\mathbf{x})\,, \\ |(m+\frac{k_j}{l_j})\tau_j|<T}} \frac{\tau_j}{\left| \det \left(\mathbb{1} - \tilde{\mathbb{M}}_j^{(\mathrm{sr})} \right) \right|} = 1, \tag{3.92}$$

or in the reduced phase space description as sum over periodic orbits:

$$\lim_{T\to\infty} \frac{1}{2T} \sum_{\substack{j:\, g_j=g\,, \\ |m^{(\mathrm{sr})}\,\tau_j^{(\mathrm{sr})}|<T}} \frac{\tau_j^{(\mathrm{sr})}}{\left| \det \left(\mathbb{1} - \tilde{\mathbb{M}}_j^{(\mathrm{sr})} \right) \right|} |G| = 1. \tag{3.93}$$

In the general form using common variable names, the modified HOdA sum rule in reduced phase space eventually reads

$$\lim_{T\to\infty} \frac{1}{\Delta T} \sum_{\substack{\gamma:\, g_\gamma=g\,, \\ T<T_\gamma^{(\mathrm{sr})}<T+\Delta T}} \frac{f_1(T_{\mathrm{ppo},\gamma}^{(\mathrm{sr})})\, f_2(T_\gamma^{(\mathrm{sr})})}{\left| \det \left(\mathbb{1} - \tilde{\mathbb{M}}_\gamma^{(\mathrm{sr})} \right) \right|} = \frac{1}{|G|} \frac{f_1(T)\, f_2(T)}{T} \qquad \forall g \in G \tag{3.94}$$

with γ indexing only periodic orbits in reduced phase space with specific ignorable coordinate $g_\gamma = g$.

If a similar sum goes over all periodic orbits in reduced phase space without restricting to one symmetry transformation, and if the summand includes a function of the group element, one gets the group average of this function. This will become especially useful in the next sections.

3.2.2 The Spectral Form Factor For Identical Particles

General Concept

The spectral form factor in general is a two point correlating property associated with a given spectrum $\{E_n\}$. Expressing the spectrum as density of states $\rho(E)$, the two point correlation function reads

$$R_2(x) = \frac{1}{\bar{\rho}^2} \left\langle \rho\left(E\right) \rho\left(E + \frac{x}{\bar{\rho}}\right) \right\rangle_E \tag{3.95}$$

where $1/\bar{\rho}$ denotes the mean level spacing and $\langle \cdots \rangle_E$ stands for averaging E over a energy window small enough so that $\bar{\rho}$ can be considered to be constant. Splitting the density into smooth and oscillating part $\rho(E) = \bar{\rho} + \tilde{\rho}(E)$ and using $\langle \tilde{\rho}(E) \rangle_E = 0$ yields

$$R_2(x) = 1 + \frac{1}{\bar{\rho}^2} \langle \tilde{\rho} \tilde{\rho}_x \rangle_E \,, \tag{3.96}$$

where the subscript x denotes evaluation at $E + x/\bar{\rho}$ instead of E.
The spectral form factor K is defined as Fourier transform of the two point correlator

$$K(\tau) = \frac{1}{\bar{\rho}^2} \left\langle \int_{-\infty}^{\infty} \mathrm{d}x \, e^{2\pi i x \tau} \left\langle \tilde{\rho}(E) \tilde{\rho}\left(E + \frac{x}{\bar{\rho}}\right) \right\rangle_E \right\rangle_\tau \,, \tag{3.97}$$

where $\langle \cdots \rangle_\tau$ stands for averaging τ over a small time window which is basically equivalent to using a damped exponential in the Fourier integral. This can easily be calculated for a Gaussian averaging

$$\int_{-\infty}^{\infty} \mathrm{d}\tau' \sqrt{\frac{\alpha}{\pi}} e^{-\alpha(\tau - \tau')^2} \int_{-\infty}^{\infty} \mathrm{d}x \, e^{2\pi i x \tau'} \, f(x) = \int_{-\infty}^{\infty} \mathrm{d}x \, e^{2\pi i x \tau - \frac{\pi^2}{\alpha} x^2} \, f(x). \tag{3.98}$$

This causes the damping of large values of x so that it suffices to analyse the approximate behaviour of $\tilde{\rho}(E + x/\bar{\rho})$ for small x.
The argument of the form factor is here time in units of the Heisenberg time:

$$\tau = \frac{T}{T_\mathrm{H}} \tag{3.99}$$

To give a semiclassical approximation of $K(\tau)$ we plug in the semiclassical density of states. We use the general form

$$\tilde{\rho}(E) = \frac{1}{\pi\hbar} \sum_{\gamma} A_\gamma \cos\left(\frac{1}{\hbar} S_\gamma(E)\right) \tag{3.100}$$

where γ indexes some variety of orbits and A_γ contains all prefactors that are supposed to slowly vary with energy. The action S_γ is defined to contain any Maslov or other phases (including any possible complex phase of prefactors, so that here A_γ can be considered real).
The product of the two densities gives a double sum over orbits

$$\sum_{\gamma,\gamma'} A_\gamma A_{\gamma'} \cos(\cdots)_\gamma \cos(\cdots)_{\gamma',x}. \tag{3.101}$$

We apply the addition theorem

$$\cos\alpha\cos\beta = \frac{1}{2}\cos(\alpha+\beta) + \frac{1}{2}\cos(\alpha-\beta), \tag{3.102}$$

and neglect the term with the sum of actions in the argument because fast oscillating functions won't survive the energy average. Furthermore we assume the prefactor to be rather constant and expand the action around $x = 0$

$$S_{\gamma',x} \approx S_{\gamma'} + \frac{\partial S_{\gamma'}(E)}{\partial E}\frac{x}{\bar{\rho}} = S_{\gamma'} + T_{\gamma'}\frac{x}{\bar{\rho}}, \tag{3.103}$$

and perform the Fourier integral for $\tau > 0$ to get

$$\begin{aligned} K(\tau) &= \frac{1}{T_{\mathrm{H}}^2}\left\langle \sum_{\gamma,\gamma'} A_\gamma A_{\gamma'}\, e^{\frac{i}{\hbar}(S_\gamma - S_{\gamma'})} \left\langle \delta\left(\tau - \frac{T_{\gamma'}}{T_{\mathrm{H}}}\right)\right\rangle_\tau \right\rangle_E \\ &= \frac{1}{T_{\mathrm{H}}^2}\frac{1}{\Delta\tau} \sum_{\substack{\gamma,\gamma' \\ \tau < \frac{T_{\gamma'}}{T_{\mathrm{H}}} < \tau+\Delta\tau}} A_\gamma A_{\gamma'} \left\langle e^{\frac{i}{\hbar}(S_\gamma - S_{\gamma'})}\right\rangle_E \end{aligned} \tag{3.104}$$

where in the last step the time average was taken as the mean value over a time window of width $\Delta\tau$.

Equation (3.104) is the starting point for calculations under further assumptions.
As orbits whose actions are uncorrelated will vanish after averaging the energy, one has to consider only pairs of orbits that are somehow correlated.

The first and most obvious is the pairing of orbits with exactly the same actions.

The corresponding part of the form factor is called the *diagonal approximation* $K^{(\mathrm{d})}(\tau)$ and has first been considered by Berry in 1985 [4]. There, the orbits are considered as members of equivalence classes $[\gamma]$ with multiplicity $g_{[\gamma]}$. Where the multiplicity arises because of symmetries like e.g. time reversal invariance that induces equality in action of periodic orbits and their time reversed versions.

The appropriate result for the diagonal approximation $K^{(\mathrm{d})}$ of the full spectrum of a chaotic system using the Gutzwiller trace formula is obtained by appliance of the HOdA sum rule (3.79).

$$K^{(\mathrm{d})}(\tau) = \frac{1}{T_{\mathrm{H}}} \frac{1}{\Delta T} \sum_{\substack{[\gamma]:\, \mathbf{x}\mapsto\mathbf{x} \\ T<T_{[\gamma]}<T+\Delta T}} \frac{T_{\mathrm{ppo},[\gamma]}^2}{\left|\det\left(\mathbb{1} - \tilde{\mathbb{M}}_{[\gamma]}\right)\right|} g_{[\gamma]} \tag{3.105}$$

$$K^{(\mathrm{d})}(\tau) = \overline{g_{[\gamma]}}\,\tau \equiv \beta\tau \qquad\qquad \tau \gg \tau_{\min} \tag{3.106}$$

$\tau_{\min}$ is the minimal period for the reliability of the ergodic hypothesis (see section 3.2.1).
The parameter β is characteristic for the symmetries the Hamiltonian obeys. Without spatial symmetries one basically distinguishes three symmetry classes of systems. That are systems without any symmetry, with time reversal invariance (TRI) and with symplectic symmetry (systems with spin) respectively. The accordant β-values are

$$\begin{aligned} &\beta = 1 && \text{no symmetry} \\ &\beta = 2 && \text{TRI} \\ &\beta = 4 && \text{symplectic} \end{aligned} \tag{3.107}$$

The considered values for τ are thereby large enough to allow the assumption that self-symmetric orbits are heavily outweighed by non-self-symmetric ones. Therefore the average multiplicity $\overline{g_{[\gamma]}}$ is taken as the multiplicity of a multiplet of non-self-symmetric orbits, which is maximal. In the case of TRI this means self-retracing periodic orbits (which are their own time flipped version) are much less in number than non-self-retracing ones for the considered periods.

It is possible to go beyond the diagonal approximation and find other pairs of orbits that are correlated somehow. Richter and Sieber [28] showed that in systems with TRI one can find pairs of loop orbits with and without avoided crossing. These are in general correlated more weakly than the pairs in the diagonal approximation and in the TRI case $\beta = 2$ give exactly the next-to-leading order contribution to K that is also predicted by random matrix theory.

$$K(\tau) = K^{(\mathrm{d})}(\tau) + K^{(1-loop)}(\tau) + \ldots = 2\tau - 2\tau^2 + \ldots. \tag{3.108}$$

Interestingly the loop construction is not possible in the $\beta = 1$ case which is consistent with the RMT prediction of a linear τ-dependence up to $\tau = 1$.

The loop corrections can be systematised to higher orders, where classes of orbits with multiple (non-)avoided encounters along the trajectory are taken into account [20]. These are giving all orders in τ in the expansion around $\tau = 0$. So far, the universal behaviour of the spectral form factor up to $\tau = 1$ is understood by means of semiclassics. In addition to that it is possible to advance to the regime $\tau > 1$ by imposing a unitarity condition to the system. But since this condition is artificial in the context of semiclassical derivation, an argument based on orbital correlations would be most welcome. Recently, orbits that partially follow other orbits repeatedly are under discussion as possible candidates [30].

Form Factor With Discrete Symmetry

Let us move on to systems with discrete symmetries. A similar derivation as in the last subsection can be done for the symmetry-projected spectra associated with irreducible representations α. It was first presented by Keating and Robbins in 1996 [16] and is based on Robbin's trace formula in reduced phase space (3.12). The main difference is that then the double sum in K_α runs over periodic orbits in reduced phase space γ and that the group characters $\chi_\alpha(g_\gamma)$ appear in the prefactors. According to Keating and Robbins the form factor $K_\alpha(\tau)$ associated with the irreducible representation α as double sum reads

$$\begin{aligned} K_\alpha(\tau) &= \frac{1}{T_{\mathrm{H},\alpha}^2} \left\langle \sum_{\gamma,\gamma'} \chi_\alpha(g_\gamma)\chi_\alpha^*(g_{\gamma'}) A_\gamma A_{\gamma'}\, e^{\frac{i}{\hbar}(S_\gamma - S_{\gamma'})} \left\langle \delta\left(\tau - \frac{T_{\gamma'}}{T_{\mathrm{H},\alpha}}\right)\right\rangle_\tau \right\rangle_E \\ &= \frac{1}{T_{\mathrm{H},\alpha}^2}\frac{1}{\Delta\tau} \sum_{\substack{\gamma,\gamma' \\ \tau < \frac{T_{\gamma'}}{T_{\mathrm{H},\alpha}} < \tau+\Delta\tau}} \chi_\alpha(g_\gamma)\chi_\alpha^*(g_{\gamma'}) A_\gamma A_{\gamma'} \left\langle e^{\frac{i}{\hbar}(S_\gamma - S_{\gamma'})}\right\rangle_E \end{aligned} \tag{3.109}$$

with the proper Heisenberg time associated with the symmetry projected spectrum

$$T_{\mathrm{H},\alpha} = 2\pi\hbar\frac{\bar{\rho}_\alpha}{d_\alpha}. \tag{3.110}$$

$T_{\mathrm{H},\alpha}$ is the characteristic time for K_α as is T_H for K. So in the context of symmetry-projected spectra, τ is time measured in units of $T_{\mathrm{H},\alpha}$. This corresponds to measurement of energy spacings in units of the mean level spacing $\bar{\rho}_\alpha^{-1}$ of the symmetry-projected density spectrum in the two-point correlator.

In (3.109), γ and γ' index all periodic orbits in reduced phase space. Note that the general form of the form factor (3.104) can be used. There, A_γ and $A_{\gamma'}$ are defined to contain the absolute values of group characters whereas their phases are absorbed in S_γ and $S_{\gamma'}$, so that the complex conjugation then arises through the $-$ sign in front of the latter. In contrast to that, in (3.109) A_γ and

$A_{\gamma'}$ are defined as the sole real stability prefactors without group characters. S_γ and $S_{\gamma'}$ here only include possible Maslov phases.

As we want to give the diagonal approximation to (3.109) we have to distinguish between systems with and without TRI. In both cases pairs of equal orbits contribute. For them, the double sum reduces to a single sum and all indexes γ' are just replaced by γ. In the TRI case in addition to that every orbit γ can be paired with its time reversed version $\gamma' = \gamma^-$. The associated group element is the inverse element and therefore the appropriate character has to be complex conjugated:

$$\chi^*_\alpha(g_{\gamma^-}) = \chi^*_\alpha(g_\gamma^{-1}) = \chi_\alpha(g_\gamma). \tag{3.111}$$

All other properties are equal to the non-reversed orbit. Thus with TRI the diagonal part may be written

$$K_\alpha(\tau) = \frac{1}{T^2_{\mathrm{H},\alpha}} \frac{1}{\Delta\tau} \sum_{\substack{\gamma \\ \tau < \frac{T_\gamma}{T_{\mathrm{H},\alpha}} < \tau + \Delta\tau}} \left[|\chi_\alpha(g_\gamma)|^2 + (\chi_\alpha(g_\gamma))^2 \right] A^2_\gamma, \tag{3.112}$$

whereas without TRI only the first summand $|\chi_\alpha(g_\gamma)|^2$ would contribute.

So far, the analysis does not differ from the presentation given in [16]. But where Keating and Robbins evaluate the sum over group characters based on a more or less heuristic argument of equal distribution of group elements, we are now able to use the modified HOdA sum rule of section 3.2.1, which exhibits a bit more rigour since it is based on the standard ergodic hypothesis only as is the original sum rule by Hannay and Ozorio de Almeida.

If we apply the modified HOdA sum rule (3.94) to (3.112), we directly see

$$K_\alpha(\tau) = \left\langle |\chi_\alpha(g)|^2 + (\chi_\alpha(g))^2 \right\rangle_g \tau. \tag{3.113}$$

$\langle \ldots \rangle_g$ stands for averaging g over the whole group G. To evaluate the group average one uses the Schur orthogonality relations for characters of irreducible representations

$$\sum_{g \in G} \chi_\alpha(g) \chi^*_\beta(g) = |G| \delta_{\alpha\beta}. \tag{3.114}$$

Thus the first summand in (3.112) gives unity. For the second summand, one has to realise that the complex conjugated characters correspond to complex conjugated matrix representation. Matrix representations $D_\alpha(g)$ can be classified as being

- real: $D^*_\alpha(g) = D_\alpha(g)$ is real. $\chi_\alpha(g)$ are real.

- pseudo-real: $D^*_\alpha(g) = D_\beta(g) \neq D_\alpha(g)$ can not be brought to real but α and β are equivalent representations. $\chi_\alpha(g)$ are real.

- complex: $D^*_\alpha(g) = D_\beta(g) \neq D_\alpha(g)$ can not be brought to real and α and β are not equivalent representations. $\chi_\alpha(g)$ are not real.

Thus the group averages evaluate to

$$\left\langle |\chi_\alpha(g)|^2 + (\chi_\alpha(g))^2 \right\rangle_g = 1 + \begin{cases} 1 & \alpha \text{ real or pseudo-real} \\ 0 & \alpha \text{ complex .} \end{cases} \tag{3.115}$$

For a rigorous derivation of the group averages the interested reader may be referred to the book of Hamermesh [11] for example.

All in all the form factor of symmetry-projected spectra (not including the symplectic case) reads

$$K_\alpha(\tau) = \beta\tau \qquad \beta = \begin{cases} 2 & \alpha \text{ real or pseudo-real} \\ 1 & \alpha \text{ complex .} \end{cases} \tag{3.116}$$

For particle exchange symmetry, the bosonic $(+)$ and fermionic $(-)$ sub-spectra correspond to one-dimensional real representations of the symmetric group $G = S_N$ with characters

$$\chi_\pm(g) = (\pm 1)^\sigma, \tag{3.117}$$

which are the only one-dimensional irreducible representations of S_N by the way. So for both, fermionic and bosonic sub-spectra we get the normal leading order GOE result of

$$K^{(\mathrm{d})}_\pm(\tau) = 2\tau. \tag{3.118}$$

Of course we could have used the trace formula by Weidenmüller (3.11) in combination with the corresponding modified HOdA sum rule for full phase space instead.

I want to close this subsection remarking that there has also been progress in doing loop corrections for symmetry projected spectra [15]. Also there the same argument of equally distributed group elements is used as in [16]. In the opinion of the author it would be worth to investigate to what extent the modified HOdA sum rule can be useful there to give a more solid ground to the argument. But since we are only interested in the diagonal approximation in the scope of this work, this shall be postponed to future projects.

Correlation Between Fermionic And Bosonic Spectra

Based on the previous subsections we are able to briefly discuss on the correlation between the fermionic and the bosonic sub-spectrum of in other respects equal systems with chaotic ergodic motion. Let us therefore in analogue to (3.97) define a correlator

$$C(\tau) = \left\langle \int_{-\infty}^{\infty} \mathrm{d}x\, e^{2\pi i x\tau} \left\langle \tilde{\rho}_+(E)\tilde{\rho}_-\left(E + \frac{x}{\bar{\rho}_-}\right)\right\rangle_E \right\rangle_\tau . \tag{3.119}$$

Similar arguments as in the previous subsection yield

$$C(\tau) \propto \frac{1}{\Delta\tau} \sum_{\substack{\gamma \\ \tau < \frac{T_\gamma}{T_{H,-}} < \tau+\Delta\tau}} \chi_+(g_\gamma)\left[\chi_-^*(g_\gamma) + \chi_-(g_\gamma)\right] A_\gamma^2, \tag{3.120}$$

for the TRI case. Since the characters are real the case without TRI gives just 1/2 of the right hand side. Applying the modified HOdA sum rule and inserting the specific group characters (3.117) obviously gives

$$C(\tau) \propto \langle (-1)^\sigma \rangle_g = 0. \tag{3.121}$$

So we see that in the ergodic regime the spectrum of a closed chaotic spinless many body quantum system of bosons is not correlated with the corresponding spectrum of spinless fermions. Since we used diagonal approximation, this statement has to be understood as asymptotic in the limit of small values for τ but still large enough to fulfil the ergodic hypothesis $\tau > \tau_{min}$. Whether this statement can be extended to higher orders in τ considering loop corrections would have to be discussed in detail separately. But let us anticipate briefly. Following the argument in Joyner's work [15] one would get terms like

$$\langle \chi_\alpha(g_\gamma)\chi_\beta(g_{\gamma'}(g_\gamma))\rangle_g \tag{3.122}$$

for real representations. γ' is one specific partner to the multi-loop orbit γ with a particular structure of reconnected encounter regions. If we take β as the bosonic representation and α as the fermionic representation we have again simply a group average over all characters $\chi_-(g)$

$$\langle (-1)^\sigma \rangle_g = 0. \tag{3.123}$$

Thus it seems reasonable to presume a vanishing correlator between associated fermionic and bosonic spectra in all orders of τ in the ergodic regime.

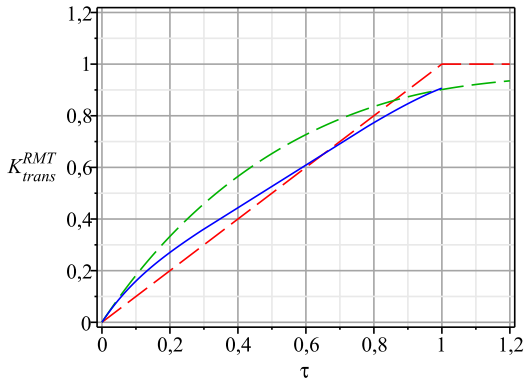


Figure 3.6: The spectral form factor in the GOE-GUE transition with a parameter $\lambda = 0.2$. For small values of τ, TRI is remained.

3.2.3 The Many Body GOE-GUE-Transition

General

In the last sections we have seen how the predictions of random matrix theory for Gaussian Orthogonal and Gaussian Unitary Ensembles coincide with semiclassical calculations of energy level fluctuations of classically chaotic systems obeying time-reversal invariance or time-reversal non-invariance respectively. This is even true for many body spectra including particle exchange symmetry. A further application of the above methods is investigating the transition between both. On the one hand, the transition in random matrix theory based on a two matrix model by Pandey and Mehta [22] is known exactly. On the other hand, a semiclassical analysis can be done for a charged particle in the presence of a weak magnetic field that is destroying TRI. The corresponding transition parameter out of RMT can be identified in the asymptotic limit of long range correlations in the energy levels [6]. This limit corresponds to the limit of small values τ in the analysis of form factors. An investigation beyond the leading diagonal approximation has been carried out by Saito and Nagao [21, 25].

The RMT result for the form factor in the transition is the closed expression

$$\begin{aligned} K_{\text{trans}}^{\text{RMT}}(\tau) &= \tau + \frac{1}{2}\int_{1-2\tau}^{1} \mathrm{d}k\, \frac{k}{k+2\tau}\, e^{-8\pi^2\lambda^2\tau(k+\tau)} \\ &= \tau + \tau e^{-8\pi^2\lambda^2\tau} - 2\tau^2 + \mathcal{O}(\tau^3) \end{aligned} \tag{3.124}$$

In works concerning this matter usually the magnetic field is considered small enough to not noticeably affect the orbital geometry. Instead, the leading effect of a vector potential in the semiclassical analysis is due to a phase shift from

the change in the action $S_\gamma(E)$

$$S_\gamma(E) \to S_\gamma(E) + \theta_\gamma(E) = \int_\gamma \mathrm{d}\mathbf{q}\cdot\mathbf{p} \;+\; e\int_\gamma \mathrm{d}\mathbf{q}\cdot\mathbf{A}. \tag{3.125}$$

Here, e denotes the charge of the particle and $\mathbf{A}$ denotes the vector potential associated with the magnetic field $\mathbf{B}$. For closed orbits γ, the line integral in θ_γ equals the magnetic flux ϕ_γ through the surface spanned by γ. The crucial point is that the magnetic phase $\theta_\gamma/\hbar$ for a time-reversed orbit is the negative of the phase of the original orbit whereas their classical actions are equal:

$$\theta_{\gamma^-} = -\theta_\gamma \tag{3.126}$$
$$S_{\gamma^-} = S_{\gamma^-} \tag{3.127}$$

The corresponding spectral form factor in diagonal approximation reads

$$K^{(\mathrm{d})}_{\mathrm{trans}}(\tau) = \frac{1}{T_\mathrm{H}^2}\frac{1}{\Delta\tau}\sum_{\substack{\gamma \\ \tau<\frac{T_\gamma}{T_\mathrm{H}}<\tau+\Delta\tau}} A_\gamma^2\left[1+\exp\left(2\frac{i}{\hbar}\theta_\gamma(E)\right)\right], \tag{3.128}$$

assuming that (like A_γ) θ_γ is varying rather smoothly with the energy so that it can be simply evaluated at the mean energy E for both, the orbit γ and its time reversed, actually energy shifted counterpart γ^-.

