Semiclassical theory of spin-orbit interaction

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Chapter 1

Introduction

The subject of spin-orbit interaction in solid state physics has been attracting much attention recently due to potential applications in spin-based electronic devices [30, 31, 32, 75]. It has often proved advantageous, on the other hand, to exploit the semiclassical description of electrons in mesoscopic systems in the ballistic regime [82]. Hence there is a substantial interest in extending the semiclassical theory to include spin.

One of the basic quantities that describes properties of a quantum system is a density of states $g(E)$ of its quantum spectrum. In the Periodic Orbit Theory developed by Martin Gutzwiller [45] the oscillating part $\delta g(E)$ of $g(E)$ is expressed by the so-called Trace Formula through the quantities of the classical periodic orbits: their classical actions and stabilities (see [18] for the review). The Periodic Orbit Theory has proved to be a successful tool for the semiclassical description of chaotic systems [10, 28, 46, 47]. Therefore, it seems quite natural to start a formulation of the semiclassical theory including spin from a generalization of the Gutzwiller's Trace Formula to systems with spin-orbit interaction.

Several attempts were made in the last decade in this direction. Littlejohn and Flynn [66] revised and improved the asymptotic theory of coupled wave equations (or multicomponent WKB theory) and applied it to systems with standard spin-orbit coupling [67]. Their approach relies on a rather large strength of the spin-orbit interaction (strong coupling limit). However, it becomes invalid at the points in classical phase space where the interaction vanishes—the so-called mode-conversion points. Frisk and Guhr [37] found that in certain cases this problem can be corrected by a heuristic procedure. However, none of these authors have developed an explicit Trace Formula.

Bolte and Keppeler [16] studied the opposite situation when the interaction is weak (weak coupling limit). They derived the Trace Formula for the Dirac equation and Pauli equation with spin 1/2. Based on the assumption that the orbital motion is not affected by spin, their approach was used to explain the anomalous magneto-oscillations in quasi-two-dimensional systems [52].

Both of the above-mentioned semiclassical methods imply the smallness of $\hbar$ compared to classical action. Therefore, in each case the semiclassical approximation involves an expansion in series of $\hbar$. It is the asymptotic behavior of the coupling constant that determines the difference between the results obtained within both methods. Their comparative analysis and applications to specific systems can be found in [3].

Another type of semiclassical approximation is usually employed for: 1) spin systems in external time-dependent field; and 2) statistical ensembles of spin particles at finite temperature (e.g., the Heisenberg ferromagnet model [63]). In such systems the semiclassical limit is understood as a limit of the large spin value. The description of spin by continuous variables is achieved by using the basis of spin coherent states. One can then construct path-integral expressions for the quantum propagator and its trace (quantum partition function in the case of statistical ensembles, respectively), and evaluate them by the stationary phase method. Recently, there has been made a substantial progress in obtaining the respective semiclassical asymptotics [56, 92], and in proving their validity [86]. Such semiclassical description has been successfully applied in Ref. [40] for the study of the spin tunneling in the molecular magnet Fe_8.

We propose a semiclassical approach to spin-orbit coupling where the orbital and spin degrees of freedom are combined in an extended phase space [78]. The starting point for further semiclassical approximation is the path-integral expression for the trace of the quantum propagator. In such representation, it is easy to introduce different semiclassical limits, depending on the coupling strength and spin value. We show that the results of the above-discussed approaches to limits of weak and strong coupling are naturally reproduced in the unified path-intgral formulation of the theory.

Our main focus, however, is the derivation of the Trace Formula in the large-spin limit. Special attention is paid to the Solari-Kochetov phase correction [85, 56, 92] which ensures the correct asymptotic result. We also advocate the point that the Trace Formula of the large-spin limit can be used for small spins as well, provided the spin-orbit interaction is linear in spin operators. Thus, it may serve useful for interpolation between the limits of weak and strong coupling discussed above.

We expect that the semiclassical methods presented in this dissertation can be effectively used in systems with relatively strong spin-orbit interaction, such as p-InAs or InGaAs-InAlAs heterostructures [49, 71], or atomic nuclei [14]. Another field of application is molecular dynamics, where similar methods were developed to map the discrete electronic states to continuous variables and then to treat those semiclassically [89].

The dissertation is organized as follows.

In **Chapter 2** we briefly review the derivation of the Trace Formula without spin, starting from the path-integral representation for the propagator. Recently proposed by Sugita [88], this new procedure reproducing the well-known result of Gutzwiller [45] will later be generalized to include spin.

In **Chapter 3** we review the different possibilities for continuous (phase-space) representation of the spin degrees of freedom. Among them are the spin coherent states, Jordan-Schwinger boson model and Stratonovich-Weyl calculus.