Further simplifications require certain assumptions regarding the chaotic dynamics of the system. Namely the accumulation of magnetic phase θ_γ along an orbit is considered a random walk process. Classical simulations are substantiating this assumption [14]. Since for every orbit the time reversed exists and has different sign in θ, the corresponding probability distribution $P(\phi_\gamma)$ must have zero expectation value. According to the central limit theorem the probability distribution of flux becomes a Gaussian in the long time limit:

$$P(\phi) = \frac{1}{\sqrt{2\pi}\sigma_\phi}\exp\left[-\frac{1}{2}\left(\frac{\phi}{\sigma_\phi}\right)^2\right] \tag{3.129}$$

with some standard deviation σ_ϕ. Then the form factor can be evaluated by taking the flux dependent part in the sum as its average $\langle\ldots\rangle_\phi$ under the distribution (3.129), where this mean value in general depends on the orbit time T_γ taken as mean orbit time T under the sum. Also the mean energy E is a parameter the mean value depends on. We were assuming that θ_γ of a specific orbit is rather independent of its energy in the considered energy window of the energy average. In contrast to that, when averaging over all orbits in a particular interval of periods, energy dependence comes back in through the variance

of flux distribution. The resulting mean value of the flux-dependent summand for general variance can easily be obtained by a Gaussian integration and reads

$$\left\langle \exp\left(2\frac{i}{\hbar}\theta_\gamma\right)\right\rangle_\phi = \left\langle \exp\left(2\pi i\frac{\phi}{\phi_0}\right)\right\rangle_\phi = \exp\left(-2\pi^2\left(\frac{\sigma_\phi}{\phi_0}\right)^2\right). \tag{3.130}$$

The variance σ_ϕ^2 is proportional to the number of effective random steps, which is of course in general dependent on the orbits transit time T and energy E. In the paper by Bohigas et al. [6], the random process is described through a time correlation function of flux accumulation

$$\left\langle \dot\theta_\gamma(0)\,\dot\theta_\gamma(t)\right\rangle_t. \tag{3.131}$$

Another approach is to consider two-dimensional quantum billiard systems with a magnetic field perpendicular to the billiard plane and makes life a bit easier. There, a single random step is associated with every orbit segment between two bounces on the billiard's boundary. So the total flux-variance σ_ϕ^2 equals the number of bounces n_B times the flux-variance of a single bounce σ_B^2. The number of bounces is the typical orbit length in the sum (3.128) divided by the typical segment length $\bar L$ of the billiard. Expressed in terms of kinetic particle energy E and transit time T the variance is

$$\sigma_\phi^2 = \sqrt{\frac{2}{m\bar L^2}}\,\sqrt{E}\,T\,\sigma_B^2 \tag{3.132}$$

The single bounce variance is clearly proportional to the square of magnetic field.

$$\sigma_B \propto B = |\mathbf{B}| \tag{3.133}$$

Furthermore the characteristic time unit in the form factor still is the Heisenberg time, so K has to be expressed in terms of τ instead of $T = T_\mathrm{H}\tau$ to be comparable with the RMT result. Therefore we have to introduce the smooth part of the density of states.

$$\bar\rho(E) = \frac{T_\mathrm{H}}{2\pi\hbar} \tag{3.134}$$

All in all, the diagonal part of the form factor for the GOE to GUE transition reads

$$K^{(\mathrm{d})}_{\mathrm{trans}}(\tau) = \tau\left(1 + e^{-b\tau}\right), \tag{3.135}$$

with

$$\begin{aligned} b &= 4\pi^3\hbar\sqrt{\frac{2}{m}}\frac{\sigma_B^2}{\bar L\phi_0^2}\,\sqrt{E}\,\bar\rho(E) \\ &= \text{const.}\cdot B^2\sqrt{E}\,\bar\rho(E), \end{aligned} \tag{3.136}$$

with some system-specific constant. In order to compare this semiclassical result with the RMT prediction, one should mind a consistent expansion in powers of τ. In linear order $\mathcal{O}(\tau)$ we obtain just an unaffected GOE form factor $K = 2\tau$. So if we want to identify the symmetry braking parameter λ we have to go to second order $\mathcal{O}(\tau^2)$. This means we are actually not allowed to compare the diagonal approximation of K_{trans} with the RMT result without taking loop corrections into account since we know that these already in the TRI limit also give corrections of the order $\mathcal{O}(\tau^2)$. Here we simply anticipate the first order loop result for the transition [21], which is

$$\Delta K_{\text{trans}}^{(\text{1-loop})} = -2\tau^2 e^{-8\pi^2\lambda^2\tau} = -2\tau^2 + \mathcal{O}(\tau^3).$$

We see that up to quadratic order in τ the loop correction is unaffected by time-reversal invariance breaking. Also in higher order loop corrections one could conjecture that the corresponding correction to K_{trans} is a product of a function of the same order in τ as the TRI correction multiplied by the exponential $\exp(-b\tau)$ coming from the Gaussian averaging of the magnetic phase factor. Indeed we see this behaviour in the second loop correction computed by Saito and Nagao [25]. Thus we consistently regard order $\mathcal{O}(\tau^2)$ by taking the diagonal approximation (3.128) and adding the unaltered first order loop correction $-2\tau^2$ of the TRI system. We then easily identify the symmetry breaking parameter by comparing with (3.124):

$$\begin{aligned} \lambda &= \left(\frac{\pi\hbar}{\sqrt{2m\bar{L}}}\right)^{\frac{1}{2}} \frac{\sigma_B}{\phi_0} E^{\frac{1}{4}} \sqrt{\bar{\rho}(E)} \\ &= \text{const.} \cdot B\, E^{\frac{1}{4}} \sqrt{\bar{\rho}(E)} \end{aligned} \tag{3.137}$$

We see that λ unsurprisingly is proportional to the magnetic field. But it also depends on the energy at which one is calculating spectral fluctuations.

Many Particles

Now let us be ambitious and try to give a similar analysis for a system of many charged particles. The interesting oddity in such a system lies in the naive expectation that the more particles in the system the more sensitive it should react to a magnetic field by means of breaking time-reversal symmetry. In the limit of infinitely many particles this would mean that there was no non-zero magnetic field for which TRI would be partially preserved. Any physical field would be supposed to destroy TRI completely, at least regarding spectral statistics. So for a system of a large number of particles it would be almost impossible to find an experimental setup in which one could measure signatures of TRI in the energy level fluctuations. We shall refer to this apparent oddity as the *many body transition catastrophe*. The reason for this naive expectation is the fact that N charged particles after some transit time will accumulate N times the magnetic

phase that would be accumulated by a single particle after the same time. But of course we have to do a careful analysis in order to make a physical statement. We will see that there are several challenging features of this issue. I want to anticipate that we will not give solutions for all of them that are completely satisfactory. So this subject will throw up open questions, where the major one will then be treated in the next chapter. In this sense, the attempt of analysing the application at hand will serve as a motivation for the investigations made in the rest of the present work.

First we want to incorporate exchange symmetry. For this purpose we use the symmetry projected form factor (3.109). In order to implement the magnetic phase of orbits we recognise that the accumulation of flux in full phase space can simply be expressed as magnetic flux in reduced phase space. Let γ be an orbit segment in full phase space description. The corresponding magnetic phase is

$$\theta_\gamma = \sum_{i=1}^{N} \theta_\gamma^{(i)} = e \sum_{i=1}^{N} \int\limits_{\gamma,\, \mathbf{q}_i(0)}^{\mathbf{q}_i(t)} \mathrm{d}\mathbf{q}^{(\mathrm{SP})} \cdot \mathbf{A}(\mathbf{q}^{(\mathrm{SP})}), \tag{3.138}$$

where due to exchange symmetry, the vector potential $\mathbf{A}(\mathbf{q}^{(\mathrm{SP})})$ is the same function of single particle coordinates for all particles. Applying any symmetry transformation $P \leftrightarrow \sigma \in S_N$ to γ gives

$$\theta_{P\gamma} = e \sum_{i=1}^{N} \int\limits_{\gamma,\, \mathbf{q}_{\sigma(i)}(0)}^{\mathbf{q}_{\sigma(i)}(t)} \mathrm{d}\mathbf{q}^{(\mathrm{SP})} \cdot \mathbf{A}(\mathbf{q}^{(\mathrm{SP})}) = \sum_{i=1}^{N} \theta_\gamma^{(\sigma(i))} = \theta_\gamma. \tag{3.139}$$

Thus by segment-wise transforming a trajectory in full phase space back into reduced phase space we see that both the unfolded and the symmetry reduced trajectory have the same magnetic phase θ. So we simply extend the orbit action S_γ by θ_γ where the flux can then be calculated in reduced or full phase space at will.

$$K^{(\mathrm{d})}_{\mathrm{trans},\,\pm}(\tau) = \frac{1}{T^2_{\mathrm{H},\,\pm}} \frac{1}{\Delta\tau} \sum_{\substack{\gamma \\ \tau < \frac{T_\gamma}{T_{\mathrm{H},\,\pm}} < \tau + \Delta\tau}} A_\gamma^2 \left[|\chi_\pm(g_\gamma)|^2 + (\chi_\pm(g_\gamma))^2 \exp\left(2\frac{i}{\hbar}\theta_\gamma(E) \right) \right], \tag{3.140}$$

where γ indexes periodic orbits in reduced phase space. Note that the term *flux* in this context is used despite the fact that exchange orbits in full phase space are not closed and therefore do not span an area with unique flux. Alternatively regarding closed periodic orbits in reduced phase space leads to the problem of how to define a spanned surface and associated flux in a space with nontrivial topology. Thus the term flux is not meant literally but instead used

synonymously for the line integral of vector potential. This arises the question of gauge invariance. To answer it, we remind ourselves that every symmetry related orbit γ in full phase space is part of a periodic orbit Γ. By multiple application of symmetry transformations to the exchange orbit and using the equality (3.139) we obtain the total magnetic phase of the full closed periodic orbit θ_Γ as a multiple of θ_γ. As θ_Γ is now gauge-invariant as a unique flux through a surface spanned by Γ, so is θ_γ.

We apply the modified HOdA sum rule to the flux independent parts in (3.140) and write the exponential as a factor with averaged flux over all orbits in the time window $\tau < \frac{T_\gamma}{T_{\mathrm{H},\pm}} < \tau + \Delta\tau$.

$$K^{(\mathrm{d})}_{\mathrm{trans},\pm}(\tau) = \tau \left\langle |\chi_\pm(g_\gamma)|^2 \right\rangle_g + \tau \left\langle (\chi_\pm(g_\gamma))^2 \right\rangle_g \left\langle \exp\left(2\frac{i}{\hbar}\theta_\gamma(E)\right) \right\rangle_\phi , \quad (3.141)$$

Again we use the fact that the group averages in (3.141) for the real representations of bosonic and fermionic symmetry give unity (see (3.115) and (3.117)) and take the fluxes of orbits as Gaussian-distributed (3.129). Then the diagonal approximation of the transition form factor of the symmetry projected spectrum of a many particle system has the same form as in the single particle case

$$K^{(\mathrm{d})}_{\mathrm{trans},\pm}(\tau) = \tau + \tau \exp\left(-2\pi^2 \left(\frac{\sigma_\phi}{\phi_0}\right)^2\right). \quad (3.142)$$

Thus we see that exchange symmetry has no direct effect in the analysis of the transition form factor. But of course the variance of flux distribution has now to be taken as a many body quantity that differs from the single particle variance.

$$\sigma_\phi = \sigma_\phi^{(\mathrm{MB})} \overset{\text{i.g.}}{\neq} \sigma_\phi^{(\mathrm{SP})} \quad (3.143)$$

One should stress that all semiclassical statements about the universal features of quantum spectra are based on fully chaotic and ergodic classical motion. In the context of many particles, this has a special implication. While in a single particle system the chaoticity can be managed by tuning a potential or billiard boundary, this is not sufficient in a many body system. There, one has to demand interaction between particles, because otherwise every periodic orbit for a single particle results in a marginally stable family of periodic many particle orbits. Consider N particles with coordinates $\mathbf{q}_i(t)$ all following the same periodic orbit. It is then possible to individually displace the single particle coordinates continuously along their orbits and thereby obtain a new periodic many body orbit

$$\mathbf{q}'(t) = (\mathbf{q}'_1(t), \ldots, \mathbf{q}'_N(t)) = (\mathbf{q}_1(t + \Delta t_1), \ldots, \mathbf{q}_N(t + \Delta t_N)), \quad (3.144)$$

which is then in general not lying on the original many body orbit in $(2ND)$-dimensional phase space but still has the same period and other classical properties. So every single particle orbit in general comes as a $(N-1)$-times degenerate family of orbits in the many body phase space. The existence of periodic orbit families is typical for nonchaotic regular motion and corresponds to the existence of constants of motion. In this case one could take the individual single particle energies E_i as independent constants. This of course destroys ergodicity in relation to the energy shell $\mathscr{E}$ of constant total energy $E = \sum E_i$. So we have to demand an interaction that is strong enough to restore chaoticity and ergodicity. How strong this would be in order to have enough chaos to compare with RMT results is one open question that is passed to future investigations.

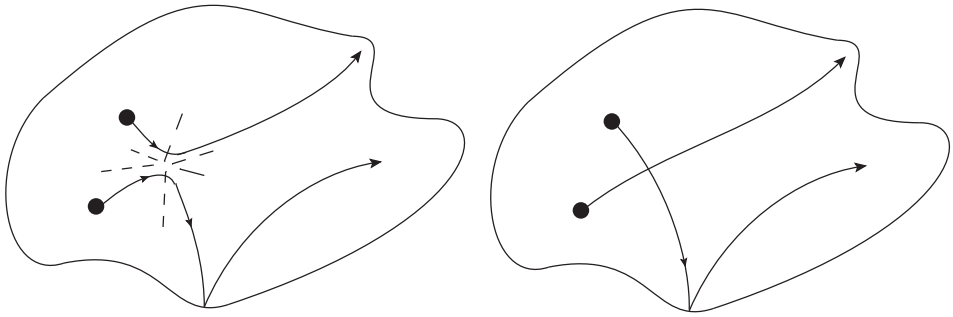
In the present context the requirement of particle-particle interaction is of special importance since we have to include statistics of classical motion regarding the magnetic phase accumulation. While in the single particle case the assumptions leading to a random walk process and the corresponding quantification of variance of magnetic flux where straightforward, the treatment of statistical many body dynamics in the presence of interaction can be difficult. One attempt is to assume short range interactions in the sense that the effect on the dynamics can approximately be reduced to two-particle collisions. Furthermore, if the effective range of interaction is short enough, the collision can be regarded to happen in a small region of coordinate space. If this region is small enough, we can assume that the two colliding particles, due to their equality of masses, just interchange their coordinates and momenta (see figure 3.7). Thus such an event will not give a change in the magnetic phase accumulation

$$\theta_\gamma(t) = e \int\limits_{\gamma,\mathbf{q}(0)}^{\mathbf{q}(t)} \mathrm{d}\mathbf{q} \cdot \mathbf{A}. \tag{3.145}$$

The many body random walk process for such a short range interaction can therefore be regarded effectively as an independent single particle processes with unaffected random walk step length.

$$(\sigma_\phi^{(\mathrm{MB})})^2 = \sum_{i=1}^{N} (\sigma_{\phi,\,i}^{(\mathrm{SP})})^2 = N(\sigma_{\phi,\,\mathrm{eff}}^{(\mathrm{SP})})^2. \tag{3.146}$$

But then the assumptions give rise to a new question regarding the single particle variances. To what extent can they be assumed to be independent and to what extent can they be assumed to be equal? And, if we assume them to be equal, what is their value? Or in other words, how can we incorporate the time dependent partitioning of energy into single particle energies in an effective description of the single particle standard deviation of flux $\sigma_{\phi,\,\mathrm{eff}}^{(\mathrm{SP})}$? A first order attempt could be the assumption of equal distribution of energy in the long time



(a) collisions /exchange (b) particles don't interact

Figure 3.7: Two particles in a cavity with short range interaction. In the context of magnetic phase accumulation, the collision of the two is effectively equivalent to an exchange which is equivalent to no interaction at all.

average due to energy transfer at collision events.

$$E_{\text{eff}}^{(\text{SP})}(E) = \frac{E}{N} \tag{3.147}$$

This seems to stand in contradiction to the assumption of exact exchange of momenta at collisions leading to exchange of single particle energies without transferring small quantities of energy to yield an effectively equal distribution. But this assumption has to hold only in the time regime of single bounces for not to affect the flux accumulation during one random walk step. Thus we can imagine a regime of the interaction range that allows a short time description through two-body collisions on the one hand, and the assumption of equal energy distribution in long time dynamics on the other hand. We can weaken the assumption of equal distributed energies by assuming that every particle over long times feels the same effective energy $E_{\text{eff}}^{(\text{SP})}$ for the random walk description but which has not necessarily to be the N-th fraction of the total energy E. In this effective description of statistical dynamics we collect all quantities and write the overall variance of flux as

$$\begin{aligned}
(\sigma_{\phi}^{(\text{MB})})^2 &= N\ (\sigma_{\phi,\,\text{eff}}^{(\text{SP})})^2 \\
(\sigma_{\phi,\,\text{eff}}^{(\text{SP})})^2 &= \sigma_{\text{B}}^2\ n_{\text{B,\,eff}}^{(\text{SP})} \\
n_{\text{B,\,eff}}^{(\text{SP})} &= T\ v_{\text{eff}}^{(\text{SP})}\ \frac{1}{\bar{L}} \qquad \text{with} \qquad v_{\text{eff}}^{(\text{SP})} = \sqrt{\frac{2}{m} E_{\text{eff}}^{(\text{SP})}} \\
(\sigma_{\phi}^{(\text{MB})})^2 &= \sqrt{\frac{2}{m\bar{L}^2}}\ N \sqrt{E_{\text{eff}}^{(\text{SP})}}\, T\, \sigma_{\text{B}}^2
\end{aligned} \tag{3.148}$$

So as in the single particle case (3.135) the form factor takes the form

$$K_{\text{trans},\,\pm}^{(\text{d})}(\tau) = \tau \left(1 + e^{-b^{(\text{MB})}\,\tau}\right) \tag{3.149}$$

with

$$b^{(\mathrm{MB})} = 4\pi^3\hbar\sqrt{\frac{2}{m}}\frac{\sigma_{\mathrm{B}}^2}{\bar{L}\phi_0^2}\, N\sqrt{E_{\mathrm{eff}}^{(\mathrm{SP})}(E)}\,\bar{\rho}(E)$$
$$= \text{const.}\cdot B^2\, N\sqrt{E_{\mathrm{eff}}^{(\mathrm{SP})}(E)}\,\bar{\rho}(E) \tag{3.150}$$

with some system-specific constant. We compare this semiclassical result with the RMT prediction (3.124) anticipating that the first loop correction to $K_{\pm}$ in the TRI case is $-2\tau^2$ [15] like in the case without discrete symmetry and presuming that TRI-breaking corrections to this loop correction are of order $\mathcal{O}(\tau^3)$ as are the associated corrections without symmetry. So we identify the symmetry breaking parameter λ in the many body system:

$$\lambda = \left(\frac{\pi\hbar}{\sqrt{2m}\bar{L}}\right)^{\frac{1}{2}}\frac{\sigma_{\mathrm{B}}}{\phi_0}\sqrt{N}\left(E_{\mathrm{eff}}^{(\mathrm{SP})}(E)\right)^{\frac{1}{4}}\sqrt{\bar{\rho}(E)} = \text{const.}\cdot B\sqrt{N}\left(E_{\mathrm{eff}}^{(\mathrm{SP})}(E)\right)^{\frac{1}{4}}\sqrt{\bar{\rho}(E)}. \tag{3.151}$$

In order to be able to use expression (3.151) one has to check to what extent the effective short range interaction description is valid. Therefore it is highly recommended to do simulations of classical dynamics. This should be a good way to see how far the made assumptions are justified. And besides fixing the range of validity thereby one could address the question on how the effective single particle energy scales as a function of total energy. A question very important to answer is then if this range of validity is compliant with the demand for strong interaction to produce sufficient chaos. These questions shall be left open and postponed to future investigations. For now, let us simply assume the likely seeming case that there is a major number of system configurations that allow us to use (3.151).

What we referred to as many body transition catastrophe in the beginning is expressed by the explicit particle number dependence $\sqrt{N}$ in λ. Taking the limit of infinitely many particles obviously results in an abrupt transition at arbitrarily small magnetic field B. But this only happens when considering $E_{\mathrm{eff}}^{(\mathrm{SP})}(E)$ and $\bar{\rho}(E)$ as constant. So the question arises how one should scale the total energy E when comparing systems with different numbers of particles. Since both, the effective single particle energy and the smooth part of the density of states are quantities which increase with E, the best chance to find a region in the many body spectrum where GOE statistics are partially preserved is to go to low energies. But then of course one falls foul of the semiclassical validity. Also the assumption of smooth varying level spacing in the considered energy average window gets bad for low excitation energies. So one has to be careful with the question under discussion.

For educational reasons let us try a rough analysis of an example of a fermionic

system. The lowest possible energies are near the ground state that we estimate to roughly scale like

$$E_{\mathrm{GS}}^{(\mathrm{f})} \propto N^2. \tag{3.152}$$

For simplicity we assume the effective single particle energies to be the N-th fraction of E. At ground state energy they scale like

$$E_{\mathrm{eff}}^{(\mathrm{SP})}(E_{\mathrm{GS}}^{(\mathrm{f})}) = \frac{E_{\mathrm{GS}}^{(\mathrm{f})}}{N} \propto N. \tag{3.153}$$

To fix the scaling of λ one would now have to fix the scaling of $\bar{\rho}(E)$ with particle number. And that is why we cannot make a quantitative statement about the symmetry breaking for now. $\bar{\rho}(E)$ is strongly varying with the energy near the ground state. Below, it should have value zero and start to increase strongly above. The way in which this strong energy dependence is manifest is in turn strongly depending on the particle number N. In order to compensate the N-scaling in λ the average energy had to be scaled in a way that the smooth part of the density of stated scales like

$$\bar{\rho}(\langle E \rangle) \propto N^{-\frac{3}{2}}. \tag{3.154}$$

How near the average energy gets to the ground state due to this scaling and whether the variation of $\bar{\rho}(E)$ with the energy is smooth enough to consider it as rather constant in the energy average window needed in the spectral two point correlator (3.95) are questions crucially depending on the behaviour of $\bar{\rho}(E)$ with energy and particle number. Even if we had the assurance, that this scaling is consistently possible, it was unclear, whether this scaling pushed us into the non-universal regime of the many body spectrum, so that the whole semiclassical argument would break down and we were not able to make any statement about the emergence of a transition catastrophe at all. All in all, we see that there are many open questions that have to be dealt with very carefully, since the interplay between many sensitive properties and effects will decide about the manifestation of something that we could call a many body transition catastrophe.

In any case it should be clear now that the most important issue at hand is the behaviour of the smooth part of the many body density of states of a system of identical particles

$$\bar{\rho}(E) = \bar{\rho}_{\pm}^{(\mathrm{MB})}(E). \tag{3.155}$$

The semiclassical derivation of this object in terms of short range propagation shall therefor be the subject of the proceeding chapter.

4 The Weyl Expansion For Systems Of Identical Particles

4.1 Naive Volume Term

In order to determine the smooth part of density of states for a system of identical particles with bosonic or fermionic exchange symmetry we write the exact symmetry projected density of states in terms of the propagator

$$\rho_{\pm}(E) = \frac{1}{\pi\hbar}\,\Re\left[\int_0^\infty \mathrm{d}t\, e^{\frac{i}{\hbar}(E+i\epsilon)t}\,\frac{1}{N!}\sum_{\sigma\in S_N}(\pm 1)^\sigma \int \mathrm{d}^{ND}q\, K(P\mathbf{q},\mathbf{q};t)\right], \qquad (4.1)$$

by expressing the symmetry projected trace of the Green's function (3.5) in terms of the propagator (2.46). We abbreviate (4.1) to

$$\rho_{\pm}(E) = \frac{1}{\pi\hbar}\,\Re\left[\int_0^\infty \mathrm{d}t\, e^{\frac{i}{\hbar}(E+i\epsilon)t}\;\int \mathrm{d}^{ND}q\, K_{\pm}(\mathbf{q},\mathbf{q};t)\right], \qquad (4.2)$$

by the definition of the *symmetry projected propagator*

$$K_{\pm}(\mathbf{q}',\mathbf{q};t) = \langle\mathbf{q}'|\,\hat{\mathbb{1}}_{\pm}e^{-\frac{i}{\hbar}\hat{H}t}\,|\mathbf{q}\rangle = \frac{1}{N!}\sum_{\sigma\in S_N}(\pm 1)^\sigma\; K(P\mathbf{q}',\mathbf{q};t). \qquad (4.3)$$

Since we want to obtain the smooth part of the density of states $\bar{\rho}(E)$ we are interested in the short time behaviour of $K_{\pm}(\mathbf{q},\mathbf{q};t)$. Any permutation P other than the identity 1_{S_N} in $K_{\pm}$ will yield the propagation between points $\mathbf{q}$ and $P\mathbf{q}$ that are not close to each other in general. To illustrate this, figure 4.1 shows the simple example of two particles in a one-dimensional billiard, where the only permutations are the identity and the exchange of first and second particle.

Since only propagation over short distances can give relevant short time contributions one could naively expect the main contribution to $\bar{\rho}_{\pm}(E)$ to be associated with the identical permutation

$$\bar{\rho}_{\mathrm{v}}(E) = \frac{1}{N!}\bar{\rho}_{\mathrm{TF}}(E), \qquad (4.4)$$

which we call the *naive volume term* and which is simply the volume Weyl term or Thomas-Fermi level density of the unsymmetrised system divided by $N!$.

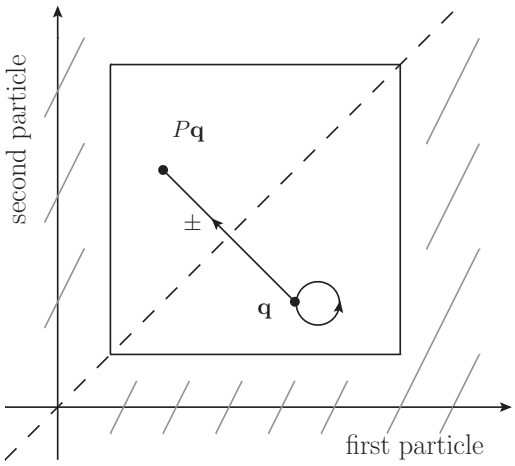


Figure 4.1: the two contributions to the symmetry projected propagator

The factor of $1/N!$ could thereby be interpreted as the correction introduced in statistical mechanics to solve the Gibbs paradox. As a first peculiarity we find that $\bar{\rho}_{\mathrm{v}}(E)$ is the same for bosons and fermions. This seems curious. So we want to check to what extent $\bar{\rho}_{\mathrm{v}}(E)$ can be considered a qualitatively good approximation to $\bar{\rho}_{\pm}(E)$. In order to do that, we consider a two-dimensional billiard of N non-interacting spinless fermions. The corresponding naive volume term reads

$$\bar{\rho}_{\mathrm{v}}(E) = \left(\frac{m}{2\pi\hbar^2}\right)^N A^N \frac{N}{(N!)^2} E^{N-1}\theta(E). \tag{4.5}$$

If the volume term was supposed to be a valuable approximation, it should asymptotically be able to provide the correct many body ground state energy $E_{\mathrm{GS}}^{(\mathrm{f})}$. Bosonic and fermionic ground state clearly differ from each other, thus already now we could stop and conclude that $\bar{\rho}_{\mathrm{v}}(E)$ can not be describing the system's properties sufficiently. Nevertheless the following calculation will substantiate this failure. The actual ground state energy of the non-interacting system can easily be calculated by filling up single particle energy levels. We do this by virtue of the smooth part of the single particle density of states

$$\bar{\rho}_0(E) = \left(\frac{m}{2\pi\hbar^2}\right) A\,\theta(E) \equiv \bar{\rho}_0\theta(E). \tag{4.6}$$

The corresponding average single particle level counting function is

$$\bar{N}_0(E) = \int_{-\infty}^{E} \mathrm{d}E'\,\bar{\rho}_0(E') = \bar{\rho}_0\,E. \tag{4.7}$$

We define the Fermi energy E_{F} by

$$N \stackrel{!}{=} \overline{N}_0(E_{\mathrm{F}}) = \bar{\rho}_0\,E_{\mathrm{F}}. \tag{4.8}$$

We get the ground state energy by counting the energies of all filled levels up to E_F

$$E_{\mathrm{GS}}^{(\mathrm{f})} = \int_{-\infty}^{E_{\mathrm{F}}} \mathrm{d}E'\, E'\, \bar{\rho}_0(E) = \frac{1}{2} N^2 \frac{1}{\bar{\rho}_0}. \tag{4.9}$$

The naive volume term expressed in terms of the single particle mean level spacing $1/\bar{\rho}_0$ reads

$$\bar{\rho}_{\mathrm{v}}(E) = \bar{\rho}_0 \, \frac{N}{(N!)^2} \, (\bar{\rho}_0 \, E)^{N-1} \theta(E), \tag{4.10}$$

and the related naive average many body level counting function has the simple form

$$\bar{N}_{\mathrm{v}}(E) = \frac{1}{(N!)^2} (\bar{\rho}_0 \, E)^N. \tag{4.11}$$

Up to the ground state energy the number of naively counted levels is

$$\bar{N}_{\mathrm{v}}(E_{\mathrm{GS}}^{(\mathrm{f})}) = \frac{N^{2N}}{2^N \, (N!)^2} \overset{N \gg 1}{\approx} \frac{1}{2\pi N} \underbrace{\left(\frac{e^2}{2} \right)^N}_{>1} \gg 1, \tag{4.12}$$

where in the last step the Stirling Formula has been used to approximate the factorial. So we naively count a number of levels below the ground state energy that is exponentially growing with particle number although it should be of the order of one. Even down to the $(e^2/2)$-th fraction of $E_{\mathrm{GS}}^{(\mathrm{f})}$ the naive term shows this behaviour. Note that (4.12) is independent of $\hbar$, meaning also the formal semiclassical limit $\hbar \to 0$ can not repair this failure. Also, adding the perimeter correction (2.80) to the single particle density can not help us out, since it effectively shifts the single particle density by some positive energy which in turn yields a higher ground state energy and hence makes the correctness of the naive picture even worse.

We conclude that the naive volume Weyl term which equals the Thomas-Fermi approximation with additional factor $1/N!$ is not sufficiently describing the average many particle density of states in a semiclassical limit. Especially when we are interested in the behaviour near the ground state energy $E_{\mathrm{GS}}^{(f)}$, we clearly have to go beyond this simple picture.

4.2 A Convolution Formula For Non-Interacting Systems

To answer the question of what is missing in the naive volume term it is advisable to stick to the non-interacting case. We will see that there it is possible to

express the exact many body density of states $\rho_{\pm}(E)$ in terms of single particle densities. A corresponding analysis has first been made by Weidenmüller [31]. As a useful basic concept first we introduce the organisation of permutations $P \in S_N$ in terms of *cycles*.

The Decomposition Into Cycles

A cycle is a basic permutation σ on a set X that maps all elements of a subset $C \subseteq X$ onto each other in a cyclic fashion, while all other elements are mapped onto themselves. Cyclic mapping thereby means that all elements in C share the same orbit, which is just C itself. An orbit of an element $c \in C$ is here defined as the union of all successive mappings $\sigma^k(c) =: c_k$.

$$C = \bigcup_{k \in \mathbb{N}} \sigma^k(c) \qquad \forall c \in C \tag{4.13}$$

$$\sigma(x) = x \qquad \forall x \notin C \tag{4.14}$$

Every element in C gets successively mapped through whole C

$$c = c_0 \mapsto c_1 \mapsto c_2 \mapsto \cdots \mapsto c_n = c \qquad , n = |C|. \tag{4.15}$$

The size $n = |C|$ of the set C is called the *length* of the cycle. Equivalently one uses the term *n-cycle*. In *cycle notation* one writes the permutation σ as the ordered sequence of all elements in C between brackets

$$\sigma = (\, c_0\, c_1\, \ldots\, c_{n-1}). \tag{4.16}$$

Every permutation $\sigma \in S_N$ can be decomposed into a commuting product of cycles with distinct subsets C. All fixed points of σ can thereby conventionally be written as one-cycles. The following examples shall illustrate the cycle decomposition.

$$\begin{aligned} \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 4 & 5 & 1 & 3 \end{pmatrix} &= (\,1\,2\,4\,) \cdot (\,3\,5\,) \\ \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix} &= (\,1\,) \cdot (\,2\,3\,) \\ \begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \end{pmatrix} &= (\,1\,) \cdot (\,2\,) \cdot (\,3\,) = 1_{S_3} \end{aligned} \tag{4.17}$$

Equipped with that we return to the symmetry projected density of states for non-interacting particles.

The Convolution Of Single Particle Densities

We remind that the many body density $\rho_{\pm}(E)$ is expressed as Fourier transform of the trace of the symmetry projected propagator (4.2). We write the real part

of the half sided Fourier transform in (4.2) as Fourier transform for all times

$$\rho_{\pm}(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \mathrm{d}t\, e^{\frac{i}{\hbar}Et - \epsilon t^2} \int \mathrm{d}^{ND}q\, K_{\pm}(\mathbf{q}, \mathbf{q}; t), \tag{4.18}$$

where we brought the ϵ-regularisation into another, more symmetric form that is equivalent in the limit $\epsilon \to 0$. To obtain (4.18), one has to use the following conjugation property of the symmetry-projected propagator from an initial point back to itself.

$$\begin{aligned} K_{\pm}(\mathbf{q}, \mathbf{q}; t)^* &= \left(\langle \mathbf{q}|\ \hat{\mathbb{1}}_{\pm}\, e^{-\frac{i}{\hbar}\hat{H}t}\ |\mathbf{q}\rangle \right)^* \\ &= \langle \mathbf{q}|\ e^{\frac{i}{\hbar}\hat{H}t}\, \hat{\mathbb{1}}_{\pm}\ |\mathbf{q}\rangle \\ &= \langle \mathbf{q}|\ \hat{\mathbb{1}}_{\pm}\, e^{\frac{i}{\hbar}\hat{H}t}\ |\mathbf{q}\rangle \\ &= K_{\pm}(\mathbf{q}, \mathbf{q}; -t). \end{aligned}$$

In (4.19) we used hermiticity of the projector (2.24) and the Hamiltonian and the commutation of both (2.32).

Essential is now the independence of non-interacting single particle propagations based on the commutation of single particle Hamiltonians $\hat{H}_i$ which are acting on different subspaces of $\mathscr{H}$.

$$e^{-\frac{i}{\hbar}\hat{H}t} = \prod_{i=1}^{N} e^{-\frac{i}{\hbar}\hat{H}_i t}. \tag{4.19}$$

The unsymmetrised many body propagator (and therefore every summand in the symmetry projected propagator (4.3)) can be factorised,

$$K(P\mathbf{q}', \mathbf{q}; t) = \prod_{i=1}^{N} K^{(\mathrm{SP})}(\mathbf{q}'_{\sigma(i)}, \mathbf{q}_i; t). \tag{4.20}$$

In every factorised summand (4.20) corresponding to a permutation P we can carry out some of the coordinate integrals by using the cycle decomposition and the general convolution property of propagators

$$\int \mathrm{d}^D q'\, K^{(\mathrm{SP})}(\mathbf{q}'', \mathbf{q}'; t_2)\, K^{(\mathrm{SP})}(\mathbf{q}', \mathbf{q}; t_1) = K^{(\mathrm{SP})}(\mathbf{q}'', \mathbf{q}; t_1 + t_2). \tag{4.21}$$

Let us write the permutation $P = \sigma \in S_N$ as a cycle-decomposition

$$\sigma = \sigma_1 \cdots \sigma_l \qquad , l \leq N \tag{4.22}$$

of l cycles σ_ω of length N_ω acting on the set of particle indexes $I := \{1, \ldots, N\}$. First, since the subsets of indexes $I_\omega = \{i_{\omega,1}, \ldots, i_{\omega,N_\omega}\}$ corresponding to the

cycles σ_ω are distinct, the appropriate summand of K can be decomposed into a product of l propagators, each associated with a cycle-subset.

$$K(P\mathbf{q}, \mathbf{q}; t) = \prod_{\omega=1}^{l} K^{(N_\omega)}((P\mathbf{q})_{I_\omega}, \mathbf{q}_{I_\omega}; t), \tag{4.23}$$

where

$$\mathbf{q}_{I_\omega} = \left(\mathbf{q}_{i_{\omega,1}}, \mathbf{q}_{i_{\omega,2}}, \ldots, \mathbf{q}_{i_{\omega,N_\omega}}\right) \tag{4.24}$$

and

$$(P\mathbf{q})_{I_\omega} = \left(\mathbf{q}_{\sigma(i_{\omega,1})}, \mathbf{q}_{\sigma(i_{\omega,2})}, \ldots, \mathbf{q}_{\sigma(i_{\omega,N_\omega})}\right) \tag{4.25}$$

are the restrictions of the vectors $\mathbf{q}$ and $P\mathbf{q}$ to components associated with each cycle's index set. The integral over coordinates of each index set I_ω then only involves the corresponding factor in (4.23), which in turn can be written again as a product of single particle propagators. For the sake of simplicity we relabel all indexes in I_ω by $\{1, \ldots, N_\omega\}$ when regarding one specific cycle σ_ω. So that the cycle simply acts as index increment

$$\begin{aligned} \sigma(i) &= i + 1 \qquad \forall i < N_\omega \\ \sigma(N_\omega) &= 1 \end{aligned} \tag{4.26}$$

Furthermore we simply write $\mathbf{q}$ by meaning $\mathbf{q}_{I_\omega}$.

$$\begin{aligned} &\int \mathrm{d}^{N_\omega D} q \; K^{(N_\omega)}(P\mathbf{q}, \mathbf{q}; t) = \\ &\int \mathrm{d}^{N_\omega D} q \; \prod_{i=1}^{N_\omega} K^{(SP)}(\mathbf{q}_{\sigma(i)}, \mathbf{q}_i; t) = \\ &\int \mathrm{d}^{N_\omega D} q \; K^{(SP)}(\mathbf{q}_1, \mathbf{q}_{N_\omega}; t) \cdots K^{(SP)}(\mathbf{q}_3, \mathbf{q}_2; t) \, K^{(SP)}(\mathbf{q}_2, \mathbf{q}_1; t) = \\ &\int \mathrm{d}^{D} q_1 \; K^{(SP)}(\mathbf{q}_1, \mathbf{q}_1; N_\omega t) = \operatorname{tr} \hat{U}^{(\mathrm{SP})}(N_\omega t) \equiv \operatorname{tr} \hat{K}_\omega(t), \end{aligned} \tag{4.27}$$

where we used the propagator convolution property (4.21). Thus the trace of the summand corresponding to P is the product of l traces of single particle propagators with modified time arguments $t_\omega = N_\omega t$.

$$\int \mathrm{d}^{ND} q \; K(P\mathbf{q}, \mathbf{q}; t) = \prod_{\omega=1}^{l} \operatorname{tr} \hat{K}_\omega(t) \tag{4.28}$$

We turn back into the density of states, knowing that the Fourier transform $\mathcal{F}$

of a product of functions gives a convolution of the Fourier transforms $\mathcal{F}[f_i](y)$ of all functions

$$\mathcal{F}[f_1(t)\cdots f_n(t)](y) = \int \mathrm{d}y_1 \ldots \mathrm{d}y_n \; \delta\left(y - \sum_{i=1}^{n} y_i\right) \mathcal{F}[f_1(t)](y_1)\cdots\mathcal{F}[f_n(t)](y_n). \tag{4.29}$$

Thus we obtain the symmetry projected density of states by substituting $t_\omega = N_\omega t$ in every Fourier transform

$$\mathcal{F}[\mathrm{tr}\, K_\omega(t)](E_\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \mathrm{d}t \; e^{\frac{i}{\hbar}Et - \epsilon t^2} \; \mathrm{tr}\, K_\omega(t) = \frac{1}{N_\omega}\rho^{(\mathrm{SP})}\left(\frac{E_\omega}{N_\omega}\right), \tag{4.30}$$

$$\rho_\pm(E) = \frac{1}{N!}\sum_{\sigma\in S_N}(\pm 1)^\sigma \int \mathrm{d}E_1 \ldots \mathrm{d}E_l \; \delta\left(E - \sum_{\omega=1}^{l} E_i\right) \prod_{\omega=1}^{l} \frac{1}{N_\omega}\rho^{(\mathrm{SP})}\left(\frac{E_\omega}{N_\omega}\right). \tag{4.31}$$

Because the sign of a permutation is determined by the number of cycles in its decomposition we can subsume all permutations in the sum that correspond to the same partition of N into integers $N = N_1 + N_1 + \cdots + N_l$.

$$\begin{aligned}\rho_\pm(E) =& \frac{1}{N!}\sum_{l=1}^{N}(\pm 1)^{N-l} \sum_{\substack{N_1,\ldots,N_l=1 \\ N_1\le\cdots\le N_l}}^{N} \delta_{N,\sum N_\omega} \; c(N_1,\ldots,N_l)\left[\prod_{\omega=1}^{l}\frac{1}{N_\omega}\right]\times \\ & \int \mathrm{d}E_1 \ldots \mathrm{d}E_l \; \delta\left(E - \sum_{\omega=1}^{l} E_\omega\right) \left[\prod_{\omega=1}^{l}\rho^{(\mathrm{SP})}\left(\frac{E_\omega}{N_\omega}\right)\right],\end{aligned} \tag{4.32}$$

where the combinatorial factor $c(N_1,\ldots,N_l)$ is the number of distinct permutations sharing the same partition $\{N_1,\ldots,N_l\}$ of N corresponding to the cycle-lengths of their cycle-decompositions.

The Correction Of Wrong Counted Single Particle Levels

Since we introduced the above formalism to answer the question of what is missing in the naive volume Weyl term $\bar{\rho}_{\mathrm{v}}(E)$, we remember that it was the contribution related to the identity permutation in the sum over the symmetric group. Therefore, we relate this to the convolution formula of non-interacting particles by taking only the contribution from the identity permutation in (4.31), which gives the convolution of all unaltered single particle densities

$$\rho_1(E) = \frac{1}{N!}\int \mathrm{d}E_1 \ldots \mathrm{d}E_N \; \delta\left(E - \sum_{\omega=1}^{N} E_i\right) \prod_{\omega=1}^{N} \rho^{(\mathrm{SP})}\left(E_\omega\right). \tag{4.33}$$

Plugging in the single particle densities expressed in terms of single particle energy levels

$$\rho^{(\mathrm{SP})}(E) = \sum_n \delta(E - E_n) \tag{4.34}$$

yields

$$\rho_1(E) = \frac{1}{N!} \sum_{n_1,\ldots,n_N} \delta\left(E - \sum_{i=1}^{N} E_{n_i}\right). \tag{4.35}$$

The term related to the identity gives us a δ-peak at every energy E that can be partitioned into single particle energies E_i. When all single particle levels are different ($n_i \neq n_j \quad \forall i \neq j$), the corresponding total energy E appears $N!$ times in the sum. Thus the prefactor of $1/N!$ yields a singly counted δ-peak for this particular energy E. Thus such a many body energy level is reproduced correctly by the identity contribution. But in the case of equality of some of the single particle levels ($\exists i \neq j \quad n_i = n_j$), (4.33) produces wrong results. In the fermionic case, such an energy should not be counted at all whereas in the bosonic case, it appears less than $N!$ times in the sum and therefore produces a δ-peak with a coefficient that is too small. We want to see now, how these failures are corrected by the terms in (4.31) related to permutations other than the identity.

Although it is possible to systematically show this correction of δ-peaks, we restrict ourselves now to the case of two particles ($N = 2$) for the sake of simplicity. The symmetry projected density (4.32) then simplifies to

$$\rho_\pm(E) = \frac{1}{2}\left((\rho^{(\mathrm{SP})} * \rho^{(\mathrm{SP})})(E) \pm \frac{1}{2}\rho^{(\mathrm{SP})}\left(\frac{E}{2}\right)\right). \tag{4.36}$$

Again, we plug in (4.34) and find

$$\rho_\pm(E) = \frac{1}{2}\sum_{n_1,n_2} \delta(E - E_{n_1} - E_{n_2}) \pm \frac{1}{2}\sum_n \delta(E - 2E_n). \tag{4.37}$$

So we see now that the correction due to the exchange of the two particles indeed retrieves the failure of wrong counted energy levels. For fermions, it cancels the peaks with equal single particle energies. And for bosons, it doubles the corresponding coefficient resulting in a fully counted many body energy level.

This partially explains what is going wrong when we take only the naive volume term related to the identity permutation in the smooth part of the density of states. Especially the incorrect reproduction of a ground state energy seems now to be unsurprising. But if we strictly want to compare Weidenmüller's convolution formula to the smooth part of the level density, we should somehow incorporate smoothness into it.

Smoothing The Convolution Of Densities

Of course, as a first attempt, one would think of simply plugging in the smooth single particle densities $\bar{\rho}^{(\mathrm{SP})}(E)$ in (4.32) in order to obtain the smooth part of the many body density $\bar{\rho}_{\pm}(E)$. And indeed, the following argument will show that, at least in some sense, this is possible.

We want to start with each summand of (4.32) and convolve every single particle density with some smoothing function δ_α with smoothing parameter α

$$\begin{aligned}\bar{\rho}^{(\mathrm{SP})}\left(\frac{E_\omega}{N_\omega}\right) &\to \int \mathrm{d}\epsilon_\omega\ \bar{\rho}^{(\mathrm{SP})}(\epsilon_\omega)\,\delta_\alpha\left(\epsilon_\omega - \frac{E_\omega}{N_\omega}\right) \\ &= \int \mathrm{d}\bar{\epsilon}_\omega\ \bar{\rho}^{(\mathrm{SP})}\left(\frac{\bar{\epsilon}_\omega}{N_\omega}\right) \underbrace{\frac{1}{N_\omega}\delta_\alpha\left(\frac{\bar{\epsilon}_\omega}{N_\omega} - \frac{E_\omega}{N_\omega}\right)}_{\stackrel{!}{=}\delta_{\alpha N_\omega}(\bar{\epsilon}_\omega - E_\omega)},\end{aligned} \tag{4.38}$$

Where we demand now that the parameter α reflects a characteristic smoothing function argument, i.e. its full width of half maximum (FWHM)

$$\delta_{c\alpha}(x) = \frac{1}{c}\delta_\alpha\left(\frac{x}{c}\right). \tag{4.39}$$

Performing now the convolution with one of the densities in the summand

$$\int \mathrm{d}E_1 \ldots \mathrm{d}E_l\ \left[\prod_{\omega=1}^{l} \rho^{(\mathrm{SP})}\left(\frac{E_\omega}{N_\omega}\right)\right]\ \delta\left(E - \sum_{\omega=1}^{l} E_i\right) \tag{4.40}$$

is equivalent to a smoothing of the delta-function

$$\begin{aligned}&\int \mathrm{d}E_\omega \int \mathrm{d}\bar{\epsilon}_\omega\ \bar{\rho}^{(\mathrm{SP})}\left(\frac{\bar{\epsilon}_\omega}{N_\omega}\right)\ \delta_{\alpha N_\omega}\left(\bar{\epsilon}_\omega - E_\omega\right)\ \delta(E - \sum_{k=1}^{l} E_k) \\ &= \int \mathrm{d}E_\omega\ \bar{\rho}^{(\mathrm{SP})}\left(\frac{E_\omega}{N_\omega}\right)\ \delta_{\alpha N_\omega}(E - \sum_{k=1}^{l} E_k),\end{aligned} \tag{4.41}$$

where we integrated over E_ω and renamed $\bar{\epsilon}_\omega$ by E_ω afterwards. So we are left with a similar expression to the summand but with the delta-function substituted by the smoothing function due to convolution of both. If we apply now the convolution corresponding to another index λ, we have to convolve $\delta_{\alpha N_\lambda}$ with the smoothing function at hand $\delta_{\alpha N_\omega}$ instead of a delta function. So we demand the additional property of the smoothing function of invariance with respect to convolution and additivity of FWHMs

$$(\delta_\alpha * \delta_\beta)(x) = \int \mathrm{d}x'\ \delta_\alpha(x - x')\delta_\beta(x') = \delta_{\alpha+\beta}(x). \tag{4.42}$$

This means the successive convolution of single particle densities effectively increases the smoothing parameter of the delta function in the summand (4.40), which can be seen as smoothing function with parameter $\alpha = 0$. After performing a total of l single particle convolutions in the summand we are eventually left with

$$\int \mathrm{d}E_1 \ldots \mathrm{d}E_l \left[\prod_{\omega=1}^{l} \rho^{(\mathrm{SP})}\left(\frac{E_\omega}{N_\omega}\right)\right] \delta_{\alpha N}\left(E - \sum_{\omega=1}^{l} E_i\right), \tag{4.43}$$

which equals the smoothing of the whole summand (4.40) with respect to the total energy E with smoothing parameter αN. This total smoothing parameter is now independent of the specific partition $N = N_1 + \cdots + N_l$ in (4.32), thus it is the same for all summands. We see now that this was the very reason to demand the additivity of smoothing parameters. The single particle smoothing (4.38) is then equal to the smoothing of the many body density of states by virtue of the same smoothing function but with the smoothing parameter multiplied by the number of particles.