In **Chapter 4** we estimate semiclassically the trace of the quantum propagator for a system with spin-orbit coupling written in the path-integral representation using spin coherent states. Three versions of the Trace Formula are derived. In the first case (Sec. 4.2) the path integral is evaluated by the stationary-phase method in both spin and orbital variables. Then, using Sugita's approach, we express the oscillating part of the density of states as a sum over the periodic orbits in the extended phase space. In the last two instances we integrate over the spin variables in the path integral exactly and then apply the stationary-phase approximation. Consequently, for weak spin-orbit interaction (Sec. 4.3) we obtain the generalization of the Trace Formula of

Bolte and Keppeler [16] to arbitrary spin, and for strong coupling (Sec. 4.4) we recover, on a restricted basis, the result by Littlejohn and Flynn (at this stage their "no-name" phase still has to be recovered).

As an application of the general theory, in **Chapter 5** we study the systems with Rashba-type spin-orbit interaction [21] and the Jaynes-Cummings model [50].

Chapter 2

Semiclassical theory without spin

2.1 Periodic Orbit Theory without spin

In this section we summarize some basic facts related to the semiclassical Trace Formula and present its derivation for systems without spin [88]. We consider a system described by the Schrödinger equation

$$\widehat{H}\,\psi_n = E_n\,\psi_n \tag{2.1}$$

with a discrete energy spectrum $\{E_n\}$. Its density of states $g(E) = \sum_n \delta(E - E_n)$ can be subdivided into smooth and oscillating parts, i.e.,

$$g(E) = \widetilde{g}(E) + \delta g(E)\,. \tag{2.2}$$

From the semiclassical point of view, the smooth part $\widetilde{g}(E)$ is given by the contribution of all orbits with zero length and can be evaluated by the (extended) Thomas-Fermi theory [11]. Numerically it can be extracted by a Strutinsky averaging of the quantum spectrum [18].

Our present subject of interest is the oscillating part $\delta g(E)$, which is semiclassically approximated by the *Trace Formula*

$$\delta g_{sc}(E) = \sum_{po} \mathcal{A}_{po}(E)\cos\left(\frac{1}{\hbar}\mathcal{S}_{po}(E) - \frac{\pi}{2}\sigma_{po}\right). \tag{2.3}$$

The sum here is over all classical periodic orbits (*po*), including all repetitions of each primitive periodic orbit (*ppo*). $\mathcal{S}_{po}(E)$ is the action integral and σ_{po} is the Maslov index of a periodic orbit. The amplitude $\mathcal{A}_{po}(E)$ depends on the integrability and the continuous symmetries of the system. When all periodic orbits are isolated in phase space, the amplitude

$$\mathcal{A}_{po}(E) = \frac{1}{\pi\hbar}\frac{T_{ppo}}{\sqrt{|\det(\widetilde{M}_{po} - I_{2(d-1)})|}} \tag{2.4}$$

specifies the *Gutzwiller's Trace Formula* [45], where T_{ppo} is the period of the primitive orbit, $\widetilde{M}_{po}$ is the stability matrix of the periodic orbit, and d is the number of degrees of freedom. I is the unit matrix, the subscript denotes the dimensionality of the space where I acts. For two-dimensional systems ($d = 2$) the stability denominator equals to $\sqrt{|\det(\widetilde{M}_{po} - I_2)|} = 2|\sin(\Lambda_{po}/2)|$, where Λ_{po} is called the stability angle of a periodic orbit. Λ_{po} is real for stable orbits, and imaginary for unstable orbits. For further details related to the amplitude (2.4), we refer to [18].

In the presence of continious symmetries the Trace Formula (2.3) is modified [26]: the amplitude $\mathcal{A}_{po}(E)$ acquires another form, and the summation in (2.3) is performed over the *families* of periodic orbits.

Recently Sugita [88] has proposed a re-derivation of the Trace Formula directly from the trace of propagator, avoiding the calculation of the semiclassical propagator itself. Since in the following we utilize his approach for systems with spin, we will briefly review it here. Sugita's starting point is the trace of the quantum propagator in the path integral representation

$$Z(T) = \lim_{N\to\infty} \int \prod_{k=1}^{N} \frac{d\mathbf{q}_k d\mathbf{p}_k}{(2\pi\hbar)^d} \exp\left\{\frac{i}{\hbar}\mathcal{R}_W^{(N)}\right\}, \tag{2.5}$$

$$\mathcal{R}_W^{(N)} = \sum_{k=1}^{N} \left\{\mathbf{p}_k \cdot (\mathbf{q}_k - \mathbf{q}_{k-1}) - \tau H_W\left(\frac{\mathbf{q}_k + \mathbf{q}_{k-1}}{2}, \mathbf{p}_k\right)\right\}, \tag{2.6}$$

where $\mathbf{q}_k = \mathbf{q}(t_k)$, $\mathbf{p}_k = \mathbf{p}(t_k)$, $\tau = T/N$, $t_k = k\tau$. We make use of the Wigner-Weyl symbol H_W of the quantum Hamitonian $\widehat{H}$ (see Appendix A.1 for details) and of the mid-point prescription for the path's dissection, which corresponds to the above choice of the symbol [62]. For the closed loops we can antisymmetrize $\mathbf{p}_k \cdot (\mathbf{q}_k - \mathbf{q}_{k-1})$ replacing it by

$$\frac{1}{2}\mathbf{p}_k \cdot (\mathbf{q}_k - \mathbf{q}_{k-1}) - \frac{1}{2}\mathbf{q}_{k-1} \cdot (\mathbf{p}_k - \mathbf{p}_{k-1}). \tag{2.7}$$

In the continuous limit (2.5) can be symbolically written as

$$Z(T) = \oint \mathcal{D}\mathbf{q}\mathcal{D}\mathbf{p} \exp\left\{\frac{i}{\hbar}\mathcal{R}_W[\mathbf{q}, \mathbf{p}; T]\right\}, \tag{2.8}$$

where the symbolic notation for the path integration measure

$$\mathcal{D}\mathbf{q}\mathcal{D}\mathbf{p} \equiv \lim_{N\to\infty} \prod_{k=1}^{N} \frac{d\mathbf{q}_k d\mathbf{p}_k}{(2\pi\hbar)^d} \tag{2.9}$$

is introduced. The continuous limit of $\mathcal{R}_W^{(N)}$ yields the Hamilton principal action function

$$\mathcal{R}_W[\mathbf{q}, \mathbf{p}; T] = \oint_0^T \left[\frac{1}{2}(\mathbf{p}\cdot\dot{\mathbf{q}} - \mathbf{q}\cdot\dot{\mathbf{p}}) - H_W(\mathbf{q}, \mathbf{p})\right] dt, \tag{2.10}$$

which appears in (2.8). By subscript "W" we indicate that it has been obtained from the "mid-point" discretization corresponding to the usage of the Wigner-Weyl symbol.

The Fourier-Laplace transform of $Z(T)$ yields, after taking the imaginary part, the density of states

$$g(E) = -\frac{1}{\pi} \operatorname{Im}\left(\frac{1}{i\hbar}\int_0^\infty e^{iET/\hbar} Z(T)\, dT\right). \tag{2.11}$$

The path integral (2.8) receives its largest contributions from the neighborhoods of the classical paths, along which the principal function $\mathcal{R}_W$ is stationary according to Hamilton's variational principle $\delta\mathcal{R}_W = 0$. The first variation hereby yields the classical equations of motion

$$\dot{\mathbf{q}} = \frac{\partial H_W}{\partial \mathbf{p}}, \quad \dot{\mathbf{p}} = -\frac{\partial H_W}{\partial \mathbf{q}}, \tag{2.12}$$

which should be solved with the periodic boundary conditions

$$\mathbf{q}(0) = \mathbf{q}(T), \quad \mathbf{p}(0) = \mathbf{p}(T). \tag{2.13}$$

One may evaluate the integrations in (2.8) using the stationary phase approximation, which becomes asymptotically exact in the classical limit $\mathcal{R} \gg \hbar$. The semiclassical approximation of the partition function $Z(T)$ then turns into a sum over all classical periodic orbits with fixed period T

$$Z_{sc}(T) = \sum_{po} e^{i\mathcal{R}_{po}/\hbar} \int \mathcal{D}\boldsymbol{\eta} \exp\left\{i\mathcal{R}_{po}^{(2)}[\boldsymbol{\eta}; T]\right\}, \quad \mathcal{D}\boldsymbol{\eta} = \lim_{N\to\infty} \prod_{k=1}^{N} \frac{d\boldsymbol{\eta}_k}{(2\pi)^d}, \tag{2.14}$$

where $\mathcal{R}_{po}$ are the principal functions (2.10), evaluated now along the classical orbits. The functional of the second variations is

$$\mathcal{R}_{po}^{(2)}[\boldsymbol{\eta}, T] = \oint_0^T \left[\frac{1}{2}\boldsymbol{\eta}\cdot\mathcal{J}\dot{\boldsymbol{\eta}} - H^{(2)}\right] dt, \tag{2.15}$$

where $\boldsymbol{\eta}$ is the $2d$-dimensional phase-space vector of small variations $\boldsymbol{\eta} = (\boldsymbol{\lambda}, \boldsymbol{\rho}) = (\delta\mathbf{q}, \delta\mathbf{p})/\sqrt{\hbar}$ and $\mathcal{J} = \begin{pmatrix} 0 & I_d \\ -I_d & 0 \end{pmatrix}$ is the $2d$-dimensional unit symplectic matrix. $H^{(2)}$ is the second variation of the classical Hamiltonian $H(\mathbf{q}, \mathbf{p}) = \lim_{\hbar\to 0} H_W(\mathbf{q}, \mathbf{p})$, calculated along the periodic orbits:

$$H^{(2)} = \frac{1}{2}\sum_{l,j=1}^{d}\left[\lambda_l\lambda_j\frac{\partial^2 H}{\partial q_l \partial q_j} + 2\lambda_l\rho_j\frac{\partial^2 H}{\partial q_l \partial p_j} + \rho_l\rho_j\frac{\partial^2 H}{\partial p_l \partial p_j}\right]. \tag{2.16}$$

Note that $Z_{sc}(T)$ does not include the contribution of the zero-length orbits.