Indeed there is a choice of $\delta_\alpha(x)$ that fulfils the conditions (4.39) and (4.42). Namely the Cauchy distribution

$$\delta_\alpha(x) = \frac{1}{\pi\alpha} \frac{1}{1 + \left(\frac{x}{\alpha}\right)^2}. \tag{4.44}$$

If we used instead for example a Gaussian smoothing, we would obtain different variances in the summands due to the additivity of variances instead of standard deviations. Therefore it was not possible to write the corresponding sum as a single unique convolution with respect to the total energy E. So we see that the incorporation of smoothness in the convolution formula by Weidenmüller is indeed possible, but only in a very specific way.

Closing one has to stress that we are interested in the smooth part of the density of states defined by the semiclassical decomposition $\rho_{\mathrm{scl}}(E) = \bar{\rho}_{\mathrm{scl}}(E) + \tilde{\rho}_{\mathrm{scl}}(E)$. In that definition $\bar{\rho}_{\pm}(E)$ is related to short time or short path propagation instead of a convolution with a Lorentzian profile or any other smoothing function. Also the single particle Weyl expansions in the case of a billiard system can not be expressed by convolution of the exact densities. So we have no strict argument at hand that allows us to use the convolution formula (4.32) in combination with smooth single particle densities in order to obtain the correct $\bar{\rho}_{\pm}(E)$. We could nonetheless close our eyes for a moment and just do what we are not allowed to do and see what happened and then try to confirm the results afterwards. But we will go the correct way from the beginning and deduce the smooth part $\bar{\rho}_{\mathrm{scl}}(E)$ out of short path propagation in the many body phase space. Especially when it comes to particle-particle interactions, the convolution formula will be of no use, whereas in principle one can include interactions as modifications to short path propagation.

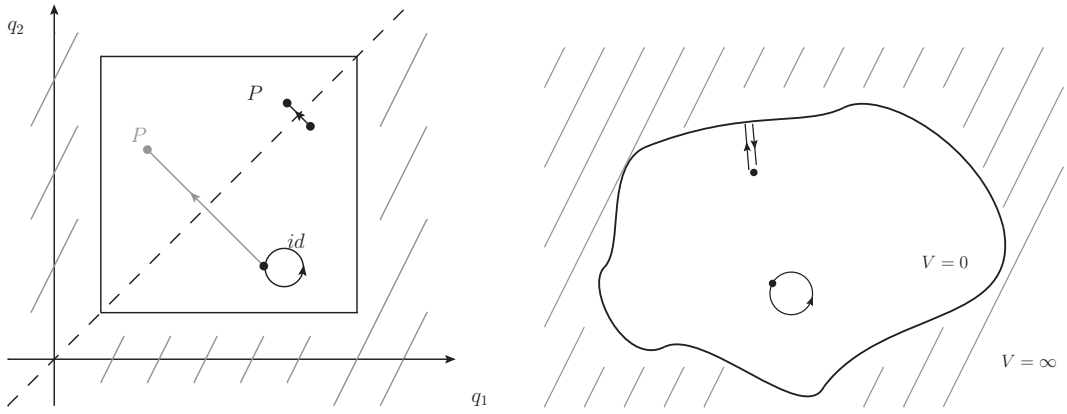
4.3 Short Path Contributions For Identical Particles

Again we want to restrict ourselves to billiard systems. As we have seen in section 2.2.2, the first term of the smooth part of the density of states corresponds to local free propagation in the interior of a billiard. In the context of identical particles we called this the naive volume term (see section 4.1). We know now that this does not give a sufficient description, so we want to include higher terms coming from permutations in (4.1) other than the identity and search for short path contributions in there. This shall happen just analogue to the single particle Weyl expansion, where additional short path contributions came from propagation modifications near the billiard boundary (2.83). In general, one should be able to obtain Weyl-like corrections in a similar manner for any kind of discrete symmetry. One should mention the work of Whelan and Lauritzen [17], who explicitly calculated Weyl-like corrections for two- and three-dimensional systems symmetric under general point transformations in this restricted number of dimensions, which can be easily parametrised. In the case of particle exchange symmetry however, no such formalism is available so far. In order to develop a formalism for calculating Weyl-like expansions in systems of identical particles, one has to explicitly account for the special structure of possible short path contributions. First we will have a look on a one dimensional billiard of two particles, where the additional short path contributions have a simple geometrical interpretation.

4.3.1 Two Non-Interacting Fermions On A Line

Consider a system of two particles confined to a line of length L. The only two permutations are the identity and the exchange of both, or in cycle notation $(1)(2)$ and (12). Figure (4.2a) illustrates the two possible contributions to the propagator. Since the system has an effective two-dimensional description we want to compare it to a single particle two-dimensional billiard, where we have contributions to the propagator from free propagation and from reflections on the boundary, which is illustrated in figure (4.2b).

We want now to understand additional symmetry related short path contributions to $\bar{\rho}_{\pm}(E)$ as Weyl-like corrections from boundaries. As discussed in section 3.1.3 we can give a simple two-dimensional single particle billiard that is exactly equivalent to the two particle system. That is, the billiard defined by the fundamental domain which we choose as $\mathscr{F} : q_1 > q_2$ with an additional hard wall boundary along the symmetry line $q_1 = q_2$. In this two dimensional picture reflections on the additional boundary are mapped to the propagation with respect to the exchange permutation in the one dimensional many body



(a) 2 particles in 1 D (b) 1 particle in 2 D

Figure 4.2: Comparison of the system of two identical particles in one dimension and one particle in two dimensions.

picture. Figure (4.3) illustrates the corresponding propagations in both pictures. In the two-dimensional single particle picture (1p2d) the Weyl expansion (2.81) includes a volume term $\bar{\rho}_{\mathrm{v}}(E)$ with area $A = L^2/2$, which is the naive volume term in the many body picture (2p1d), where the factor of $1/2$ corresponds to the factor $1/N!$. The perimeter correction $\bar{\rho}_{\mathrm{p}}(E)$ induced by the additional boundary in the single particle picture comes with the perimeter $\sqrt{2}L$. For now we do not take into account single particle one dimensional boundary corrections, so all remaining boundaries are consistently untreated in both pictures. This means the perimeter correction is just the correction due to symmetry related short path propagation near the symmetry line that we were searching for. The smooth part of density of states without single particle confinement corrections then reads

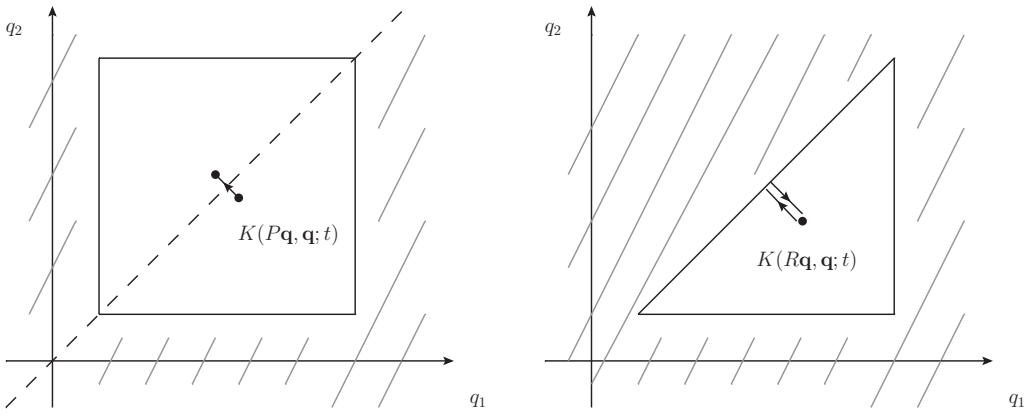
$$\bar{\rho}_{-}^{(\mathrm{2p1d})}(E) = \bar{\rho}_{\mathrm{Weyl}}^{(\mathrm{1p2d})}(E) = \frac{L^2}{8\pi}\left(\frac{2m}{\hbar^2}\right)\theta(E) \; - \; \frac{\sqrt{2}L}{8\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} E^{-\frac{1}{2}}\theta(E). \quad (4.45)$$

For a moment, let us take the convolution formula (4.36) and simply plug in the full Weyl expansion of a one-dimensional billiard

$$\bar{\rho}_0(E) := \bar{\rho}_{\mathrm{Weyl}}^{(\mathrm{1d})}(E) = \frac{L}{2\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} E^{\frac{1}{2}}\theta(E) - \frac{1}{2}\delta(E), \quad (4.46)$$

which we have to remind is strictly not justified at this stage, as we discussed at the end of section 4.2. Nonetheless, the convolution formula in total gives

$$\begin{aligned}&\frac{1}{2}\left((\bar{\rho}_0 * \bar{\rho}_0)(E) - \frac{1}{2}\bar{\rho}_0\left(\frac{E}{2}\right)\right)\\ =&\frac{L^2}{8\pi}\left(\frac{2m}{\hbar^2}\right)\theta(E) \; - \; (2+\sqrt{2})\frac{L}{8\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} E^{-\frac{1}{2}}\theta(E) \; + \; \frac{3}{8}\delta(E), \quad (4.47)\end{aligned}$$



(a) 2 particles in 1 D (b) 1 particle in 2 D

Figure 4.3: Comparison of the system of two identical particles in one dimension and one particle in two dimensions.

which exactly equals the full Weyl expansion in the (1p2d)-picture (2.81) including all boundary segments and all three corners. The perimeter correction from the two boundary segments of length L are thereby identified with the one-dimensional volume term convoluted with the one-dimensional confinement correction. The correction from the corner that is built by both of them can be identified with the convolution of the two one-dimensional confinement corrections. The other two corners give corrections corresponding to the one-dimensional confinement correction in the symmetry correction term $-\frac{1}{2}\bar{\rho}_0\left(\frac{E}{2}\right)$ due to particle exchange. So we see that in this case indeed we are able to obtain $\bar{\rho}_-(E)$ by simply using the single particle Weyl expansion in the convolution formula. This justification is based on the equivalence of the single particle and two particle pictures in this simple case. So we can not extend this argument to the general case of N particles in D dimensions by now.

4.3.2 General Case - Propagation In Cluster Zones

Invariant Manifolds And Cluster Zones

Consider the rather general case of N identical particles in a D-dimensional billiard. In more than one dimension we can not give an easy geometrical interpretation as in the last subsection by mapping the system that is symmetric under particle exchange onto a simple effective single particle system without that symmetry. Note that although in section 3.1.3 we discussed the possibility of mapping a bosonic system in $D > 1$ to the system of a multidimensional single particle moving in the wrapped fundamental domain, we can not use this equivalence to obtain the smooth part of density of states. That is because of the non-trivial topology of the wrapped fundamental domain. Despite the existence

of a formula for the smooth part of density of states in billiards of arbitrary dimension and arbitrary curvature [1], the author is not aware of a generalisation to arbitrary topologies. In the case of two bosons one might think about conformal mapping of the wrapped fundamental domain to the full domain by virtue of quadrature. This would correspond to the mapping of for example the lower complex half plane onto whole $\mathbb{C}$ by the conformal map $z \mapsto z^2$. But since Schrödinger's equation is not homogeneous, this process produces an effective potential term concentrated around the symmetry plane, so one no longer had to deal with a billiard system in the mapped system (see Appendix B of [27]). This of course would affect the smooth part of the density of states in a non-trivial way that would demand the treatment of hard walls and smooth potentials at the same time. Thus we see that the description in the wrapped fundamental domain leads to complications whose treatment lies beyond the scope of this work and may be postponed to future analysis. Nevertheless we note that it should be of value to do such an analysis, especially in the context of symmetry-induced effective forces in unsymmetric analogues of the actual symmetric system (see Appendix B in [27]). For now, we stick to the general description in full phase space with a symmetry projected propagator.

In the last section we saw that in the example of two particles on a line the correction to $\bar{\rho}(E)$ due to the exchange permutation is related to the propagation in the vicinity of the symmetry line $q_1 = q_2$. The important property of the symmetry line is that it is invariant under $P = (\,1\,2\,)$, so that the distance $|P\mathbf{q} - \mathbf{q}|$ becomes zero. This is the very reason to assume short path contributions to come from its vicinity. So we extend the concept of invariant manifolds to the general case by finding the manifolds associated with each permutation P, defined by

$$\mathcal{M}_P = \big\{\mathbf{q} \in \mathbb{R}^{ND} \;\big|\; |P\mathbf{q} - \mathbf{q}| = 0\big\}. \tag{4.48}$$

We write P as a composition of cycles (see section 4.2)

$$P = \sigma_1 \cdots \sigma_l, \tag{4.49}$$

with distinct cycle subsets of particle indexes

$$I_1, I_2, \ldots, I_l \tag{4.50}$$

of size

$$N_1, N_2, \ldots, N_l. \tag{4.51}$$

So we see that $\mathcal{M}_P$ is the manifold defined by the equality of the coordinates of all particles associated with each cycle

$$\mathcal{M}_P = \bigcap_{\omega=1}^{l} \big\{\mathbf{q} \in \mathbb{R}^{ND} \;\big|\; \mathbf{q}_i = \mathbf{q}_j \quad \forall i, j \in I_\omega\big\}. \tag{4.52}$$

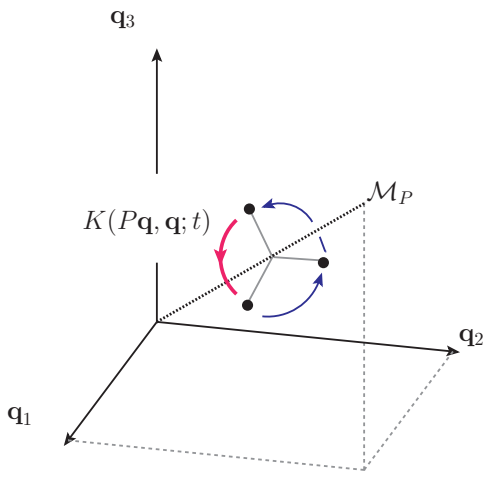


Figure 4.4: three particles in one dimension. The invariant manifold corresponding to the cycle through all three particles is just a line, not a surface.

As a simple example take the permutation

$$P = (\,1\,2\,4\,)\,(\,3\,5\,), \tag{4.53}$$

whose associated manifold $\mathcal{M}_\mathcal{P}$ corresponds to the condition

$$\big(\mathbf{q}_1 = \mathbf{q}_2 = \mathbf{q}_4\big) \wedge \big(\mathbf{q}_3 = \mathbf{q}_5\big). \tag{4.54}$$

In contrast to the symmetry line in the one-dimensional two particle case, these manifolds in general can not be seen as a boundary or surface in coordinate space in the sense of dividing the space into distinct pieces as illustrated in figure 4.4 for the example of three particles in one dimension and the permutation $(\,1\,2\,3\,)$.

The vicinities of these invariant manifolds, which will be the places to find short path contributions, shall from now on be referred to as *cluster zones*. All particles associated with a particular cycle index subset will be subsumed to the notion of a *cluster*. A system that is momentarily arranged in a particular cluster zone is composed of l clusters, each associated with a cycle in P. Each cluster ω is composed of N_ω particles according to the length of the cycle.

We separate coordinates parallel to $\mathcal{M}_P$ and perpendicular to it, since the propagation near $\mathcal{M}_P$ will not depend on shifting the position along them. This holds at least as long as one does not get too close to the single particle billiard boundaries. But we want to restrict to the symmetry corrections without single particle boundary corrections. We will refer to this as the *unconfined case*. Of course, one should treat confinement corrections too in order to give consistent

results. But this lies beyond the scope of this work and is passed to future investigations. Maybe one could also want to think of softened billiard walls with some smooth potential slope, which would result in an effective damping of single particle boundary corrections. For now, assume the propagation to be invariant along $\mathcal{M}_P$.

Furthermore, the invariance of propagation along the invariant manifolds is in a strict treatment also broken in the case of interaction. But the sense lying behind this construction is that when restricting to interactions of rather short range, the propagation can be assumed to be invariant along $\mathcal{M}_P$ as long as one does not get too close to other invariant submanifolds. In other words, as long as the coordinates corresponding to different cycles do not become too close. Or to put it into a more intuitive picture, the different clusters should not collide. One can pick up this idea when discussing the implementation of such short range interactions. A promising approach could be to build up a hierarchy of interaction modifications in the sense that the main modification in a particular cluster zone is related to the independent motion of clusters throughout the zone, the propagation in each cluster feeling the modification due to interaction within the cluster but independent from other clusters. This has the consequence that interaction modifications related to a submanifold have to be altered, since then one has to account only for the difference of the propagator modification of the merged clusters to the product of the propagator modifications of the independent clusters. This is because in the relevant merged clusterzone corresponding to the submanifold only the propagation of the merged cluster is relevant but partially already counted by the product of subcluster propagations in the vicinity of parent manifolds. For example in the interaction modification to a three cluster correction, the propagator modification of a pair of two particles multiplied with the independent single particle propagator of the third particle can be subtracted from the actual three particle propagator modification. And this for any of the three possible pairings corresponding to the three parent manifolds. Thus there is hope that these modification differences become very small with growing cluster sizes and that one can probably give approximations to interacting systems by neglecting modification differences related to larger cluster sizes. In the end this remains an open question which we look forward to give answers in the future.

The Measure Of Invariant Manifolds

We have to first calculate the measure of the invariant manifold $\mathcal{M}_P$. For a better understanding let us start with a clustering of the first k particles $(1 \leq k \leq N)$

$$P_k = (\,1\,2\,\ldots\,k\,)\,(\,k+1\,)\,\cdots\,(\,N\,). \tag{4.55}$$

For the determination of the infinitesimal volume element $\mathrm{d}\mu$ on $\mathcal{M}_{P_k}$ we determine the infinitesimal vectors in full (ND)-dimensional coordinate space lying in $\mathcal{M}_{P_k}$ that correspond to the variations of independent coordinates. We use again the notation $\mathbf{q} = (\mathbf{q}_1, \ldots, \mathbf{q}_N)$ and $\mathbf{q}_i = (q_i^{(1)}, \ldots, q_i^{(D)})$. As a set of independent Cartesian coordinates we choose the D coordinates of the first particle and the D coordinates of all particles with indexes $k+1, \ldots, N$

$$\bigcup_{d=1}^{D} \{q_1^{(d)}, q_{k+1}^{(d)}, \ldots, q_N^{(d)}\}. \tag{4.56}$$

Let $\mathrm{d}\mathbf{s}_k^{(d)}$ denote the infinitesimal vector on $\mathcal{M}_{P_k}$ that corresponds to a variation of the d-th spatial component of $\mathbf{q}_1$. When shifting $\mathbf{q}_1$ by $\mathrm{d}\mathbf{q}_1$, all particle coordinates up to the k-th particle have to follow this shift in order to stay on $\mathcal{M}_{P_k}$. Therefore, the shifting vector is

$$\mathrm{d}\mathbf{s}_k^{(d)} = (\underset{\substack{\uparrow \\ 1\text{st}}}{\mathbf{e}_d}, \ldots, \underset{\substack{\uparrow \\ k\text{-th}}}{\mathbf{e}_d}, \mathbf{0}, \ldots, \mathbf{0}) \cdot \mathrm{d}q_1^{(d)}, \tag{4.57}$$

where $\mathbf{e}_d = (\ldots, 0, \underset{\substack{\uparrow \\ d\text{-th}}}{1}, 0, \ldots)$ denotes the d-th unit vector in $\mathbb{R}^D$. All shifting vectors for the various spatial components are orthogonal to each other and therefore $\mathrm{d}\mu$ is the product of their norms $\mathrm{d}s_k^{(d)}$ and the volume elements of all other particle coordinates.

$$\begin{aligned} \mathrm{d}s_k^{(d)} &= \sqrt{k}\, \mathrm{d}q_1^{(d)} \\ \mathrm{d}\mu &= \prod_{d=1}^{D} \mathrm{d}s_k^{(d)}\ \mathrm{d}^D q_{k+1} \cdots \mathrm{d}^D q_N \\ &= \sqrt{k}^D \underbrace{\prod_{d=1}^{D} \mathrm{d}q_1^{(d)}}_{=\mathrm{d}^D q_1}\ \mathrm{d}^D q_{k+1} \cdots \mathrm{d}^D q_N. \end{aligned} \tag{4.58}$$

To obtain the measure of the manifold $\mu(\mathcal{M}_{P_k})$ we have to integrate all independent coordinates over the interior Ω of the billiard.

$$\mu(\mathcal{M}_{P_k}) = \int \mathrm{d}\mu = \sqrt{k}^D\, V_D^{N-k+1} \tag{4.59}$$

with the D-dimensional volume of the billiard

$$V_D = \int_{\Omega} \mathrm{d}^D q_i. \tag{4.60}$$

Figure (4.5) illustrates the above construction for the clustering of two particles.

Now we can generalise the construction to arbitrary permutations P in cycle

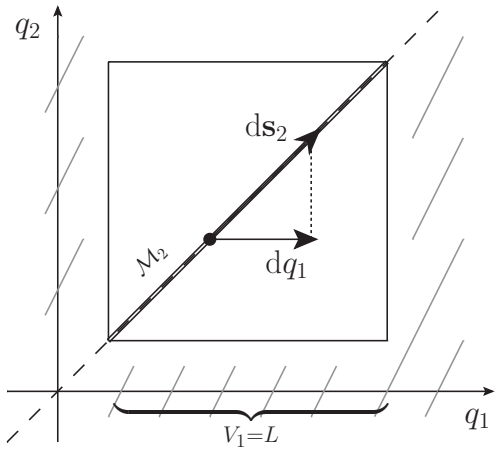


Figure 4.5: calculating the measure of the invariant manifold for a two-cycle

decomposition (4.49 - 4.51) Since all particles associated with one cycle have to fulfil the condition of equal coordinates, we get exactly one independent D-dimensional vector for each cycle σ_ω , $\omega = 1, \ldots, l$, while all other particles in the same cycle have to follow in order to remain on the invariant manifold $\mu(\mathcal{M}_P)$. For the sake of simplicity, let us simply write the l independent vectors as $\mathbf{q}_\omega$, $\omega = 1, \ldots, l$. Furthermore we order the particles in a way that the first cycle σ_1 involves the first N_1 particles, the second cycle σ_2 involves the N_2 subsequent particles, and so on. Due to symmetry, we can do so without changing the measure of the manifold. Similar to before but now for each cycle σ_ω, we get D shifting vectors $\mathrm{d}\mathbf{s}^{(d)}_{N_\omega}$, $d = 1, \ldots, D$ for the D spatial components of the variation of the associated independent vector $\mathrm{d}\mathbf{q}_\omega$

$$\mathrm{d}\mathbf{s}^{(d)}_{N_\omega} = (\underbrace{\mathbf{0}, \ldots, \mathbf{0}}_{N_1+\cdots+N_{\omega-1}}, \underbrace{\mathbf{e}_d, \ldots, \mathbf{e}_d}_{N_\omega}, \mathbf{0}, \ldots) \cdot \mathrm{d}q^{(d)}_\omega \tag{4.61}$$

with norm

$$\mathrm{d}s^{(d)}_{N_\omega} = \sqrt{N_\omega}\, \mathrm{d}q^{(d)}_\omega. \tag{4.62}$$

Since all shifting vectors of all cycles are pairwise orthogonal, the volume element $\mathrm{d}\mu$ of $\mathcal{M}_P$ is the product of all their lengths

$$\begin{aligned} \mathrm{d}\mu &= \prod_{d=1}^{D} \mathrm{d}s^{(d)}_{N_1} \cdot \cdots \cdot \prod_{d=1}^{D} \mathrm{d}s^{(d)}_{N_l} \\ &= \mathrm{d}^D q_1 \cdots \mathrm{d}^D q_l \cdot \sqrt{N_1}^D \cdots \sqrt{N_l}^D. \end{aligned} \tag{4.63}$$

Integrating all independent particle coordinates over the interior Ω of the billiard yields the total measure

$$\mu(\mathcal{M}_P) = V_D^l \cdot \left(\prod_{\omega=1}^{l} N_\omega\right)^{\frac{D}{2}} . \tag{4.64}$$

This measure is only depending on the partition of N into integers $N_1 + \cdots + N_l$ corresponding to the decomposition of P into cycles with lengths $N_1, \ldots, N_l$. So for each permutation associated with the particular partition $\{N_1, \ldots, N_l\}$ we get an invariant manifold of the same measure (4.64). Furthermore the contributions from short path propagation in their vicinities will be the same due to the symmetry with respect to relabelling particle indexes. This means we can replace the sum over all permutations by a sum over all distinct partitions of N and multiply each summand by the combinatorial factor

$$c(N_1, \ldots, N_\omega) = N! \left(\prod_{\omega=1}^{l} \frac{1}{N_\omega}\right) \left(\prod_{n=1}^{N} \frac{1}{m_n!}\right), \tag{4.65}$$

which is the number of permutations $P \in S_N$ with cycle lengths $\{N_1, \ldots, N_l\}$ in their cycle decomposition. Thereby, m_n denotes the multiplicity with which the cycle length n appears. The combinatorial factor (4.65) is just the same as in Weidenmüller's convolution formula (4.32), where also the permutations were subsumed by means of the corresponding cycle lengths.