After a stationary-phase evaluation of the Fourier-Laplace integral (2.11) with $Z_{sc}(T)$ instead of $Z(T)$, one finally obtains the Gutzwiller's Trace Formula (2.3), where the actions $\mathcal{S}_{po}(E) = \mathcal{R}_{po} + ET_{po}$ are calculated at fixed energy E and the periods of the orbits are $T_{po} = d\mathcal{S}_{po}/dE$. The monodromy matrix M_{po} is defined by $\boldsymbol{\eta}(T_{po}) = M_{po}\,\boldsymbol{\eta}(0)$ in terms of the solutions of the linearized equations of motion $\dot{\boldsymbol{\eta}} = \mathcal{J}\,\partial H^{(2)}/\partial\boldsymbol{\eta}$, which are purely classical. After removing the trivial parabolic block from M_{po} that appears due to the time translation symmetry, one obtains the reduced $2(d-1)$-dimensional monodromy matrix $\widetilde{M}_{po}$. The latter enters the formula (2.4), and, since it contains information about the stability of periodic orbits [18], it is often referred to as the stability matrix. For the Maslov indices $\sigma_{po} \equiv \sigma_r$ (r - repetition number) Sugita has also given general formulae [88]:

$$\sigma_r = \sum_{i=1}^{n_{\rm ell}}\left(1 + 2\left[\frac{r\chi_i}{2\pi}\right]\right) + rn_{\rm ih} + 2rm, \tag{2.17}$$

where n_{ell} is a number of elliptic blocks of $\widetilde{M}_{po}$, χ_i is a stability angle, n_{ih} is a number of inverse hyperbolic blocks, m is a winding number; $[x]$ denotes the largest integer $\leq x$ (see Appendix B.1 for details).

In the presence of continuous symmetries the formula (2.17) is modified so as to take into account the contribution from parabolic blocks which emerge due to these symmetries [88, 74].

Sometimes it is also necessary to include extra-phase corrections to the classical action $\mathcal{S}_{po}(E)$ in (2.3). It happens when the quantum Hamiltonian contains the terms that mix $\hat{q}_j$ and $\hat{p}_j$ for the same j. Unless $\hat{H}$ is Weyl- (symmetrically) ordered, it is not sufficient to take into account just the principal symbol (classical Hamiltonian) $H(\mathbf{q}, \mathbf{p})$ for the calculation of $\mathcal{R}_{po}$. The following proposition can be formulated [80]: in the semiclassical evaluation of the propagator (or its trace (2.14)) the Wigner-Weyl symbol of the quantum Hamiltonian should be taken including the next-to-leading order term

$$H_W(\mathbf{q}, \mathbf{p}) = H(\mathbf{q}, \mathbf{p}) - \delta H(\mathbf{q}, \mathbf{p}) + O(\hbar^2), \quad \delta H(q,p) \sim O(\hbar). \tag{2.18}$$

The classical dynamics is governed by the principal symbol, or naive classical Hamiltonian, $H(\mathbf{q}, \mathbf{p})$, and the next order term $\delta H(\mathbf{q}, \mathbf{p})$ divided by $\hbar$ contributes to the phase of the semiclassical propagator. This extra phase then also appears in the Trace Formula (2.3) correcting the classical action:

$$\frac{1}{\hbar}\mathcal{S}_{po} \to \frac{1}{\hbar}\mathcal{S}_{po} + \delta\Phi, \quad \delta\Phi = \frac{1}{\hbar}\oint \delta H(\mathbf{q}_{po}(t), \mathbf{p}_{po}(t))dt \sim O(\hbar^0). \tag{2.19}$$

If the quantum Hamiltonian $\hat{H}$ is a polynomial in $\hat{q}_j$ and $\hat{p}_j$, it is easy to calculate $\delta H(\mathbf{q}, \mathbf{p})$ using the Moyal formula (Appendix A.1).

We will face the problem of the extra-phase corrections in the next section.

2.2 Coherent-state semiclassical approximations

The problem of the extra-phase corrections discussed in the previous section is often encountered in the coherent-state semiclassical approximations. It is related to the scheme of ordering of annihilation and creation operators. This problem is actual, since the quantum Hamiltonians with the terms mixing

$$\hat{A} = \frac{1}{\sqrt{2}}\left(\hat{q} + i\hat{p}\right), \quad \hat{A}^\dagger = \frac{1}{\sqrt{2}}\left(\hat{q} - i\hat{p}\right), \tag{2.20}$$

are often used in various physical applications. We note that the operators (2.20) satisfy the commutation relation

$$[\hat{A}, \hat{A}^\dagger] = \hbar, \tag{2.21}$$

and differ from the conventional annihilation $\hat{a}$ and creation $\hat{a}^\dagger$ operators by a factor, according to $\hat{a} = \hat{A}/\sqrt{\hbar}$ and $\hat{a}^\dagger = \hat{A}^\dagger/\sqrt{\hbar}$.

In this section we will discuss the coherent-state representation of the semiclassical propagator and its trace. We will show that the extra-phase corrections correspond to the restoration of zero-point energy. They also enable one to reproduce the correct asymptotic result obtained in the standard (q,p) formulation of the semiclassical theory. For simplicity, we restrict ourselves to a single degree of freedom (or a single bosonic mode), the generalization for higher-dimensional systems being straightforward.