4.4 The Non-Interacting Case

4.4.1 The Weyl Expansion Of Non-Interacting Particles

Derivation Of The Density Of States

Up to this point, the analysis is quite general and is valid also for particle-particle interaction. We believe it to be feasible in the context of interaction. But for now, we will explicitly carry out the non-interacting case. We are interested in the trace of the symmetry projected free propagator

$$\int \mathrm{d}^{ND} q \, K_{0,\pm}(\mathbf{q}, \mathbf{q}; t) = \frac{1}{N!} \sum_{\sigma \in S_N} (\pm 1)^\sigma \int \mathrm{d}^{ND} q \, K_0(P\mathbf{q}, \mathbf{q}; t). \tag{4.66}$$

We are now going to explicitly calculate the summand corresponding to a particular permutation P. Again we use the form of P decomposed into cycles. The particle indexes of different cycles don't mix up, so we get a product of independent propagators, which can be traced separately, each factor corresponding to a specific cycle in the decomposition of P. We consider now the trace of all coordinates corresponding to the cycle σ_ω. For this purpose, we relabel the particles, so that the indexes associated with σ_ω are simply $I_\omega = \{1, \ldots N_\omega\}$. For

the sake of simplicity we write $\mathbf{q}$ by meaning $\mathbf{q}_{I_\omega}$ and $P\mathbf{q}$ by meaning $(P\mathbf{q})_{I_\omega}$. Furthermore we write $n = N_\omega$. The integral over the associated coordinates reads

$$\int \mathrm{d}^{nD}q\, K_0(P\mathbf{q}, \mathbf{q}; t) = \int \mathrm{d}^{nD}q\, \left(\frac{m}{2\pi\hbar i t}\right)^{\frac{nD}{2}}\, e^{\frac{i}{\hbar}\frac{m}{2t}|P\mathbf{q}-\mathbf{q}|^2}. \tag{4.67}$$

Where the equality of a product of n free propagators in D dimensions and one (nD)-dimensional free propagator has been used. The distance vector between point and permuted point is

$$P\mathbf{q} - \mathbf{q} = (\mathbf{q}_2 - \mathbf{q}_1, \mathbf{q}_3 - \mathbf{q}_2, \ldots, \mathbf{q}_1 - \mathbf{q}_n). \tag{4.68}$$

The squared distance is

$$\begin{aligned} |P\mathbf{q} - \mathbf{q}|^2 &= |\mathbf{q}_2 - \mathbf{q}_1|^2 + \cdots + |\mathbf{q}_1 - \mathbf{q}_n|^2 \\ &= \sum_{d=1}^{D} \left[(q_2^{(d)} - q_1^{(d)})^2 + \cdots + (q_1^{(d)} - q_n^{(d)})^2\right] \end{aligned} \tag{4.69}$$

The overall squared distance is the sum of squared distances according to one spatial component, which are just the summands in (4.69). The following calculation proceeds in equal manner for all spatial components $d = 1, \ldots, D$. So we further simplify the notation by calculating only one spatial component and by omitting the superscript (d). Thus we are moving in n-dimensional space for now. For this calculation we simply write $\mathbf{q}$ and $P\mathbf{q}$ by meaning the corresponding tuples of one particular spatial component.

$$\begin{aligned} \mathbf{q} &= (q_1, q_2, \ldots, q_{n-1}, q_n) \\ P\mathbf{q} &= (q_2, q_3, \ldots, q_n, q_1). \end{aligned} \tag{4.70}$$

Each summand in (4.69) in this simplified notation is

$$|P\mathbf{q} - \mathbf{q}|^2 = (q_2 - q_1)^2 + \cdots + (q_n - q_{n-1})^2 + (q_1 - q_n)^2 \tag{4.71}$$

The trace to calculate is

$$\int \mathrm{d}^{n}q\, K_0(P\mathbf{q}, \mathbf{q}; t) = \int \mathrm{d}^{n}q\, \left(\frac{m}{2\pi\hbar i t}\right)^{\frac{n}{2}}\, e^{\frac{i}{\hbar}\frac{m}{2t}|P\mathbf{q}-\mathbf{q}|^2}. \tag{4.72}$$

The squared distance is of second order in all coordinates, so one could think about performing the integral (4.72) as a generalised multidimensional Gaussian integral

$$\int \mathrm{d}^{m}x\, e^{-\frac{1}{2}\mathbf{x}^T A \mathbf{x}} = \sqrt{\frac{(2\pi)^m}{\det(A)}}. \tag{4.73}$$

But we see that the determinant of A equals zero. It has one eigenvalue $\lambda = 0$ corresponding to the direction parallel to the invariant manifold, expressing the local translational invariance

$$\hat{\mathbf{q}}_{\parallel} = \frac{1}{\sqrt{n}}(1, \ldots, n), \tag{4.74}$$

since the distance vector is invariant in this direction,

$$P(\mathbf{q} + a\hat{\mathbf{q}}_{\parallel}) - (\mathbf{q} + a\hat{\mathbf{q}}_{\parallel}) = P\mathbf{q} - \mathbf{q} \; + \; a(\underbrace{P\hat{\mathbf{q}}_{\parallel} - \hat{\mathbf{q}}_{\parallel}}_{=0}) = P\mathbf{q} - \mathbf{q}. \tag{4.75}$$

This is the very reason why we introduced the separation into coordinates parallel and perpendicular to the invariant manifolds in the beginning. Also in the case with short range interaction the invariance of propagation along the manifolds is a valuable concept. Thus the normal way to proceed would be to introduce suitable perpendicular coordinates, perform the corresponding lower dimensional integral of the propagator and in the end multiply it by the measure of the invariant manifold. One has to stress that in the interacting case this is most likely the most convenient way to calculate the trace of the propagator. And indeed, one can follow this procedure in the non-interacting case. But the introduction of perpendicular coordinates is rather uncomfortable since naturally one is lead to non-orthogonal coordinate systems and therefore has to introduce a metric tensor and pay extra attention to the arising volume elements. Although the calculation for the free case can be carried out in this manner, we will present an alternative approach in the non-interacting case that is more convenient and straightforward.

For the following analysis, let us assume a minimum cycle length of $n \geq 2$. The trivial case $n = 1$ will be included automatically in the resulting expressions. In the n-dimensional space of particle coordinates corresponding to only one cycle and only one spatial dimension, the subspace of vectors under which the squared distance is invariant is only one-dimensional (there is only one $\hat{\mathbf{q}}_{\parallel}$). Accordingly, the matrix A has exactly one eigenvalue that is vanishing, when we bring the trace (4.72) into the form of a multidimensional Gaussian integral (4.73). Therefore it is sufficient to separate one of the n coordinates, e.g. q_1 and calculate the integral over all others as a generalised multidimensional Gaussian integral with linear term

$$\int \mathrm{d}^m x \; e^{-\frac{1}{2}\mathbf{x}^T A \mathbf{x} + \mathbf{B}^T \mathbf{x}} = \sqrt{\frac{(2\pi)^n}{\det(A)}} \; e^{\frac{1}{2}\mathbf{B}^T A^{-1} \mathbf{B}}. \tag{4.76}$$

The remaining integral $\int \mathrm{d}q_1$ can then be kept and eventually, when merging together all spatial components and cycles, it will automatically produce the measure of $\mathcal{M}_P$ together with the determinant prefactors. Parts of the prefactors

will thereby act as the Jacobian determinant associated with the relation of the volume element of the manifold to the independent coordinates $q_{1,\omega}^{(d)} \quad , d = 1, \ldots, D \, , \omega = 1, \ldots, l$. We abbreviate

$$\alpha = \frac{i}{\hbar} \frac{m}{2t} \tag{4.77}$$

and write (4.72) as

$$\left(-\frac{\alpha}{\pi}\right)^{\frac{n}{2}} \int \mathrm{d}q_1 e^{\alpha \, 2q_1^2} \int \mathrm{d}q_2 \cdots \mathrm{d}q_n \, \exp\left[-\frac{\alpha}{2} \sum_{i,j=1}^{n-1} A_{ij} q_{i+1} q_{j+1} \, + \, \alpha \sum_{i=1}^{n-1} B_i q_{i+1}\right]. \tag{4.78}$$

We identify A and $\mathbf{B}$ by separating all q_1 dependent terms in (4.71):

$$\begin{aligned} |P\mathbf{q} - \mathbf{q}|^2 &= 2q_1^2 + \underbrace{\sum_{i=2}^{n} 2q_i^2 - \sum_{i=2}^{n-1} 2q_i q_{i+1}}_{=-\frac{1}{2}\sum A_{ij} q_{i+1} q_{j+1}} \underbrace{- 2q_1 q_2 - 2q_1 q_n}_{=\sum B_i q_{i+1}} \\ A_{ij} &= -4\left[\delta_{ij} - \frac{1}{2}(\delta_{i,j+1} + \delta_{i+1,j})\right] \\ B_i &= -2q_1(\delta_{i1} + \delta_{i,n+1}) \qquad\qquad i, j = 1, \ldots, n-1. \end{aligned} \tag{4.79}$$

A is a tridiagonal matrix of dimension $n - 1$

$$A = (-4) \cdot \begin{pmatrix} 1 & -\frac{1}{2} & 0 & 0 & \cdots \\ -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & \cdots \\ 0 & -\frac{1}{2} & 1 & -\frac{1}{2} & \\ 0 & 0 & -\frac{1}{2} & \ddots & \ddots \\ \vdots & \vdots & & \ddots & \ddots \end{pmatrix} \tag{4.80}$$

whose inverse is

$$(A^{-1})_{ij} = \begin{cases} -\frac{1}{2} j(1 - \frac{i}{n}) & i \geq j \\ (A^{-1})_{ji} & i < j, \end{cases} \tag{4.81}$$

and whose determinant is

$$\det(A) = n(-2)^{n-1}. \tag{4.82}$$

Using (4.79) and (4.81) we compute

$$\begin{aligned} \mathbf{B}^T A^{-1} \mathbf{B} &= 4q_1^2[(A^{-1})_{11} + (A^{-1})_{1,n-1} + (A^{-1})_{n-1,1} + (A^{-1})_{n-1,n-1}] \\ &= 4q_1^2 \left(-\frac{1}{2n}\right)[n - 1 + 2 + n - 1] \\ &= -4q_1^2. \end{aligned} \tag{4.83}$$

With this and (4.76) the whole integral (4.78) becomes

$$\left(-\frac{\alpha}{\pi}\right)^{\frac{n}{2}} \sqrt{\frac{(2\pi)^{n-1}}{\alpha^{n-1}\det(A)}} \int \mathrm{d}q_1 e^{\alpha\, 2q_1^2}\; e^{\alpha\frac{1}{2}\mathbf{B}^T A^{-1}\mathbf{B}} = \left(-\frac{\alpha}{\pi}\right)^{\frac{1}{2}}\; n^{-\frac{1}{2}} \int \mathrm{d}q_1 \quad (4.84)$$

By collecting all spatial components we get the contribution (4.67) corresponding to a particular cycle

$$\int \mathrm{d}^{nD}q\, K_0((P\mathbf{q})_{I_\omega}, \mathbf{q}_{I_\omega}; t) = \left(-\frac{\alpha}{\pi}\right)^{\frac{D}{2}}\; n^{-\frac{D}{2}} \int\limits_{\Omega} \mathrm{d}^D q_1 = \left(\frac{m}{2\pi\hbar i t}\right)^{\frac{D}{2}}\; N_\omega^{-\frac{D}{2}}\; V_D, \quad (4.85)$$

where we reintroduced the notations $(P\mathbf{q})_{I_\omega}, \mathbf{q}_{I_\omega}$ (see equations (4.24, 4.25)) and $n = N_\omega$ for the length of the particular cycle under investigation. Note that this general form also includes the case of a one-cycle $N_\omega = 1$.

By merging together all traces corresponding to the cycles of one particular permutation we get

$$\int \mathrm{d}^{ND}q\, K_0((P\mathbf{q}), \mathbf{q}; t) = \left(\frac{m}{2\pi\hbar i t}\right)^{\frac{lD}{2}} \left(\prod_{\omega=1}^{l} N_\omega\right)^{-\frac{D}{2}} V_D^l. \quad (4.86)$$

Again, we have an expression associated with a permutation P that is only depending on the partition of N into cycle lengths. Thus we collect all permutations with the same partition in the sum over S_N to write the trace of the symmetry projected propagator (4.66) as

$$\begin{aligned}\int \mathrm{d}^{ND}q\, K_{0,\pm}(\mathbf{q}, \mathbf{q}; t) =& \frac{1}{N!}\sum_{l=1}^{N}(\pm 1)^{N-l} \sum_{\substack{N_1,\ldots,N_l=1 \\ N_1\le\cdots\le N_l}}^{N} \delta_{N,\sum N_\omega}\; c(N_1,\ldots,N_l) \\ &\times \left(\frac{m}{2\pi\hbar i t}\right)^{\frac{lD}{2}} \left(\prod_{\omega=1}^{l} N_\omega\right)^{-\frac{D}{2}} V_D^l.\end{aligned} \quad (4.87)$$

As before, $c(N_1,\ldots,N_l)$ denotes the number of permutations with a cycle decomposition of lengths $N_1,\ldots,N_l$ (4.65). Finally, we have to take the Fourier transform of the trace, as we want to calculate the smooth part of the density of states. Using the Laplace transformation rule

$$\frac{1}{2\pi i}\int\limits_{\epsilon-i\infty}^{\epsilon+i\infty} \mathrm{d}\tau\, \frac{\Gamma(\nu)}{\tau^\nu}\, e^{\tau x} = x^{\nu-1} \qquad \nu > 0 \quad (4.88)$$

for $\tau = it$, $x = E/\hbar$ and $\nu = lD/2$, the final result for the smooth part of the symmetry projected density of states for a system of N identical bosons $(+)$ or fermions $(-)$ in a D-dimensional billiard of volume V_D reads

$$\begin{aligned}\bar{\rho}_{\mathrm{scl},\pm} =& \frac{1}{N!}\sum_{l=1}^{N}(\pm 1)^{N-l}\sum_{\substack{N_1,\ldots,N_l=1\\ N_1\leq\cdots\leq N_l}}^{N}\delta_{N,\sum N_\omega}\;\; c(N_1,\ldots,N_l)\\ &\times\;\left(\frac{m}{2\pi\hbar^2}\right)^{\frac{lD}{2}}\left(\prod_{\omega=1}^{l}\frac{1}{N_\omega}\right)^{\frac{D}{2}}\;V_D^l\;\frac{E^{\frac{lD}{2}-1}}{\Gamma\left(\frac{lD}{2}\right)}\,\theta(E).\end{aligned} \tag{4.89}$$

In general (4.89) is a sum of powers of E with coefficients that are, besides their dependence on the billiard volume, expressed as sums over partitions $N = N_1 + \cdots + N_l$ only depending on the parts N_ω. The relevant partitions of a particular coefficient are restricted to a particular number of parts l. So we see that these coefficients are not system specific but instead universal. The highest power in the sum has the exponent $(ND)/2 - 1$, which we recognise as the power of E appearing in the Thomas-Fermi approximation (2.77) or equivalently the naive volume term (see section 4.1). This is not surprising, since the highest power is related to the value $l = N$, meaning a partition of N into unities $N = 1 + \cdots + 1$ that is corresponding to permutations P with a decomposition into one-cycles. There is only one such permutation, namely the identity $1_{S_N} = (1)(2)\cdots(N)$. In the geometrical picture, this corresponds to the propagation of individual particles. None of them are clustered. The corresponding term in (4.89) can easily be calculated. The combinatorial factor is (see (4.65))

$$c(1,\ldots,1)) = N!\,\left(\prod_{\omega=1}^{l}\frac{1}{N_\omega}\right)\left(\prod_{n=1}^{N}\frac{1}{m_n!}\right) = N!\cdot 1\cdot\frac{1}{N!} = 1, \tag{4.90}$$

since all parts N_ω are unity and this cycle length appears with multiplicity $m_1 = N$. So the highest order term in E reads

$$\frac{1}{N!}\left(\frac{m}{2\pi\hbar^2}\right)^{\frac{ND}{2}}\;V_D^N\;\frac{E^{\frac{ND}{2}-1}}{\Gamma\left(\frac{ND}{2}\right)}\,\theta(E) = \bar{\rho}_{\mathrm{v}}(E) = \frac{1}{N!}\bar{\rho}_{\mathrm{TF}}(E). \tag{4.91}$$

Confirmation Of The Smoothed Convolution Formula

Before we turn into analysing formula (4.89) and its consequences one should point out that it is indeed equivalent to the convolution of single particle densities (4.32) using the Weyl volume terms for the single particle densities instead of the exact ones. In section 4.2 we argued that it is not clear whether this process is producing useful results or not. But in this subsection we want to derive the corresponding convolution for a D-dimensional billiard system since

we have now the semiclassical result (4.89) at hand and are therefore able to compare both in order to evaluate the convolution.

The single particle Weyl volume term reads

$$\bar{\rho}_0(E) = \left(\frac{m}{2\pi\hbar^2}\right)^{\frac{D}{2}} \; V_D \, \frac{E^{\frac{D}{2}-1}}{\Gamma\left(\frac{D}{2}\right)} \, \theta(E) \equiv c \, E^{\frac{D}{2}-1} \, \theta(E) \tag{4.92}$$

Using (4.32) we get the sum

$$\bar{\rho}_{\mathrm{conv},\pm}(E) = \frac{1}{N!} \sum_{l=1}^{N} (\pm 1)^{N-l} \sum_{\substack{N_1,\ldots,N_l=1 \\ N_1 \leq \cdots \leq N_l}}^{N} \delta_{N,\sum N_\omega} \; c(N_1,\ldots,N_l) \left[\prod_{\omega=1}^{l} \frac{1}{N_\omega}\right] \; \mathcal{C}(E) \tag{4.93}$$

of convolutions $\mathcal{C}(E)$ of the form

$$\begin{aligned} \mathcal{C}(E) &= \int \mathrm{d}E_1 \ldots \mathrm{d}E_l \; \left[\prod_{\omega=1}^{l} \bar{\rho}_0\left(\frac{E_\omega}{N_\omega}\right)\right] \; \delta\left(E - \sum_{\omega=1}^{l} E_i\right) \\ &= c^l \, \frac{\partial}{\partial E} \underbrace{\int \mathrm{d}E_1 \ldots \mathrm{d}E_l \; \left[\prod_{\omega=1}^{l} \left(\frac{E_\omega}{N_\omega}\right)^{\frac{D}{2}-1} \theta(E_\omega)\right] \; \theta\left(E - \sum_{\omega=1}^{l} E_\omega\right)}_{=:\, \mathcal{I}(E)} . \end{aligned} \tag{4.94}$$

We can now calculate the integral by successively performing the integrals of single particle energies and solving an emerging recursion relation. First, we separate a factor containing all N_ω.

$$\mathcal{I}(E) = \left[\prod_{\omega=1}^{l} \frac{1}{N_\omega}\right]^{\frac{D}{2}-1} \; \int_0^\infty \mathrm{d}E_1 \ldots \mathrm{d}E_l \; \prod_{\omega=1}^{l} E_\omega^{\frac{D}{2}-1} \; \theta\left(E - \sum_{\omega=1}^{l} E_\omega\right) . \tag{4.95}$$

We write $r = D/2 - 1$ and define a new variable for the energy to be distributed among the first n particles for every n

$$e_n = E - \sum_{\omega=n+1}^{l} E_\omega, \qquad\qquad n = 0, \ldots, l-1. \tag{4.96}$$

The first step in the integral of $\mathcal{I}(E)$ is then

$$\begin{aligned} \int_0^\infty \mathrm{d}E_1 E_1^r \theta(e_1 - E_1) &= \frac{1}{r+1} e_1^{r+1} \theta(e_1) \\ &= \frac{1}{r+1} (e_2 - E_2)^{r+1} \theta(e_2 - E_2). \end{aligned} \tag{4.97}$$

The next integral over E_2 is of the form

$$\int_0^a \mathrm{d}x\; x^r\,(a-x)^s\theta(a) = a^{s+r+1}\frac{\Gamma(1+r)\Gamma(1+s)}{\Gamma(2+r+s)}\theta(a) \tag{4.98}$$

with $a = e_2 = e_3 - E_3$. Therefore, also the third integral and all others are of this form. We define A_n as the total prefactor and s_n as the exponent s in (4.98) appearing in the n-th integral step. Therefore we get the recurrence relation

$$\begin{aligned} A_1 &= 1 \\ s_1 &= 0 \\ A_{n+1} &= A_n\frac{\Gamma(1+r)\Gamma(1+s_n)}{\Gamma(2+r+s_n)} \\ s_{n+1} &= r + s_n + 1. \end{aligned} \tag{4.99}$$

The solution of the recurrence reinserting $r = D/2 - 1$ is

$$\begin{aligned} A_{n+1} &= \frac{\left[\Gamma\left(\frac{D}{2}\right)\right]^n}{\Gamma\left(\frac{nD}{2}+1\right)} \\ s_{n+1} &= \frac{nD}{2} \qquad\qquad n \geq 0. \end{aligned} \tag{4.100}$$

The total integral in $\mathcal{I}(E)$ reads

$$A_{l+1}\,E^{s_{l+1}}\,\theta(E). \tag{4.101}$$

Now we are only left with the task of differentiating to obtain

$$\mathcal{C}(E) = \left[\prod_{\omega=1}^{l}\frac{1}{N_\omega}\right]^{\frac{D}{2}-1} c^l\,A_{l+1}\,s_{l+1}\,E^{s_{l+1}-1}\theta(E). \tag{4.102}$$

Using the recurrence solution and the definition of c we get the final result

$$\begin{aligned} \bar{\rho}_{\mathrm{conv},\pm}(E) =& \frac{1}{N!}\sum_{l=1}^{N}(\pm 1)^{N-l}\sum_{\substack{N_1,\ldots,N_l=1\\ N_1\leq\cdots\leq N_l}}^{N}\delta_{N,\sum N_\omega}\;\; c(N_1,\ldots,N_l) \\ &\times\;\left(\frac{m}{2\pi\hbar^2}\right)^{\frac{lD}{2}}\left(\prod_{\omega=1}^{l}\frac{1}{N_\omega}\right)^{\frac{D}{2}}\;\; V_D^l\;\frac{E^{\frac{lD}{2}-1}}{\Gamma\left(\frac{lD}{2}\right)}\,\theta(E) = \bar{\rho}_{\mathrm{scl},\pm}(E). \end{aligned} \tag{4.103}$$

So, we see now that indeed the convolution of smooth single particle densities gives the same result as the semiclassical Weyl expansion. Therefore we will from now on omit the subscripts scl and conv. The usage of the volume term in the single particle Weyl expansion is thereby consistent with neglecting of

single particle billiard boundaries in the calculation of short path propagations. This gives rise to the question whether it is possible to relate corrections from propagation in cluster zones to the correction of delta peaks that is inherent to the exact convolution formula (4.32) of Weidenmüller. And indeed one can relate each cluster zone correction to the correction of delta peaks for total energies. The corrected total energy is the energy that is a partition of single particle energies just the way the cluster zone corresponds to a partition of all particles into clusters. The cluster zone correction is associated to the correction of the total energy that is built of single particle energies, where all particles in a cluster share the same energy. A more careful treatment of this statement is left for future discussions.

Utilisation In Two Dimensions

As often in the context of semiclassics the case of a two-dimensional billiard is of special interest. On the one hand, this is because of possible technical applications. We think of confined two dimensional electron gases in semiconductor hetero structures or two-dimensional superconducting structures with bosonic description due to Cooper pairing for example. On the other hand, the existence of equally distributed energies in a $2D$ single particle billiard is a valuable special feature. This is not only because of the exceptionally simple form that the density of states takes in these systems. The constantness of the single particle smooth part also opens the possibility to make connections to number theory. Namely approximations for average distributions of partitions of integers can be related, as we will see in the next section.