The Heisenberg-Weyl coherent state $|\alpha\rangle$ is defined as an eigenstate of the annihilation operator

$$\hat{A}|\alpha\rangle = \alpha|\alpha\rangle, \tag{2.22}$$

where α is a complex number. In contrast to the standard definition, α has the dimension of $\sqrt{\hbar}$.

With the choice of the normalization $\langle\alpha|\alpha\rangle = 1$, the coherent state $|\alpha\rangle$ has the following expansion in the basis of the Fock states:

$$|\alpha\rangle = e^{-|\alpha|^2/2\hbar} e^{\alpha\hat{A}^\dagger/\hbar}|0\rangle = e^{-|\alpha|^2/2\hbar} \sum_{n=0}^{\infty} \frac{\hbar^{-n/2}\alpha^n}{\sqrt{n!}}|n\rangle. \tag{2.23}$$

One can easily check the overlap relation

$$\langle\alpha'|\alpha\rangle = e^{(2\bar{\alpha}'\alpha - |\alpha|^2 - |\alpha'|^2)/2\hbar}, \tag{2.24}$$

which means that coherent states $|\alpha\rangle$ and $|\alpha'\rangle$ are not orthogonal.

The basis of coherent states is (over)complete, and this allows for the resolution of unity

$$\int d\mu(\bar{\alpha}, \alpha)|\alpha\rangle\langle\alpha| = \hat{I}, \tag{2.25}$$

where the measure of integration is given by

$$d\mu(\bar{\alpha}, \alpha) = \frac{d(\mathrm{Re}\alpha)\, d(\mathrm{Im}\alpha)}{\pi\hbar} \equiv \frac{d^2\alpha}{\pi\hbar}. \tag{2.26}$$

This property is very important for the construction of the path-integral representation. In particular, in order to express the coherent-state propagator

$$K(\bar{\alpha}_f, \alpha_i; T) = \langle \alpha_f | T e^{-\frac{i}{\hbar}\int_0^T \hat{H}(t)dt} | \alpha_i \rangle \tag{2.27}$$

by path integral, we divide the time interval T into N small intervals $\tau = T/N$ and define $t_k = k\tau$, $\alpha_k = \alpha(t_k)$, $0 \leq k \leq N$. The time-discrete expression for the propagator (2.27) reads

$$K(\bar{\alpha}_f, \alpha_i; T) = \lim_{N\to\infty} \int \prod_{k=0}^{N} d\mu(\bar{\alpha}_k, \alpha_k) \langle \alpha_f | \alpha_N \rangle \langle \alpha_0 | \alpha_i \rangle \prod_{k=1}^{N} \langle \alpha_k | e^{-\frac{i\tau}{\hbar}\hat{H}(t_k)} | \alpha_{k-1} \rangle. \tag{2.28}$$

Proceeding further, we note that

$$\begin{aligned} \langle \alpha_k | e^{-\frac{i}{\hbar}\tau H(t_k)} | \alpha_{k-1} \rangle &= \langle \alpha_k | \alpha_{k-1} \rangle \{ \exp\{ -\frac{i\tau}{\hbar} H(\bar{\alpha}_k, \alpha_{k-1}; t_k) \} + O(\tau^2) \}, &(2.29) \\ \ln \langle \alpha_k | \alpha_{k-1} \rangle &= \frac{1}{2\hbar} (\bar{\delta}_k \alpha_{k-1} - \bar{\alpha}_k \delta_k) + O(\delta^2), \quad \delta_k = \alpha_k - \alpha_{k-1}, &(2.30) \end{aligned}$$

where

$$H(\bar{\alpha}_k, \alpha_{k-1}; t_k) = \frac{\langle \alpha_k | \hat{H}(t_k) | \alpha_{k-1} \rangle}{\langle \alpha_k | \alpha_{k-1} \rangle}. \tag{2.31}$$

Discarding terms of orders $O(\tau^2)$ and $O(\delta^2)$, we obtain

$$\begin{aligned} K(\bar{\alpha}_f, \alpha_i; T) &= \lim_{N\to\infty} \int_{\alpha_0=\alpha_i}^{\bar{\alpha}_N=\bar{\alpha}_f} \prod_{k=1}^{N-1} d\mu(\bar{\alpha}_k, \alpha_k) \langle \alpha_f | \alpha_{N-1} \rangle \langle \alpha_1 | \alpha_i \rangle \\ &\times \prod_{k=2}^{N-1} \langle \alpha_k | \alpha_{k-1} \rangle \exp \left\{ -\frac{i\tau}{\hbar} \sum_{k=1}^{N} H(\bar{\alpha}_k, \alpha_{k-1}; t_k) \right\} \\ &= \lim_{N\to\infty} \int_{\alpha_0=\alpha_i}^{\bar{\alpha}_N=\bar{\alpha}_f} \prod_{k=1}^{N-1} d\mu(\bar{\alpha}_k, \alpha_k) \langle \alpha_f | \alpha_{N-1} \rangle \langle \alpha_1 | \alpha_i \rangle \\ &\times \exp \left\{ \frac{1}{2\hbar} \sum_{k=2}^{N-1} (\bar{\delta}_k \alpha_{k-1} - \bar{\alpha}_k \delta_k) - \frac{i\tau}{\hbar} \sum_{k=1}^{N} H(\bar{\alpha}_k, \alpha_{k-1}; t_k) \right\}. \end{aligned} \tag{2.32}$$