In two dimensions the density of states and reads

$$\bar{\rho}_{\pm}(E) = \bar{\rho}_0 \sum_{l=1}^{N} (\pm 1)^{N-l} \, S_l \frac{(\bar{\rho}_0 E)^{l-1}}{(l-1)!} \, \theta(E), \tag{4.104}$$

its integral is the level counting function

$$\bar{\mathcal{N}}_{\pm}(E) = \sum_{l=1}^{N} (\pm 1)^{N-l} \, S_l \frac{(\bar{\rho}_0 E)^{l}}{l!} \, \theta(E), \tag{4.105}$$

with the constant single particle Weyl volume term

$$\bar{\rho}_0 \cdot \theta(E) \equiv \bar{\rho}_{\mathrm{v}}^{(\mathrm{SP})}(E) = \frac{A}{4\pi} \left(\frac{2m}{\hbar^2} \right) \theta(E), \tag{4.106}$$

and the system-independent purely combinatorial universal constants

$$S_l = \frac{1}{N!} \sum_{\substack{N_1,\ldots,N_l=1 \\ N_1 \leq \cdots \leq N_l}}^{N} \delta_{N,\sum N_\omega} \; c(N_1,\ldots,N_l) \prod_{\omega=1}^{l} \frac{1}{N_\omega}. \tag{4.107}$$

We insert the explicit form of the combinatorial factors $c(N_1, \ldots, N_l)$ (see (4.65)) and rewrite the sum over partitions in an unordered manner by dropping the restriction $N_1 \leq \cdots \leq N_l$ and dividing by $l!$ in order to get rid of the inconvenient multiplicity factors in (4.65). In terms of ordered partitions, the factor reads

$$S_l = \sum_{\substack{N_1,\ldots,N_l=1 \\ N_1 \leq \cdots \leq N_l}}^{N} \delta_{N,\sum N_\omega} \prod_{\omega=1}^{l} \frac{1}{N_\omega^2} \prod_{n=1}^{N} \frac{1}{m_n!}, \tag{4.108}$$

whereas in terms of unordered partitions, without multiplicities, it reads

$$S_l = \frac{1}{l!} \sum_{N_1,\ldots,N_l=1}^{N} \delta_{N,\sum N_\omega} \prod_{\omega=1}^{l} \frac{1}{N_\omega^2}. \tag{4.109}$$

We see that for positive arguments the density is a polynomial of degree $N-1$ in the energy. If we measure energy in units of the single particle mean level spacing and the density in units of the single particle mean density, the coefficients of the polynomials are just rational numbers

$$\frac{1}{\bar{\rho}_0} \bar{\rho}_\pm \left(\frac{\epsilon}{\bar{\rho}_0} \right) = \sum_{l=1}^{N} (\pm 1)^{N-l} \frac{S_l}{(l-1)!} \epsilon^{l-1} \theta(\epsilon), \tag{4.110}$$

$$\bar{\mathcal{N}}_\pm \left(\frac{\epsilon}{\bar{\rho}_0} \right) = \sum_{l=1}^{N} (\pm 1)^{N-l} \frac{S_l}{l!} \epsilon^{l} \theta(\epsilon), \tag{4.111}$$

So far, the author has not found a way to give simple expressions for the values of S_l. A few attempts to simplify, reformulate or approximate the expressions will be listed in the following sections. Nonetheless, the S_l can be summed up exactly for explicit values of N and l albeit with computation time increasing very strongly with N when using the form at hand (4.108) or (4.109). Note that the form (4.108) in terms of ordered partitions corresponds to less computation time while the form (4.109) seems to be a better starting point for simplifications or analytical calculations.

The Reproduction Of The Ground State Energy

For the time being let us examine the behaviour of $\bar{\rho}_\pm(E)$ by giving the explicit polynomials based on computer-assisted calculations of the factors S_l. Figure 4.6 shows the case of two particles. The bosonic and fermionic cases are shown in comparison to the naive volume term. We see already here, that the symmetry corrections give qualitatively the right picture. With respect to the naive

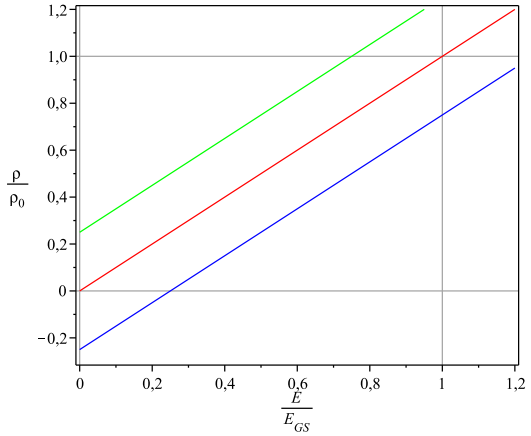
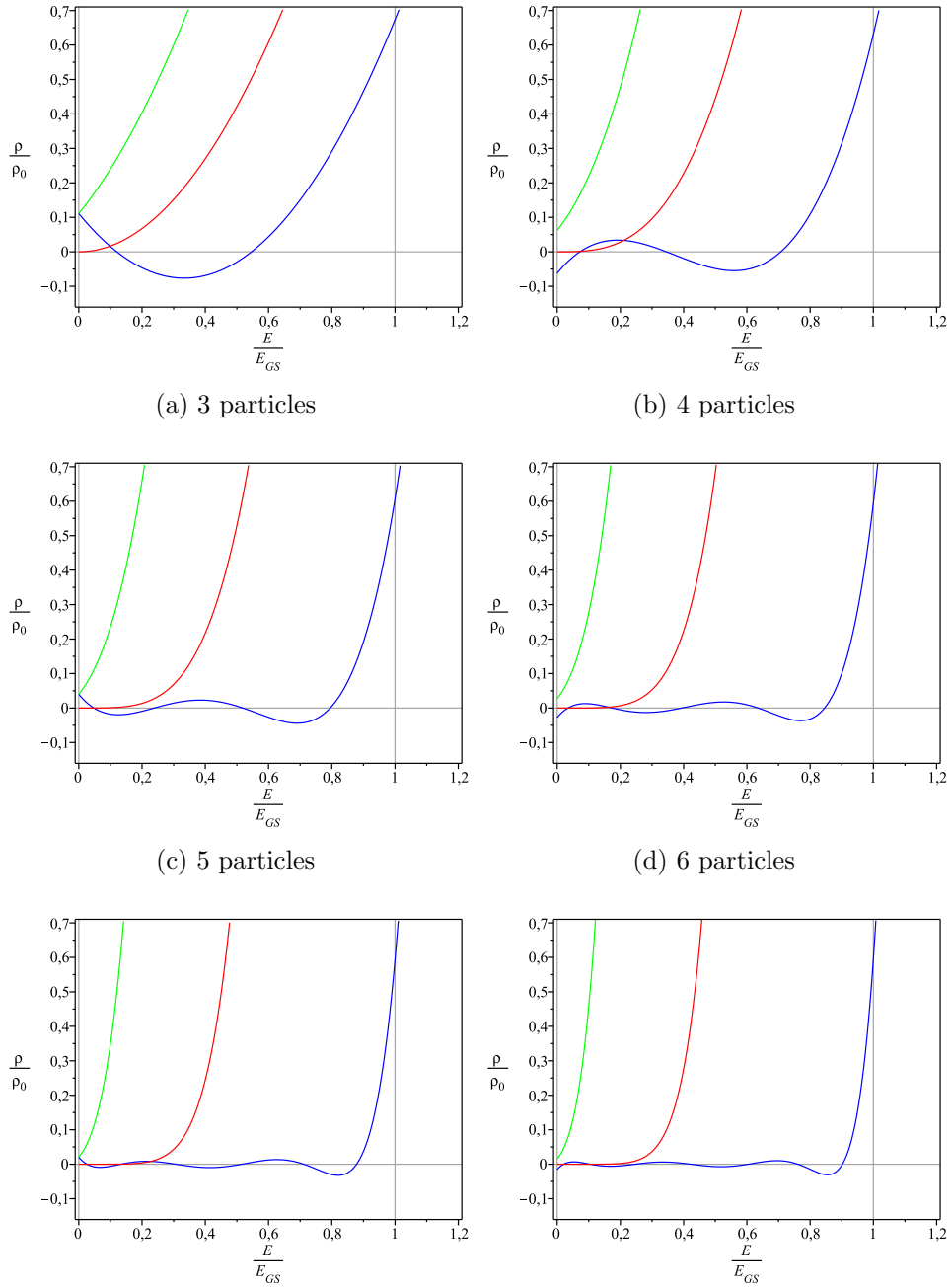


Figure 4.6: symmetry projected density of states in two dimensions for two bosons (green) and two fermions (blue) in comparison to the naive volume term (red). Energy is measured in units of the expected many body ground state energy $E_{\mathrm{GS}}^{(\mathrm{f})}$ for fermions (4.9). Densities ρ are measured in units of the constant single particle density ρ_0.

term, the fermionic density is shifted to higher energies, which is according to the expectation of the many body ground state energy below which effectively no level should appear. Whereas the bosonic density is shifted to lower energies, which accords to the full counting of many body levels corresponding to shared single particle energies in contrast to the naive term (see section 4.2).

Figure 4.7 shows the cases of three to eight particles. We see that in the fermionic case the lower powers in E in the polynomial produce oscillations around the axis $\bar{\rho} = 0$. With increasing particle number these oscillations get smaller in amplitude and larger in frequency. An energy gap opens. The density is effectively shifted to higher energies. The energy gap coincides with the fermionic ground state energy $E_{\mathrm{GS}}^{(\mathrm{f})}$ calculated by counting single particle levels by virtue of the smooth single particle density (4.9). But instead of explicitly filling up single particle energy levels by hand, this time the ground state energy occurs as a consequence out of exchange symmetry incorporated as a modification of the propagator. The corrections from cluster zone propagations are sufficient to automatically reproduce the expected ground state energy. The symmetry projected density at the expected ground state energy keeps moderate values $\bar{\rho}_-(E_{\mathrm{GS}}^{(\mathrm{f})}) \approx \mathcal{O}(1)$ while the naive density at this energy grows exponentially (see section 4.1). In contrast to the fermionic density, the bosonic density does not have these oscillations. The polynomial in E has only positive coefficients. The density is effectively shifted to lower energies as expected intuitively.



(a) 3 particles

(b) 4 particles

(c) 5 particles

(d) 6 particles

(e) 7 particles

(f) 8 particles

Figure 4.7: symmetry-projected density of states in two dimensions for bosons (green) and fermions (blue) in comparison to the naive volume term (red) for three to eight particles. Energy is measured in units of the particular expected many body ground state energy $E_{\mathrm{GS}}^{(\mathrm{f})}$ for fermions (4.9). Densities ρ are measured in units of the constant single particle density ρ_0.

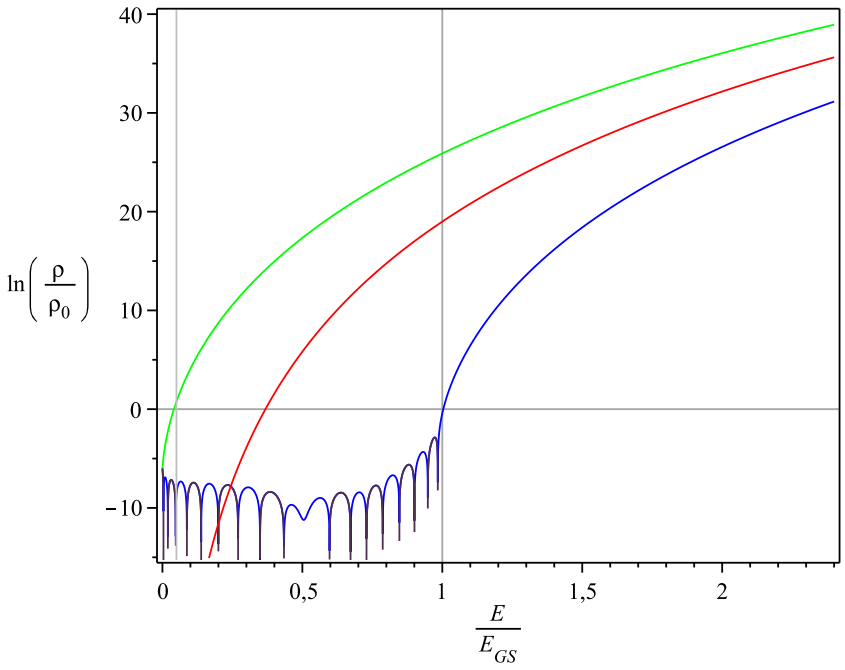


Figure 4.8: symmetry-projected density of states in two dimensions for bosons (green) and fermions (blue) in comparison to the naive volume term (red) for $N = 20$ particles. The densities ρ, measured in units of the constant single particle density ρ_0, are plotted logarithmically. Negative values of the fermionic density are plotted as logarithm of its absolute value (violet). Energy is measured in units of the particular expected many body ground state energy $E_{\mathrm{GS}}^{(\mathrm{f})}$ for fermions (4.9). The expected bosonic ground state is represented by the left vertical grey line.

When we go to higher particle numbers we have to plot $\bar{\rho}$ in a logarithmic scale in order to see at the same time the oscillations that are becoming very small and the growth behaviour around and above the ground state energy which is becoming very strong. Figure 4.8 shows the smooth part of the density in the case of $N = 20$ particles. Again the fermionic energy gap accurately reproduces the ground state energy, indicated by crossing the axis of abscissa. Also in the bosonic case, the corresponding density $\bar{\rho}_+(E)$ apparently keeps moderate values at the expected bosonic ground state energy $E_{\mathrm{GS}}^{(\mathrm{b})}$.

The definition of $E_{\mathrm{GS}}^{(\mathrm{b})}$ used here is in complete analogue with the definition of the fermionic $E_{\mathrm{GS}}^{(\mathrm{f})}$. This means, by virtue of single particle level counting in a smoothed manner. Each boson is supposed to fill up the lowest possible energy level. Thus, using the smooth density, it occupies the energy interval from 0 up

to E_1 defined by

$$\int_0^{E_1} \mathrm{d}E\ \bar{\rho}_0 = 1. \tag{4.112}$$

The energy associated with the boson is then

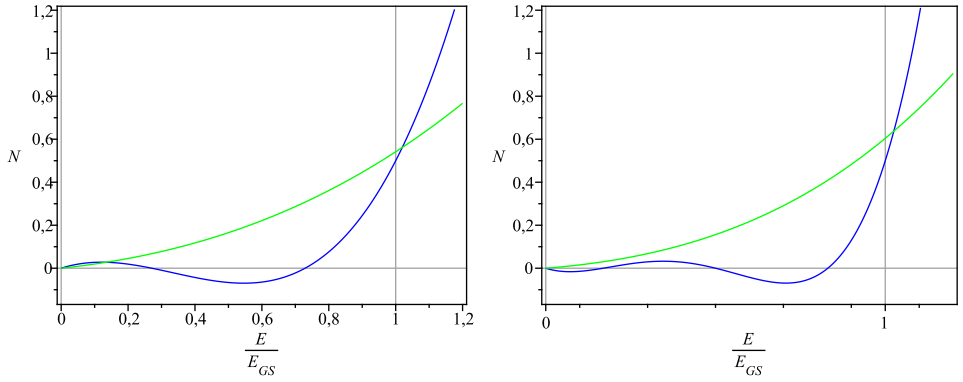
$$\int_0^{E_1} \mathrm{d}E\ \bar{\rho}_0\, E = \frac{\bar{\rho}_0\, E_1^2}{2} = \frac{1}{2}\bar{\rho}_0^{-1}. \tag{4.113}$$

The total energy of N bosons in the ground state is then

$$E_{\mathrm{GS}}^{(\mathrm{b})} = \frac{N}{2}\bar{\rho}_0^{-1}. \tag{4.114}$$

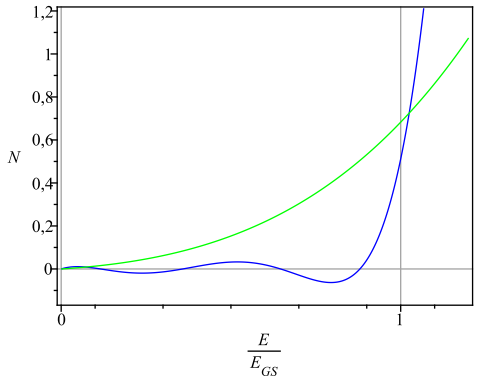
In order to check whether the behaviour of the symmetry projected densities is producing the correct ground state energy, one should actually rather regard the corresponding values of the level counting function around this energy, since it will tell us the number of many body levels we effectively produce up to the ground state energy. Figure 4.9 shows the smooth part of the symmetry projected level counting functions for three to eight particles. In contrast to the plots of the densities, we use a different energy scale for fermions and bosons. Namely, the corresponding energies are measured in units of the individual ground state energies associated with the particular type of exchange symmetry.

We see that also the level counting functions keep moderate values at the particular expected ground state energies. In order to get a picture that this behaviour also is manifest for higher particle numbers, figure 4.10 shows a logarithmic plot of the level counting functions for twenty particles. Also here, the expected ground state energies are reproduced. The crossing of the axis of abscissa in a sense indicates the produced ground state energy, since the level density produces exactly one state up to this energy. So indeed, $\bar{\rho}_\pm$ effectively does not produce energy levels below the particular ground state energy $E_{\mathrm{GS}}^{(\mathrm{b})}$ respectively $E_{\mathrm{GS}}^{(\mathrm{f})}$.

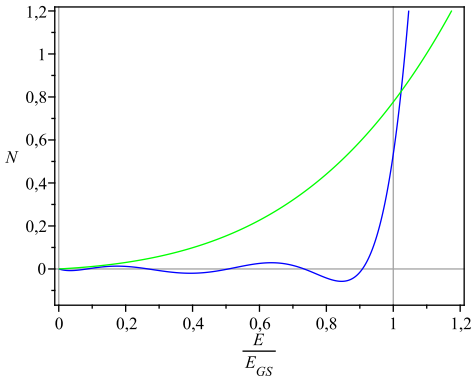


(a) 3 particles

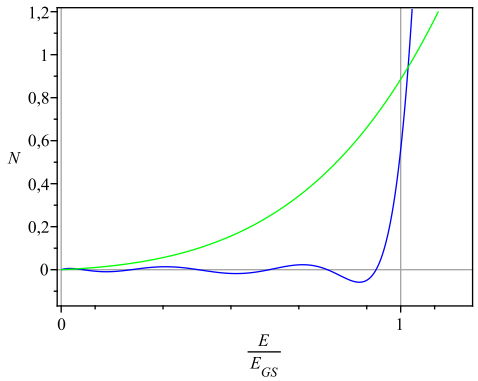
(b) 4 particles



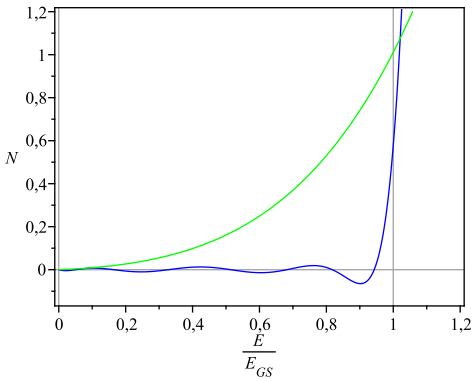
(c) 5 particles



(d) 6 particles



(e) 7 particles



(f) 8 particles

Figure 4.9: symmetry projected level counting function in two dimensions for bosons (green) and fermions (blue) for three to eight particles. Energy is measured in units of the particular expected many body ground state energy $E_{\mathrm{GS}}^{(\mathrm{f})}$ for fermions and $E_{\mathrm{GS}}^{(\mathrm{b})}$ for bosons.

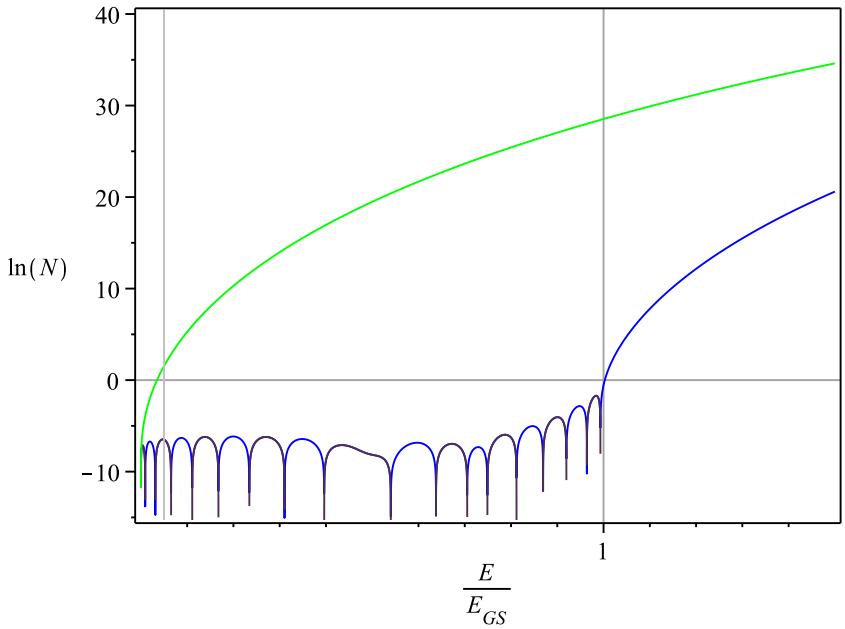
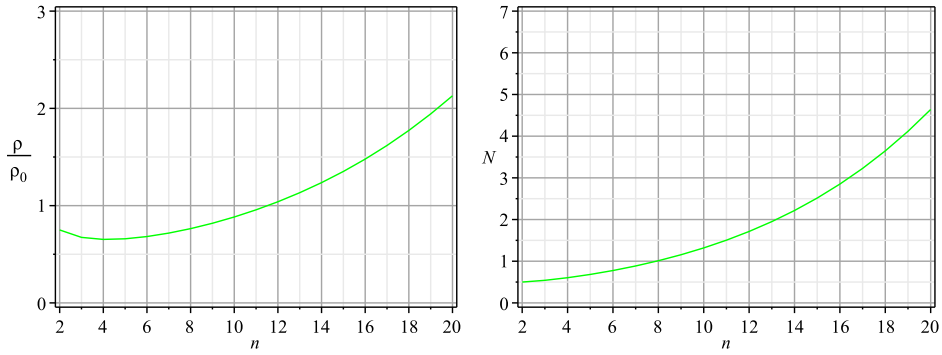
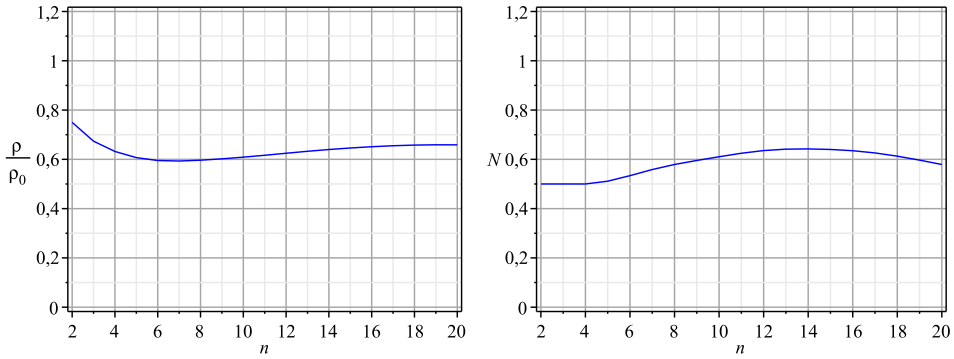


Figure 4.10: symmetry-projected level counting function in two dimensions for bosons (green) and fermions (blue). The level counting functions are plotted logarithmically. Negative values of the fermionic function are plotted as logarithm of its absolute value (violet). Energy is measured in units of the expected many body ground state energy $E_{\mathrm{GS}}^{(\mathrm{f})}$ for fermions (4.9). The expected bosonic ground state is represented by the left vertical grey line.



(a) $\bar{\rho}_+(E^{(\mathrm{b})}_{\mathrm{GS}})$: bosons (b) $\bar{\mathcal{N}}_+(E^{(\mathrm{b})}_{\mathrm{GS}})$: bosons



(c) $\bar{\rho}_-(E^{(\mathrm{f})}_{\mathrm{GS}})$: fermions (d) $\bar{\mathcal{N}}_-(E^{(\mathrm{f})}_{\mathrm{GS}})$: fermions

Figure 4.11: Density of states and level counting function at particular ground state energy in dependence on the number of particles, which in this figure is denoted by n to provide distinguishability with respect to the level counting function denoted by N in the plots.

To see this behaviour for different particle numbers in a more compact way, figures 4.11a, 4.11b, 4.11c and 4.11d show the quantities $\bar{\rho}_\pm$ and $\bar{\mathcal{N}}_\pm$ at the ground state energies associated with the particular symmetry in dependence on the particle number.

Large Cancellations

One might guess that only the highest orders in E in the polynomials (4.110) and (4.110) are relevant. Therefore, we want to analyse the relative importance of different contributions in the fermionic level density. For this purpose we take the level density of twenty fermions at ground state energy and separate all contributions corresponding to the particular powers in E. Denote these

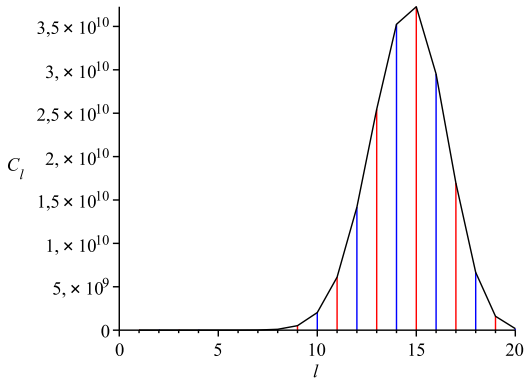


Figure 4.12: Contributions to the ground state value of the level density in a two-dimensional billiard of twenty fermions. Each contribution corresponds to a particular term in the polynomial in E. Plotted are the absolute values, while the signs are indicated by the vertical red (negative) and blue (positive) lines

contributions by C_l

$$\frac{1}{\bar{\rho}_0}\,\bar{\rho}_-(E) = \sum_{l=1}^{N}(-1)^{N-l}C_l\,\left(\frac{E}{E_{\mathrm{GS}}^{(\mathrm{f})}}\right)^{l-1}\theta(E). \tag{4.115}$$

Figure 4.12 shows the contributions C_l for $l = 1..20$. The contribution C_{20} corresponds to the permutation $1_{S_{20}}$ and equals the naive volume term evaluated at the ground state energy. It corresponds to the rightmost point in the graph. So we see that many of the other powers in E yield contributions at the ground state energy that are even of larger order of magnitude. This is not restricted to the highest values of l. From figure 4.12 we already see that at least down to a l-value of approximately 9 the contributions are at least equal in order of magnitude to the naive contribution. Since the contributions to the density come with alternating sign, the signs associated with the particular C_l are indicated by red and blue vertical lines. The naive contribution already has a huge value of

$$\frac{\bar{\rho}_{\mathrm{v}}(E_{\mathrm{GS}}^{(\mathrm{f})})}{\bar{\rho}_0} = C_{20} \approx 1.8 \times 10^8. \tag{4.116}$$

But the sum of all the large contributions with alternating signs in the end yields a value of

$$\frac{1}{\bar{\rho}_0}\,\bar{\rho}_-(E_{\mathrm{GS}}^{(\mathrm{f})}) = \sum_{l=1}^{N}(-1)^{N-l}C_l \approx 0.66 \qquad ! \tag{4.117}$$

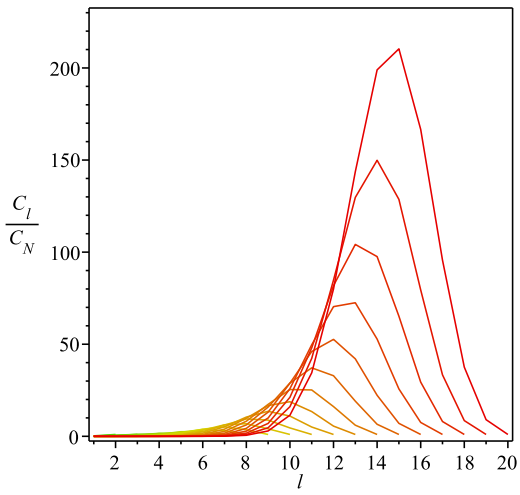
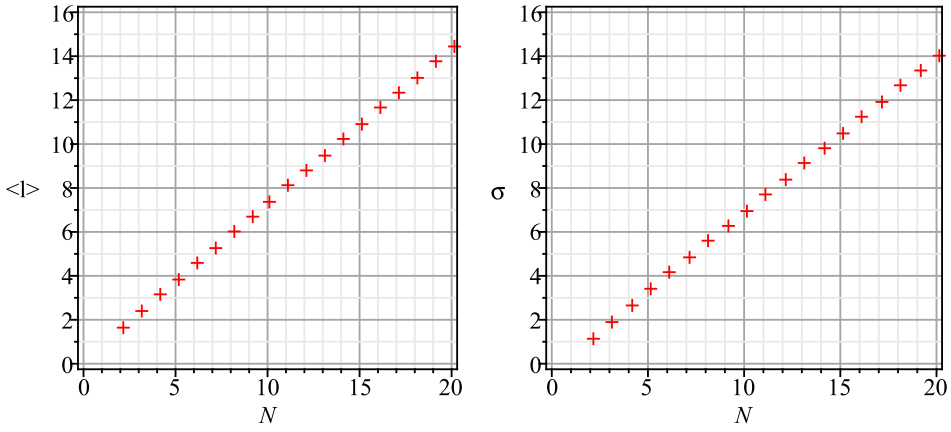


Figure 4.13: Contributions C_l to the ground state value of the level density for two to twenty fermions. $N = 2$ corresponds to leftmost curve (light green), $N = 20$ corresponds to the rightmost curve (red). To allow the comparison, all graphs are normed by their value C_N at highest abscissa $l = N$

So, we see that there are large cancellations involved to produce the right behaviour. Omitting any of the summands of the polynomial will completely destroy the right behaviour of the level density. One probably really needs all of them for a sufficient description of the system. In order to check whether and how the relative importance of particular contributions C_l is affected by varying the particle number, we want to compare the C_l distributions for different values of N. Therefore, figure 4.13 shows all C_l-graphs from 2 to 20 particles. All C_l distributions seem to have similar shape with their maximum and width increasing with particle number. So it seems that the relative importance of C_l is proportionally distributed among the l-values in a similar way for all particle numbers. To substantiate this statement a bit more, figures 4.14a and 4.14b are showing the expectation value (4.118) and standard deviation (4.119) of l under the C_l distributions in dependence on the particle number N,



(a) expectation value of l (b) standard deviation of l

Figure 4.14: mean value $\bar{l}$ and standard deviation σ_l of l under the distributions C_l in dependence on the particle number N.

$$\bar{l} = \langle l \rangle = \frac{\sum_{l=1}^{N} l\, C_l}{\sum_{l=1}^{N} C_l}, \tag{4.118}$$

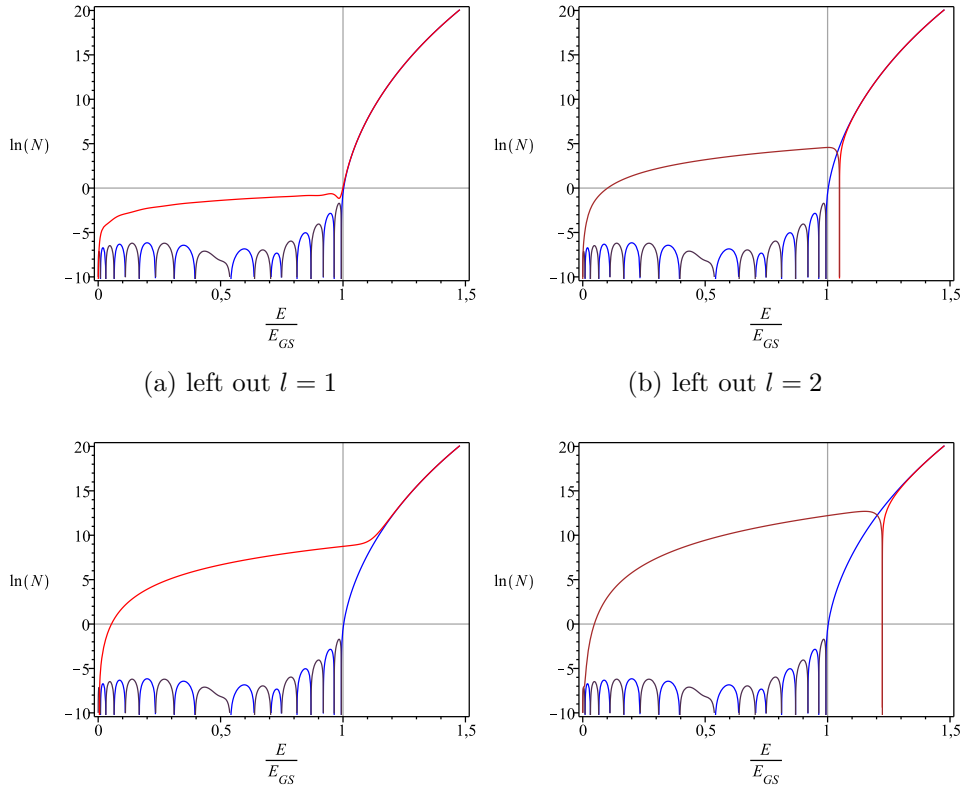
$$\sigma_l = \sqrt{\langle l^2 \rangle - \langle l \rangle^2} = \sqrt{\frac{\sum_{l=1}^{N} l^2\, C_l}{\sum_{l=1}^{N} C_l} - \bar{l}^2} \tag{4.119}$$

The mean value and standard deviation of l seem both to grow linearly with N

$$\begin{aligned} \bar{l} &\approx 0.38 + 0.71 \cdot N \\ \sigma_l &\approx -0.17 + 0.72 \cdot N, \end{aligned} \tag{4.120}$$

which substantiates that the C_l distributions are of similar shape and therefore implies that also for higher numbers of particles , the relative importance of the contributions associated with l remains.

Since the values of C_l get smaller at the lower end of the l axis, it is not clear, if probably the lowest contributions could be omitted without a big failure in the ground state behaviour. But it turns out that this is not the case. To make this point clear, we just try and exemplarily leave out the contribution of a rather small l-value. For this purpose let us take the system of $N = 20$ fermions and look at the level counting function when leaving out one of the contributions $l = 1, \ldots, 4$. The corresponding graphs are shown in figure 4.15. For the case



(a) left out $l = 1$ (b) left out $l = 2$

(c) left out $l = 3$ (d) left out $l = 4$

Figure 4.15: symmetry projected level counting function $\bar{\mathcal{N}}_-$ in two dimensions for $N = 20$ fermions. Ordinates are plotted logarithmically. In order to see negative values, the logarithm is taken of the absolute value of the function. The blue line shows the actual smooth part of the level counting function (negative values are plotted in violet), while the red line shows the wrong results produced by leaving out particular contributions associated with l (negative values are plotted in dark red).

of leaving out only the lowest order contribution $l = 1$ linear in energy (fig. 4.15a), the incomplete graph still crosses the axis of abscissa, meaning that the corresponding density effectively produces one state up to the ground state energy. But in contrast to the complete function, where oscillations of very small amplitude indicate the absence of any effective level below $E_{\mathrm{GS}}^{(f)}$, the incomplete level counting function counts a non-negligible partial energy level already at energies way below $E_{\mathrm{GS}}^{(f)}$. This means the incomplete density produces part of the first level below the ground state distributed over a large energy interval. Which makes it rather useless for applications crucially depending on its behaviour around and also slight below the ground state energy. Proceeding to higher l-values of left out contributions (fig. 4.15b - 4.15d), we see immediately that the correct reproduction of the ground state energy is completely absent, although the curves become asymptotically equal for higher energies, just as expected. In figures 4.15b and 4.15d a crossing of the value $\bar{\mathcal{N}} = 1$ is still existent, even though the corresponding energy deviates from the correct ground state energy. Up to this energy, a large negative number of levels is produced which is then compensated by positive levels within a small energy interval around the deviated ground state energy. So this behaviour is unphysical and improper for any application depending on the behaviour around the ground state.

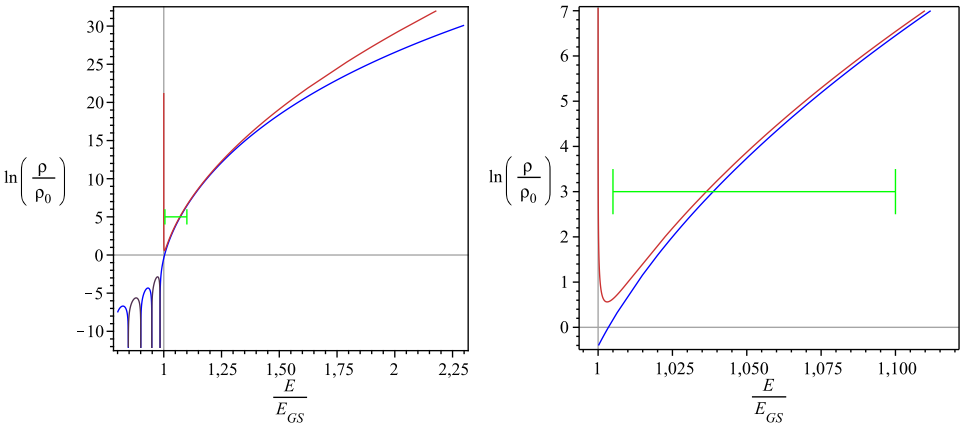
To close this subsection we finally will compare the results for fermions with an asymptotic approximation of the many body density of states in terms of the excitation energy. The speak is of the *Bethe estimate* which was already formulated in 1936 [18].

The Bethe Estimate

Based on thermodynamical calculations of the partition function incorporating the Fermi-Dirac distribution, Hans Bethe [5] calculated an approximation $\bar{\rho}_{\mathrm{Bethe}}$ to the smooth part of the density of states for fermions moving in a mean field, effectively dealing with non-interacting fermions, which makes it possible to compare it with our result. The approximation is asymptotically valid in the limit of large particle numbers $N \to \infty$ and has a restricted range of excitation energies for which it is good. The Bethe approximation reads

$$\bar{\rho}_{-}(E) \approx \bar{\rho}_{\mathrm{Bethe}}(Q) = \frac{1}{\sqrt{48}Q} \exp \sqrt{\frac{2}{3}\pi^2 \bar{\rho}_0 Q}, \tag{4.121}$$

where Q denotes the many body excitation energy. Note that the Bethe estimate is purely depending on the excitation energy instead of the total energy. Thus it is not providing a ground state energy. In order to give an expression fully comparable with our result for the level density in terms of the total energy E, one has to artificially include a ground state energy by setting $Q = E - E_{\mathrm{GS}}$. In (4.121), $\bar{\rho}_0$ denotes the single particle mean density of states at the Fermi energy $\bar{\rho}_0(E_{\mathrm{F}})$. (4.121) is supposed to be approximately valid when restricted



(a) deviation at high energies (b) range of validity

Figure 4.16: Comparison of the semiclassical smooth part of the density of states (blue) with the Bethe estimate (red) for a system of $N = 20$ fermions. The green bar indicates the range of validity of the Bethe estimate.

to excitations that are larger than the mean level spacing $Q \gg \bar{\rho}_0^{-1}$ and much smaller than the Fermi energy $Q \ll E_F$.

In order to compare our result for the smooth part of the symmetry projected density of states with the Bethe estimate, we use the ground state $E_{\mathrm{GS}}^{(\mathrm{f})}$ calculated out of smoothly counting single particle levels, which we confirmed to be consistent with our result for $\bar{\rho}_{\pm}(E)$ in the last subsection.

Figures 4.16a and 4.16b show that we have good agreement in the range of validity. For higher energies, the approximation of Bethe deviates from the actual semiclassical smooth part. In a number theoretical context [18], this deviation can also be related to the difference between unrestricted and restricted integer partitions, that becomes more and more significant for increasing integers while keeping constant restriction. For a further discussion on that, the reader may be referred to the appropriate subsection. Before going into that, let us list a few attempts to investigate the prefactors S_l analytically.

Some Suggestions For Analytical Investigation Of S_l

As many objects expressed in terms of sums over partitions, also the quantity S_l (4.109) can be investigated by virtue of the concept of *generating functions*. The factors S_l (4.109) can be expressed as derivatives of a generating function. This generating function is the l-th power of the dilogarithm, as we see using

its power series definition

$$\mathrm{Li}_2(y)^l = \left[\sum_{n=1}^{\infty} \frac{y^n}{n^2}\right]^l = \ldots + y^N \cdot \sum_{N_1,\ldots,N_l=1}^{N} \delta_{N,\sum N_\omega} \prod_{\omega=1}^{l} \frac{1}{N_\omega^2} + \ldots, \tag{4.122}$$

so that

$$S_l = \frac{1}{l!N!} \frac{\mathrm{d}^N}{\mathrm{d}y^N} \left[\mathrm{Li}_2(y)\right]^l \Big|_{y=0}. \tag{4.123}$$

On the one hand, (4.123) could be a good starting point to find recurrence relations for S_l in terms of all other S_l with lower values of l and lower values of N. This is passed to future investigations. On the other hand, we can simply plug this definition of S_l in the smooth density (4.110) to obtain

$$\frac{1}{\bar{\rho}_0}\bar{\rho}_\pm\left(\frac{\epsilon}{\bar{\rho}_0}\right) = \frac{(\pm 1)^N}{N!} \frac{\mathrm{d}^N}{\mathrm{d}y^N} \left[\sum_{l=1}^{\infty} \frac{(\pm 1)^l}{(l-1)!l!} \mathrm{Li}_2(y)(\mathrm{Li}_2(y)\,\epsilon)^{l-1}\right] \Bigg|_{y=0}, \tag{4.124}$$

where we raised the upper limit of the sum over l to infinity. We can do this because the summand corresponding to a particular value of l is of order $\mathcal{O}(y^l)$, since the smallest power in the dilogarithm is a linear term. Using the power series expansion of the Bessel function $\mathrm{J}_1(z)$

$$\begin{aligned} \mathrm{J}_1(z) &= \left(\frac{z}{2}\right) \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(k+1)!} \left(\frac{z}{2}\right)^{2k}, \\ \mathrm{I}_1(z) &= -i\,\mathrm{J}_1(iz), \end{aligned} \tag{4.125}$$

the level densities for bosons respectively fermions can be expressed as

$$\begin{aligned} \frac{1}{\bar{\rho}_0}\bar{\rho}_+\left(\frac{\epsilon}{\bar{\rho}_0}\right) &= \frac{1}{N!} \frac{\mathrm{d}^N}{\mathrm{d}y^N} \left[\sqrt{\frac{\mathrm{Li}_2(y)}{\epsilon}}\ \mathrm{I}_1\left(2\sqrt{\mathrm{Li}_2(y)\,\epsilon}\right)\right] \Bigg|_{y=0} \\ \frac{1}{\bar{\rho}_0}\bar{\rho}_-\left(\frac{\epsilon}{\bar{\rho}_0}\right) &= \frac{(-1)^{N+1}}{N!} \frac{\mathrm{d}^N}{\mathrm{d}y^N} \left[\sqrt{\frac{\mathrm{Li}_2(y)}{\epsilon}}\ \mathrm{J}_1\left(2\sqrt{\mathrm{Li}_2(y)\,\epsilon}\right)\right] \Bigg|_{y=0}. \end{aligned} \tag{4.126}$$

The advantage of these representations is that they potentially provide a starting point to gain asymptotic expressions in the limit $N \to \infty$. The origin of this suggestion lies in the representation of derivatives as closed contour integrals in the complex plain $\mathbb{C}$

$$\frac{\mathrm{d}^N}{\mathrm{d}z^N} f(z)\Big|_{z=0} = \frac{N!}{2\pi i} \oint_\gamma \frac{\mathrm{d}z}{z^{N+1}} f(z), \tag{4.127}$$

where γ is a closed contour around the origin $z = 0$ with unit winding number. The asymptotic limit $N \to \infty$ can then be achieved by writing the $1/z^{N+1}$ factor in (4.127) as an exponential

$$\frac{1}{z^{N+1}} = e^{-(N+1)\,\ln(z)}. \tag{4.128}$$

This opens the possibility of performing a saddle point approximation by distorting the contour so that it contains the point of vanishing derivative of the whole phase function including $\ln(f(z))$. Since in the limit $N \to \infty$, the integrand becomes infinitely fast oscillating, the saddle point approximation should become asymptotically exact. By this process, one should be able to obtain the Bethe approximation (4.121) for fermions, since it is also valid asymptotically. In addition to that, the ground state energy should emerge in the corresponding analysis, splitting the axis of energy in two pieces. The small oscillations below the ground state should be reachable too. Furthermore, an asymptotic level density for bosons similar to $\bar{\rho}_{\mathrm{Bethe}}$ should be achievable. Indeed, recent progress in this direction has been made in the context of an approach via spectral determinants, but a careful analysis shall be postponed for the time being.

Another approach to a better understanding of the factors S_l and the corresponding polynomials lies in the comparison with results in number theory.

4.4.2 Connection To Number Theory

The possibility of connecting $\bar{\rho}_{\pm}(E)$ to number theory has its origin in the equal distribution of single particle energy levels according to the first Weyl term in the two dimensional case. The associated number theoretical analogue is thereby the set of integers on the real axis. As pointed out by Leboeuf [18], the density of states of a system of non-interacting fermions with equally distributed single particle energy levels (e.g. a harmonic oscillator or approximately a two-dimensional quantum billiard) is related to the mathematical problem of partitioning an integer. The number of ways to decompose an integer n into a sum of integers may be denoted by $p(n)$. If we take now energy values measured in units of single particle mean level spacings, $p(e)$ is the number of energy levels that can be found at many body excitation energy e, as long as this energy is smaller than the particle number. Since we assume exactly equal distribution of single particle levels, no non-integer energy level will be available. In other words, in this ideal case, the exact many body density of states is

$$\rho_{-}(e) = \sum_{n=0}^{\infty} p(n)\delta(e-n). \tag{4.129}$$

This equivalence can be easily understood in the following way. The total excitation energy can be partitioned among single particle excitations. Each summand

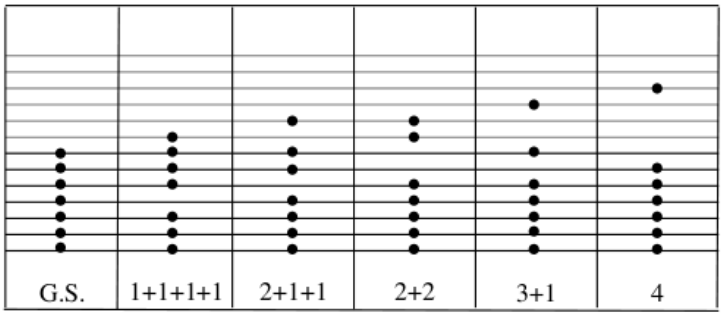


Figure 4.17: Ground state and excited states at excitation energy $e = 4$ in units of single particle level spacing. The picture is taken of [18]

in the decomposition of e is associated with the excitation of a particular single particle. Thus the number of possible decompositions $p(e)$ equals the number of antisymmetric many body states that share this total excitation energy e. Figure 4.17 illustrates this. The restriction of e to a maximum value of N corresponds to the restriction that we can only distribute the excitation energy among a maximum of N particles. As long as $e \leq N$ this restriction is not relevant, because then all possible partitions involve only sums of at most N integers. For higher energies, one would have to use the number of *restricted partitions* $p_N(e)$ instead of the number of *unrestricted partitions* $p(e)$. $p_N(e)$ is thereby the number of partitions with the restriction of at most N parts. Interestingly, this restriction is equivalent to demanding a maximum value N of each part instead. In number theory, asymptotic expressions for the number of partitions, unrestricted and restricted, are available. The first asymptotic formula for $p(e)$ has been given by Hardy and Ramanujan [13]. The highest order term in the corresponding expansion is exactly the density approximation given by Bethe (4.121). We see now how the restriction of excitation energies to values smaller than the Fermi energy in Bethe's asymptotic formula is related to the restriction $e \leq N$ to allow the equality $p_N(e) = p(e)$. The further the excitation energy lies out of the range of validity, the bigger the deviation of $p(e)$ with respect to $p_N(e)$. In order to give better approximations to the density of states by means of number theoretical results, we need an asymptotic formula for restricted partitions $p_N(e)$. One correction to the Bethe result is given by the so-called Erdos-Lehner formula [8] for the mean restricted partition number

$$\bar{p}_N(e) \approx \bar{p}(e)\ \exp\left[-\left(\frac{\sqrt{6e}}{\pi} - \frac{1}{2}\right)\exp\left(-\frac{\pi N}{\sqrt{6e}}\right)\right]. \tag{4.130}$$

Actually, the Erdos-Lehner formula slightly differs from (4.130) by the absence of the term of $1/2$ in the exponent. But the given formula can be obtained as a saddle point approximation of the density of states in a physical analogue.