In the continuous limit it can be symbolically written as

$$K(\bar{\alpha}_f, \alpha_i; T) = \int \mathcal{D}\mu(\bar{\alpha}, \alpha) \exp\{i\Phi\}, \tag{2.33}$$

where $\Phi = (\mathcal{R}_{cov} + \Gamma)/\hbar$ contains the action funtion $\mathcal{R}_{cov}$ as well as the boundary term Γ. The latter is necessary to properly fix the boundary conditions. These terms are given by

$$\begin{aligned} \mathcal{R}_{cov} &= \int_0^T \left[\frac{1}{2i} (\alpha d\bar{\alpha} - \bar{\alpha} d\alpha) - H_{cov}(\bar{\alpha}, \alpha) dt \right], &(2.34) \\ \Gamma &= \frac{1}{2} \left[\bar{\alpha}_f \alpha(T) + \bar{\alpha}(0) \alpha_i - |\alpha_f|^2 - |\alpha_i|^2 \right]. &(2.35) \end{aligned}$$

The subscript "*cov*" indicates that we use the coherent-state (covariant) symbol of the Hamiltonian

$$H_{cov}(\bar{\alpha},\alpha) = \langle\alpha|\hat{H}|\alpha\rangle, \tag{2.36}$$

which corresponds to the dissection of the path such that the variables $\bar{\alpha}(t)$ and $\alpha(t)$ are associated to the discretized variables displaced by one time step, $\bar{\alpha}(t_k)$ and $\alpha(t_{k-1})$, respectively. For a discussion of this point, see [12].

Imposing the periodic boundary condition $\alpha_f = \alpha_i$, we observe that the boundary term Γ (2.35) drops out. Integrating over $d\mu_s(\bar{\alpha}_N, \alpha_N = \alpha_0)$, we obtain an expression for the trace of a propagator

$$Z(T) = \mathrm{Tr}[K] = \lim_{N\to\infty} \oint \prod_{k=1}^{N} d\mu(\bar{\alpha}_k, \alpha_k) \exp\left\{\frac{i}{\hbar}\mathcal{R}^{(N)}\right\}, \tag{2.37}$$

where

$$\mathcal{R}^{(N)} = \sum_{k=1}^{N}\left(\frac{1}{2i}(\bar{\delta}_k\alpha_{k-1} - \bar{\alpha}_k\delta_k) - \tau H(\bar{\alpha}_k, \alpha_{k-1}; t_k)\right). \tag{2.38}$$

In the continuous limit

$$Z(T) = \oint \mathcal{D}\mu(\bar{\alpha},\alpha)\exp\left\{\frac{i}{\hbar}\mathcal{R}_{cov}\right\}, \tag{2.39}$$

where $\mathcal{R}_{cov}$ (2.34) is calculated along closed loops. However, we still need to keep in mind the shift of arguments of $\bar{\alpha}(t)$ and $\alpha(t)$, which takes place in the discretized expression (2.38).

When seeking a semiclassical approxiamtion to the coherent-state propagator (2.33), we will obtain the classical equations of motion from the stationary phase condition $\delta\Phi = 0$:

$$\dot{\alpha} = -i\frac{\partial H_{cov}}{\partial\bar{\alpha}}, \quad \alpha(0) = \alpha_i, \tag{2.40}$$

$$\dot{\bar{\alpha}} = i\frac{\partial H_{cov}}{\partial\alpha}, \quad \bar{\alpha}(T) = \bar{\alpha}_f. \tag{2.41}$$

We have to consider the variables $\bar{\alpha}$ and α as independent so that to ensure the compatibility of the equations of motion with the boundary conditions. It implies that we should distinguish between a canonical ($\bar{\alpha}$) and a complex (α^*) conjugation: $\bar{\alpha} \neq \alpha^*$.

The semiclassical approximation for the coherent-state propagator (2.33) is expressed in terms of classical solutions $\bar{\alpha}_{cl}(t)$ and $\alpha_{cl}(t)$ [55]:

$$K_{sc} = \left(i\frac{\partial^2\mathcal{R}_{cov}}{\partial\bar{\alpha}_f\partial\alpha_i}\right)^{1/2} \exp\left\{i\frac{\mathcal{R}_{cov}}{\hbar} + \frac{i}{2}\int_0^T Bdt\right\}, \tag{2.42}$$

where

$$\begin{aligned}\mathcal{R}_{cov}(\bar{\alpha}_f,\alpha_i,T) &= -\frac{i}{2}\left(\bar{\alpha}_f\alpha_{cl}(T) + \bar{\alpha}_{cl}(0)\alpha_i - |\alpha_f|^2 - |\alpha_i|^2\right) \\ &+ \int_0^T dt\left(-\frac{i}{2}(\dot{\bar{\alpha}}_{cl}\alpha_{cl} - \bar{\alpha}_{cl}\dot{\alpha}_{cl}) - H_{cov}(\bar{\alpha}_{cl},\alpha_{cl})\right)\end{aligned} \tag{2.43}$$

and

$$B = \Delta H_{cov}. \tag{2.44}$$

Hereby Δ denotes the Laplace oprator on the complex plane α

$$\Delta = \frac{\partial^2}{\partial\bar{\alpha}\partial\alpha}. \tag{2.45}$$

The phase correction expressed through the B-term appears due to the accurate account of the shift of arguments in the discretized expression for path integral (2.32). Its emergence can be otherwise interpreted in terms of the operator ordering (Appendix B.2). Here we just illustrate this idea with the following particular example.

Let us consider the normally ordered operator

$$\hat{H}^{no} = \sum_{m,n} h_{mn}\hat{A}^{\dagger m}\hat{A}^{n}. \tag{2.46}$$

Its coherent-state (covariant) symbol

$$(\hat{H}^{no})_{cov}(\bar{\alpha},\alpha) = \langle\alpha|\hat{H}^{no}|\alpha\rangle = \sum_{m,n} h_{mn}\bar{\alpha}^m\alpha^n \tag{2.47}$$

obviously coincides with the principal symbol, while its Wigner-Weyl symbol is

$$H_W = \sum_{m,n} h_{mn}\bar{\alpha}^m\alpha^n + \frac{i\hbar}{2}\sum_{m,n} h_{mn}\{\bar{\alpha}^m,\alpha^n\}_{\bar{\alpha},\alpha} + O(\hbar^2) = H_{cov} - \frac{\hbar}{2}\Delta H_{cov} + O(\hbar^2). \tag{2.48}$$

We can deduce that the phase correction in (2.42) coincides with that introduced in (2.19):

$$\frac{\delta H}{\hbar} = \frac{1}{2}\Delta H_{cov}. \tag{2.49}$$

In the case $h_{11} = \omega$ and $h_{mn} = 0$ for $m,n \neq 1$, we see that $\delta H/\hbar = \omega/2$. When multiplied by T, it exactly coincides with the required phase correction to the semiclassical coherent-state propagator of the harmonic oscillator [39]. Its inclusion is sometimes referred to as a restoration of zero-point energy in the first order of $\hbar$.

Thus, we summarize that for the semiclassical approximation of the trace of propagator (2.39) in the coherent-state basis, we can neglect the difference between $\bar{\alpha}$ and α^* in the equations of motion (2.40)-(2.41), which should be solved with the periodic boundary conditions. We can then consider the variables $\bar{\alpha}$ and α in the continuous limit as being complex conjugated to each other and taken at the same time instant. To restore the correct semiclassical result, we have to just add the phase correction to $\mathcal{R}_{cov}$ according to (2.19). It effectively takes account, with the accuracy required for the semiclassical approximation, of the shift of discretized arguments which has been neglected when we passed to the continuous limit.

It is worth also mentioning that a more rigorous construction of a path integral representation for the coherent-state propagator (2.33) exploits a contravariant symbol $H_{ctr}(\bar{\alpha},\alpha)$. The latter is implicitly given by

$$\hat{H} = \int d\mu(\bar{\alpha},\alpha) H_{ctr}(\bar{\alpha},\alpha)|\alpha\rangle\langle\alpha| \tag{2.50}$$

and differs, in general, from the covariant symbol H_{cov}, as it follows from the non-orthogonality of the coherent states (2.24). Due to the generalized Lie-Trotter formula

$$\lim_{N\to\infty}\left[\hat{K}\left(\frac{T}{N}\right)\right]^N = \exp\left\{-\frac{i}{\hbar}T\hat{H}\right\}, \tag{2.51}$$

where $\hat{H}$ does not depend on t, and $\hat{K}$ satisfies the equation

$$i\hbar\frac{d\hat{K}}{dt} = \hat{H}\hat{K}, \quad \hat{K}(0) = \hat{I}, \tag{2.52}$$

one can write the following expression for the coherent-state propagator (2.27):

$$\begin{aligned} K(\bar{\alpha}_f, \alpha_i; T) &= \lim_{N\to\infty}\int\prod_{k=1}^{N} d\mu(\bar{\alpha}_k, \alpha_k)\langle\alpha_f|\alpha_N\rangle\langle\alpha_1|\alpha_i\rangle\prod_{k=2}^{N}\langle z_k|z_{k-1}\rangle \\ &\times \exp\left\{-\frac{i}{\hbar}\tau\sum_{k=1}^{N} H_{ctr}(\bar{\alpha}_k, \alpha_k)\right\}. \end{aligned} \tag{2.53}$$

For the semiclassical approximation of $K(\bar{\alpha}_f, \alpha_i; T)$ within the contravariant quantization scheme we also refer to Appendix B.2.