As is possible with the Bethe formula. The analysis is based on the representation of the density of states expressed as inverse Laplace transform of the thermodynamical partition function.

$$\rho(E) = \frac{1}{2\pi i} \int_{\epsilon - i\infty}^{\epsilon + i\infty} \mathrm{d}\beta \; e^{\beta E} Z(\beta), \tag{4.131}$$

$$Z(\beta) = \sum_n e^{-\beta E_n} = \int \mathrm{d}E \; \rho(E) e^{-\beta E}, \tag{4.132}$$

where n is counting all many-body energy levels E_n. We define the ground state energy to be $E = 0$. For a non-interacting system, one can then express the total energy (equivalent to the many body excitation energy) as the sum of single particle excitations.

$$Z(\beta) = \sum_{\{n_k\}} \exp\left[-\beta \sum_{k=1}^{\infty} E_k n_k \right], \tag{4.133}$$

where E_k denotes the k-th single particle excitation energy. n_k denotes the number of particles sharing the k-th excitation. The subscript $\{n_k\}$ indicates that the sum runs over all possible values $n_k \in \mathbb{N}_0 \quad \forall k \in \mathbb{N}$. In the case of bosons, n_k literally is the occupation number of the according energy level. For fermions, $n_k > 1$ only means, that more than one particle are sharing the same excitation with respect to their individual energies in the ground state (leaving the notion of indistinguishability aside by identifying particles with particular occupied energy levels in the ground state). So they don't share the same level. The excitations are distributed among the particles from top to bottom, meaning the highest excitation energy is related to the particle occupying the highest single particle level in the many body ground state. We consider only systems with equally distributed single particle levels. Thus by relating all energies to the particular ground state, the bosonic and fermionic partition functions are equal. In the limit of infinitely many particles it reads

$$Z_\infty(\beta) = \prod_{k=1}^{\infty} \sum_{n=0}^{\infty} e^{-\beta k n} = \prod_{k=1}^{\infty} \frac{1}{1 - e^{-\beta k}} \quad \equiv \prod_{n=1}^{\infty} \frac{1}{1 - x^n} = \sum_{n=1}^{\infty} p(n)\, x^n, \tag{4.134}$$

where we measure energy in units of the single particle level spacing and introduced the abbreviation $x = e^{-\beta}$. Comparing the final expression with (4.132) directly shows the identity (4.129). $Z_\infty(-\ln(x))$ is therefore the generating function for the partition numbers $p(n)$. The last step can easily be seen when

expanding the infinite product of sums in x

$$\begin{aligned}\prod_{n=1}^{\infty}\frac{1}{1-x^n} =&[1+x^1+x^2+\underline{x^3}+\cdots]\\ &\times[1+\underline{x^2}+x^4+x^6+\cdots]\\ &\times[1+x^3+\underline{x^6}+x^9+\cdots]\\ &\times[\underline{1}+\cdots\\ &\quad\vdots \qquad\qquad .\end{aligned} \tag{4.135}$$

After multiplying all sums and ordering the result in powers of x, the term x^N has a coefficient equal to the number of different ways the exponent N can be distributed among the exponents in the infinite sums in (4.135). Interpreting the line number as size $1, 2, \ldots$ of one part and the position to the right in each brace as multiplicity of this part size, we see that this number of partitioning is exactly the number of possible unrestricted integer partitions. The underlined terms in (4.135) give one example of a possible partitioning of $N = 11 = 1 + 1 + 1 + 2 + 3 + 3$. The semiclassical approximation of the smooth part of the density of states $\bar{\rho}(E)$ or equally the smooth partition number function $\bar{p}(n)$ can then be obtained by writing the integrand in (4.131) as exponential, expanding the infinite sum in the corresponding phase function as a Euler-MacLaurin series and finally apply a saddle point approximation to the integral over β. In leading order of the energy, one is left with the Bethe formula (4.121). Due to the used approximations, Bethe's density is only applicable for energies larger than the single particle level spacing $e \gg 1$. For higher energies it improves in describing either the density of states $\bar{\rho}_\infty(e)$ of a system of infinitely many non-interacting particles with constant single particle level spacing or equivalently the partition number function $p(e)$. Note that the original intention of the Bethe estimate is to describe a system of non-interacting fermions not restricted to equally distributed single particle energies. The reason for the applicability is that the single particle mean level spacing can be regarded as asymptotically constant around the Fermi energy. This is another assumption that implies the restriction to excitation energies much smaller than the Fermi energy $E \ll E_\mathrm{F}$. The more irregular the single particle density at the Fermi level, the smaller the range of validity of (4.121). Since in bosonic systems the non-interacting ground state consists of particles that share the lowest single particle level, the assumption of constant single particle mean level spacing in general is not allowed. This is the reason why Bethe's estimate only regards fermions.

Similar to that one can take the partition function of a system of N non-interacting particles with ground state energy $E = 0$ and equally distributed

single particle energy levels

$$Z_N(\beta) = \prod_{m=1}^{N} \frac{1}{1-e^{-\beta m}} \equiv \prod_{m=1}^{N} \frac{1}{1-x^m} = \sum_{n=1}^{\infty} p_N(n)\, x^n, \tag{4.136}$$

do saddle point approximations to obtain an approximation for the smooth part of the density of states of the finite system respectively the smooth restricted partition number function $\bar{p}_N(n)$. By doing an analysis similar to the one that leads to Bethe's formula, one gets the slightly modified Erdos-Lehner formula (4.130). But although the restriction to finite numbers N of parts is now incorporated, the made approximations in the corresponding analysis imply a restriction $\zeta(2) \ll e \ll \zeta(2)N^2$. So the restriction to low excitations is inherent anyway. Figure 4.18 shows a comparison of the Bethe approximation $\bar{\rho}_{\mathrm{Bethe}}$, the Erdos-Lehner approximation for $\bar{p}_N$, the smooth part of the symmetry-projected density of states $\bar{\rho}_{\pm}$ and some exemplary values of unrestricted respectively restricted partition numbers $p(n)$ and $p_N(n)$. Although the Erdos-Lehner formula seems to have improved validity in comparison to the Bethe approximation for finite systems, it shows wrong behaviour for higher energies. The semiclassical symmetry projected density is in good agreement with the actual restricted partition numbers.

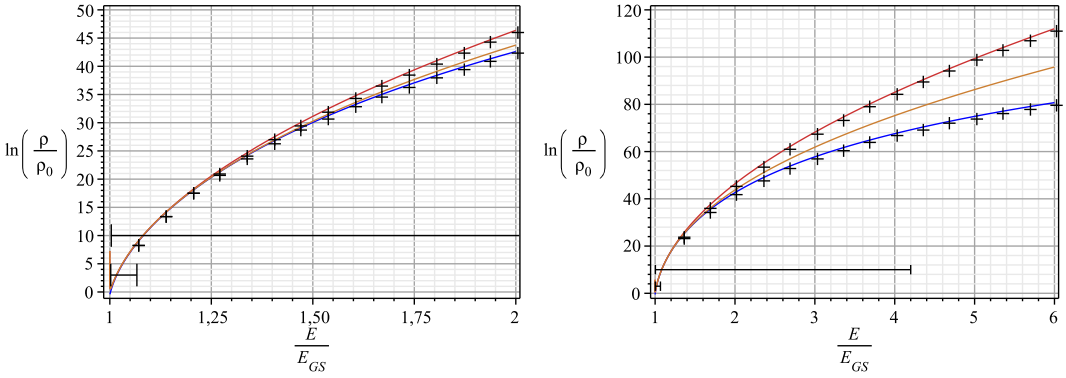
Interestingly, another approximation to the smoothed restricted partition number function $\bar{p}_N(n)$ can be found in literature. It is the complete polynomial part of the function, where the deviation is a sum of periodic functions with average value 0. The polynomial part was in its first form given by Beck, Gessel and Komatsu [2] and later refined by Rubinstein [24]. It is given in terms of a polynomial $W_1(n)$ of degree $N-1$, as is $\bar{\rho}_-$ for a two-dimensional billiard. In addition to that in its later form given by Rubinstein it is naturally given for function arguments x where the number to partition n is the excess $n = x - s_N$ over the sum of the first N integers

$$s_N = \sum_{i=1}^{N} = \frac{1}{2}N(N+1). \tag{4.137}$$

Which reminds us of the density of states which is also naturally given for total energies so that the excitation energy related to the number to partition is the difference of the function argument $e = E\bar{\rho}_0$ and the ground state energy

$$e_{\mathrm{GS}} = E^{(\mathrm{f})}_{\mathrm{GS}}\bar{\rho}_0 = \frac{1}{2}N^2. \tag{4.138}$$

The difference between s_N and e_{GS} can be related to the many body energy shift of $\delta e^{(\mathrm{MB})} = N/2$ corresponding to the single particle energy shift $\delta e = 1/2$ one has to apply the single particle density in order to give an average density



(a) improvement of validity (b) deviation at high energies

Figure 4.18: Comparison of the semiclassical smooth part of the density of states in 2 D (blue) with the Bethe estimate (red) and the Erdos-Lehner approximation (orange) for a system of $N = 30$ fermions. The two bars indicate the range of validity of the Bethe estimate (lower bar) and the Erdos-Lehner approximation (upper bar). Crosses correspond to exemplary partition numbers in the unrestricted case $p(e)$ (upper points) and the restricted case $p_N(e)$ (lower points). Energy is measured in units of the fermionic ground state energy.

for integers among real numbers. The shifted density

$$\frac{1}{\bar{\rho}_0}\bar{\rho}_0((e+\delta e)\bar{\rho}_0^{-1}) = \theta\left(e-\frac{1}{2}\right) \tag{4.139}$$

is exactly produced when the density of integers $\sum_n \delta(e-n)$ is smoothed with a window function of full width of unity. Furthermore, the polynomial given by Rubinstein produces small oscillations in the range $0 < x < s_N$. The polynomial is symmetric under the parity transformation $x \mapsto s_N/2 - x$, which means negative x-values correspond to positive n-values. This behaviour can also be found when investigating $\bar{\rho}_-(E)$, since turning to negative energy values (omitting the θ-function) simply gives the corresponding bosonic density $\bar{\rho}_+(E)$, which is also supposed to reproduce restricted partition numbers. Obviously there are many similarities between Rubinstein's polynomial $W_1(n)$ and the smooth level density $\bar{\rho}_-(E)$, which leads us to the question whether we can gain analytical information about the factors S_l out of this resemblance. Unfortunately, $W_1(n)$ is given as a Bernoulli polynomial of higher order, which is defined by a multi recursion formula.

$$W_1(n,N) = \frac{1}{N!(N-1)!}B_{N-1}^{(N)}(n+s_N \,|\, \{\overline{N}\}), \tag{4.140}$$

where $\{\overline{N}\}$ denotes the set of integers $1,\ldots,N$ and the Bernoulli polynomials of higher order are defined symbolically as

$$B_{N-1}^{(N)}(x \,|\, \{\overline{N}\}) = \left(x + \sum_{k=1}^{N} k \;\; {}^kB\right)^{N-1}, \tag{4.141}$$

where the product has to be expanded in powers of all individual ${}^kB$. Afterwards the exponents of all ${}^kB$ have to be pulled down to a subscript and understood as the subscript of Bernoulli numbers. All left superscripts k are then omitted.

$${}^kB^m \mapsto {}^kB_m \mapsto B_m, \tag{4.142}$$

with B_m denoting the m-th Bernoulli number. Equivalently, the Bernoulli polynomials of higher order can be defined by recursion.

$$B_n^{(m)}(x|\{\overline{N}\}) = \sum_{k=0}^{n}\binom{n}{k}N^k\, B_k\, B_{n-k}^{(m-1)}(x|\{\overline{N-1}\}). \tag{4.143}$$

starting with the ordinary Bernoulli polynomial

$$B_n^{(1)}(x|\{1\}) = B_n(x). \tag{4.144}$$

Unfortunately, these Bernoulli polynomials are hard to handle and there is at this stage no obvious analytical information one could gain about the coefficients in $\bar{\rho}_-(E)$.

At least, we can give explicit expressions for the coefficients corresponding to the highest orders in the function argument in the case of Rubinstein's approximation and also in the case of the smooth density of states including the earlier mentioned energy shift δe. For this purpose, we used the earlier definition by Beck, Gessel and Komatsu, where the polynomial is given in terms of the number to partition n. Unit mean level spacing shall be used for the density. We shift the density by the ground state energy to obtain a polynomial in $n = e - e_{\mathrm{GS}}$. We write the corresponding polynomial as

$$\bar{\rho}_-(n + e_{\mathrm{GS}}) = \sum_{m=0}^{N-1} a_m^{(N)} n^{N-m-1} \tag{4.145}$$

and the polynomial part of the restricted partition number function as

$$\bar{p}_N(n) = \sum_{m=0}^{N-1} b_m^{(N)} n^{N-m-1}. \tag{4.146}$$

We calculate the coefficients of the three leading orders in n to find

$$\begin{aligned}
a_0^{(N)} &= b_0^{(N)} = \frac{1}{N!(N-1)!} \\
a_1^{(N)} &= b_1^{(N)} = \frac{1}{N!(N-2)!}\left[\frac{1}{4}N(N+1)\right] \\
a_2^{(N)} &= \frac{1}{N!(N-3)!}\left[\frac{1}{32}N^4 + \frac{7}{144}N^3 + \frac{1}{96}N^2 + \frac{5}{144}N\right] \\
b_2^{(N)} &= \frac{1}{N!(N-3)!}\left[\frac{1}{32}N^4 + \frac{7}{144}N^3 + \frac{1}{96}N^2 - \frac{1}{144}N\right] \\
a_2^{(N)} &\neq b_2^{(N)}.
\end{aligned}$$

So we obtain similar but not equal coefficients for the leading terms. Note that the highest coefficient $a_0^{(N)}$ is independent of the particular used energy shift, while the equality of the second highest coefficients demands exactly the shift to the ground state energy $n = e - e_{\mathrm{GS}}$. The third coefficients already have a slight deviation from each other. Thus one can at least conclude that the two polynomials give similar results but are not equal. Whether and to what extent the computation time of coefficients is longer in one of the cases is not clear at the moment and remains to be investigated.

5 Concluding Remarks

In this thesis we have incorporated the concepts of quantum mechanical many body systems of identical particles into the semiclassical formalism. The many body generalisation of the Gutzwiller trace formula was already given by Weidenmüller or as the application of Robbins' formulation in reduced phase space to the exchange symmetry of identical particles. To use the latter, we had to construct the reduced phase space for this particular symmetry. To our knowledge, this has not been done so far. For future investigations, it will be interesting to use this construction by applying conformal mapping methods in order to map many body systems to equivalent systems without symmetry but additional interaction potentials. We think of deducing effective repulsive or attractive potentials appearing in fermionic respectively bosonic systems. Such effective potentials can also be derived in statistical mechanics [27]. It will be interesting to see if one is able to reproduce these known potentials.

Furthermore, we used the symmetry projected trace formula to obtain universal features in spectral statistics of many body systems. While there is a variety of works on the subject of semiclassical level statistics for systems obeying discrete symmetries, all of these works simply assume the symmetry group elements related to open orbits to be equally distributed among the group in the limit of long transit times. This assumption is usually justified by arguing with ergodicity. But no treatment in a rigorous manner similar to the HOdA sum rule has been given so far. We derive the corresponding formula, which should be useful not only in the context of identical particles but also for other discrete symmetries.

In a brief discussion of the apparent many body transition catastrophe we find that a less superficial treatment than the given can not be done without profound knowledge of the smooth part of the density of states. Especially the behaviour around the ground state is of interest. This was the reason to derive the semiclassical smooth part of the density of states in terms of short time (respectively short path) propagation. The special form of the particle exchange symmetry led us to the geometrical concept of cluster zones. Then, all relevant short path contributions are organised by these cluster zones. We give a calculation of the measures of the according invariant manifolds which will be useful when including short range interactions in the future. We solved for the free case and find the emergence of the correct ground state energy. We also find good agreement with the asymptotic formula by Bethe and understand

our expression as to be valid for all energies and therefore as a generalisation of Bethe's approximation to finite particle numbers and energies near and below the ground state energy. In the two-dimensional case we also found good agreement with restricted partition number functions which are equal to average densities of states for non-interacting systems with equally distributed single particle energies. This substantiates the validity of the derived expressions for all energies.

The most important possibility opened by our formal construction is the potential inclusion of short range interactions. The reason for this is the fact that the cluster zone structure is exactly the structure one needs in order to give modifications due to short range interactions, since those will only affect the propagation of particles within one cluster because they are at short distances of each other. Recent progress has been made in calculating two-cluster modifications due to hard-disk interactions. Thereby we could obtain modifications that correspond to an effective adaption of billiard properties like the reduction of available volume by the disk sizes and the increase in overall perimeter due to their circumferences. These changes are related to the identity permutation in two-cluster zones. We understand this to be the final confirmation of the potential applicability to interacting systems.

A Boundary Multiplets In Reduced Phase Space

Consider a system with two-dimensional discrete translational invariance. For simplicity let us assume periodicity respective a square lattice. One might impose periodic boundary conditions with an integer number of distinct squares though it doesn't matter for the current issue.
Consider the spatial coordinates (x, y) with symmetry respective the transformations

$$(x, y) \mapsto (x + k\,a, y + l\,a) \qquad \forall k, l \in \mathbb{Z} \tag{A.1}$$

We choose the primitive cell as the Cartesian product of $\mathbb{R}^2$ for free momentum and the coordinate square spanned from the origin into the first quadrant

$$\mathscr{P}^{(sr)} = [0, a] \times [0, a] \times \mathbb{R}^2 \tag{A.2}$$

Opposite lines of the square are then related by symmetry. They can be identified. But in contrast to the interior of that lines, the corners do not come as symmetry related pairs but as quadruplet. All four points are related by symmetry.
As with exchange symmetry, one has to find the correct mapping of pairs in order to maintain correct dynamics. That is mapping of diagonal opposites. All four points are identified when wrapping $\mathscr{P}^{(sr)}$ to the reduced phase space with 2-torus topology. And the correct dynamics in that point are given by the mapping of the derivative $\dot{\xi}(t)$ by virtue of the unique mapping that lets $\dot{\xi}(t)$ point into $\mathscr{P}^{(sr)}$ again. (see figure A.2

So everything is well defined and the formalism works fine.
Nonetheless the boundary pair argument does not hold. And that is because of the assumption that the part of a vicinity U_r of the boundary point r that is part of the exterior of the reduced phase space $B_r := U_r \backslash \mathscr{P}^{(sr)}$ should be mapped completely into the interior $B_s := g\,(B_r) \subseteq \mathring{\mathscr{P}}^{(sr)}$ by the transformation that relates the two boundary points r and $s = g(r)$. In figure (A.1) we see that this is not the case for two corner points.

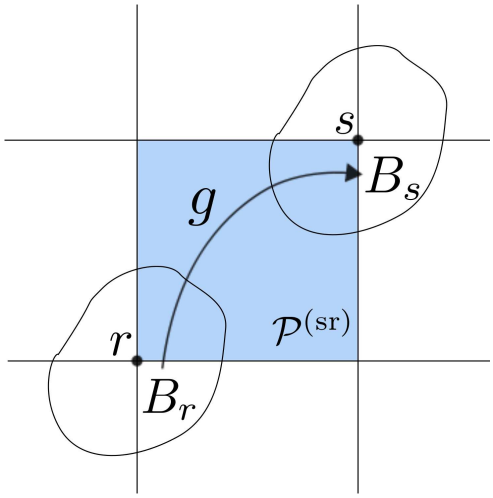


Figure A.1: The assumption that every part of a vicinity that lies outside the reduced phase space is mapped to the interiour is not valid for the shown part B_r.

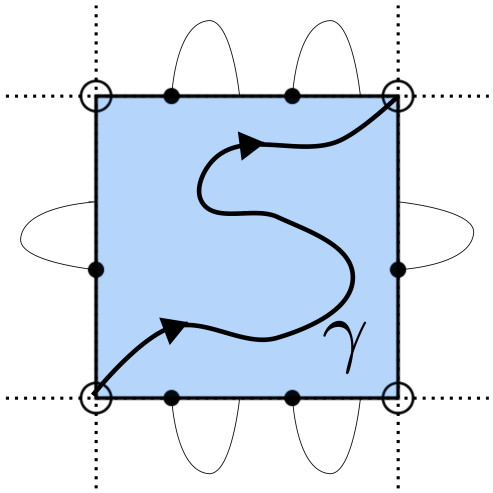


Figure A.2: Reduced phase space for discrete translational invariance in two directions. Identification of surface points yields the topology of a torus. Although the trajectory γ is at four symmetry related positions when crossing the surface, the dynamics are unique.

B HOdA Sum Rule For Maps

This section mainly follows the scheme given by Fritz Haake in [10]. The reader may also be referred to the original paper by Hannay and Ozorio de Almeida [12]. Especially the second appendix could be of interest when dealing with maps.

Let $\mathbf{r}_n$ be the n-th map of an arbitrary phase space point $\mathbf{r}_0$. The set of all points that successive mapping produces will be referred to as *orbit*. The essential ingredient to the analysis is the formulation of the assumption of ergodic behaviour. To put it into words, ergodicity means the uniform filling of all available phase space for long time dynamics. We assume this property to hold for systems showing fully chaotic dynamics. There are very special cases of *non generic* systems that are not obeying this rule but will be passed over here.

The uniformity assumption or *ergodic hypothesis* estimates

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \delta(\mathbf{r} - \mathbf{r}_n) = \frac{1}{\Omega} \tag{B.1}$$

for any $\mathbf{r}$, almost every $\mathbf{r}_0$ and Ω being the volume of available phase space. (B.1) holds also for the restriction to longtime maps replacing

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \qquad \to \qquad \lim_{N\to\infty} \frac{1}{\Delta N} \sum_{n=N}^{N+\Delta N} \tag{B.2}$$

when remaining $1 \ll \Delta N \ll N$ in the limit.

Equation (B.1) actually strictly holds only for non periodic orbits

$$\mathbf{r}_n(\mathbf{r}_0) \neq \mathbf{r}_0 \qquad\qquad \forall n \in \mathbb{N}. \tag{B.3}$$

This excludes a countable set of $\mathbf{r}_0$, so that the term 'almost every' has to be understood in its usual mathematical definition. This exclusion will lead us to an apparent contradiction that is solved when we recognise that the hypothesis holds for a somewhat smeared delta function $\delta_\epsilon(\mathbf{x})$ in the limit $\epsilon \to 0$. Then we are free to include periodic orbits as long as their period is long enough to allow the broadened δ-peaks to fill up the interspaces not hit by the orbit. Of course this process lacks of rigour. Thus strictly the relation has to be understood as

asymptotic in the sense that the definition of minimal period $N_{min}(\epsilon)$ demanded for a specific value of the smearing parameter ϵ becomes infinitely large. The product of N_{min} and ϵ somehow reflects the quality of the approximation. Since eventually we want to take the limit $\epsilon \to 0$, the minimal period will have to be very large in some sense in order to remain a good approximation. In the end, this was the reason for restriction to long times $N \to \infty$. We see that one should be careful with the way one takes the different occurring limits.

Set $\mathbf{r} = \mathbf{r}_0$ and integrate over $\mathbf{r}_0$ to get a sum over points of periodic orbits

$$\lim_{N\to\infty} \frac{1}{\Delta N} \sum_{n=N}^{N+\Delta N} \int_{\Omega} \mathrm{d}^D r_0 \sum_p \left| \det \left(\frac{\partial f_i}{\partial r_{0,j}} \right) \right|^{-1} \delta(\mathbf{r}_0 - \mathbf{x}_p) = 1 \tag{B.4}$$

with $\mathbf{x}_p$ being all points of periodic orbits of period n. p indexes all these periodic orbits

$$\mathbf{r}_n(\mathbf{x}_p) = \mathbf{x}_p. \tag{B.5}$$

$\mathbf{f}(\mathbf{r}_0)$ is the previous argument of the delta function regarded as a function of $\mathbf{r}_0$

$$\mathbf{f}(\mathbf{r}_0) = \mathbf{r}_n(\mathbf{r}_0) - \mathbf{r}_0. \tag{B.6}$$

As there exist as many different points $\mathbf{x}_p$ on a periodic orbit as is its *primitive period* n_0 one can further write the ergodic hypothesis as

$$\lim_{N\to\infty} \frac{1}{\Delta N} \sum_{n=N}^{N+\Delta N} \sum_p n_0 \left| \det \left(\left(\frac{\partial r_{n,i}}{\partial r_{0,j}} \right)_p - \delta_{ij} \right) \right|^{-1} = 1. \tag{B.7}$$

Primitive periodic orbits clearly dominate the sum, as they are much more in number and similar in stability compared to repetitions of shorter orbits with same full period n. This justifies the replacement $n_0 \to n$ which can often be seen in applications using the sum rule.

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Plagiatserklärung

Hiermit erkläre ich, dass ich die Diplomarbeit selbstständig angefertigt und keine Hilfsmittel außer den in der Arbeit angegebenen benutzt habe.

Regensburg, den 31.05.2011

(Quirin Hummel)