Chapter 3

Continuous representations for spin

For the semiclassical description of spin systems it is desirable to express the spin propagator in terms of path integrals. For this purpose we need to exploit a representation in which a spin operator is associated to a continuous function (a symbol of an operator) which is defined on some smooth manifold (phase space). There actually exist several different ways to introduce such a representation, but in every case the spin phase space naturally appears as the sphere $\mathbb{S}^2$.

In this chapter we review the spin coherent-state and the Jordan-Schwinger representations for spin systems, and show their equivalence. We also discuss the so-called Stratonovich-Weyl calculus, which can be regarded as a counterpart of the Wigner-Weyl calculus (Appendix A.1) for the case of spin. The generalization of the Stratonovich-Weyl calculus to include the spin coherent-state representation is presented as well.

3.1 Spin coherent-state representation

3.1.1 Spin coherent states

We intend to generalize the path-integral representation for the trace of propagator (2.8) to include the spin degree of freedom. The main issue then is to be able to describe spin on the quantum-mechanical level by a continuous variable. One can achieve this by using the (over)complete basis of spin coherent states [cf. Sec. 2.2]. The path integral for a system with spin in the SU(2) (spin) coherent-state representation originally appeared in a paper by Klauder [53] as an integral on the sphere $\mathbb{S}^2$. Kuratsuji *et al* [60, 61] have represented it as an integral over paths in the extended complex plane $\bar{\mathbb{C}}^1$.

The SU(2) coherent state $|z\rangle$ for spin s is defined by

$$|z\rangle = (1+|z|^2)^{-s} e^{z\hat{s}_+}|s,-s\rangle = \sum_{m=-s}^{s} \sqrt{\frac{(2s)!}{(s-m)!(s+m)!}} \frac{z^{s+m}}{(1+|z|^2)^s} |s,m\rangle, \qquad (3.1)$$

where $z \in \bar{\mathbb{C}}^1$ is a complex number. The spin operators $\hat{s}_\pm = \hat{s}_1 \pm i\hat{s}_2$ and $\hat{s}_3$ are the generators of the spin su(2) algebra:

$$[\hat{s}_3, \hat{s}_\pm] = \pm\hat{s}_\pm\,, \qquad [\hat{s}_+, \hat{s}_-] = 2\hat{s}_3\,. \qquad (3.2)$$

$|s,m\rangle$ are the eigenstates of $\hat{s}_3$. From the group-theoretical point of view, $s \in \mathbb{N}/2$ labels irreducible representations of SU(2).

In spherical coordinates

$$|z\rangle \equiv |\mathbf{n}\rangle = \sum_{m=-s}^{s} |s,m\rangle \mathcal{D}^s_{ms}(\phi,\theta,\phi), \tag{3.3}$$

where $\mathcal{D}^s$ denotes the matrix of the $(2s+1)$-dimensional representation of SU(2) parametrized by the Euler angles $\alpha = \gamma \equiv \phi$ and $\beta \equiv \theta$ (Appendix C). The relation between z and $\mathbf{n}$ is given by means of the stereographic projection

$$n_1 + in_2 = \frac{2\bar{z}}{1+|z|^2}, \quad n_3 = -\frac{1-|z|^2}{1+|z|^2}. \tag{3.4}$$

From (3.4) and the relation

$$z = \cot\frac{\theta}{2} e^{-i\phi} \tag{3.5}$$

it also follows the standard parametrization of $\mathbb{S}^2$ by polar angles (θ,ϕ):

$$n_1 + in_2 = \sin\theta e^{i\phi}, \quad n_3 = \cos\theta. \tag{3.6}$$

The irreducibility, as well as the existence of the SU(2) invariant measure

$$d\mu_s(\bar{z},z) = \frac{2s+1}{\pi}\frac{d^2z}{(1+|z|^2)^2} \equiv d\mu_s(\mathbf{n}) = \frac{2s+1}{4\pi}\sin\theta d\theta d\phi, \tag{3.7}$$

ensures that the resolution of unity holds in the spin coherent-state basis:

$$\int |z\rangle\langle z|\, d\mu_s(\bar{z},z) \equiv \int |\mathbf{n}\rangle\langle\mathbf{n}|\, d\mu_s(\mathbf{n}) = \hat{I}_{2s+1}\,. \tag{3.8}$$

Like in the case of the Heisenberg-Weyl coherent states discussed in Sec. 2.2, the property (3.8) allows for the path-integral construction. We note that the measure $d\mu_s$ (3.7) takes account of the curvature of the sphere $\mathbb{S}^2$.

Spin coherent states are not orthogonal either, and the following overlap property holds

$$\langle z'|z\rangle = \frac{(1+\bar{z}'z)^{2s}}{(1+|z'|^2)^s(1+|z|^2)^s} \equiv \langle\mathbf{n}'|\mathbf{n}\rangle = \left[\sin\frac{\theta'}{2}\sin\frac{\theta}{2} + \cos\frac{\theta'}{2}\cos\frac{\theta}{2}e^{i(\phi'-\phi)}\right]^{2s}. \tag{3.9}$$

As a consequence, we get

$$|\langle\mathbf{n}'|\mathbf{n}\rangle|^2 = \left(\frac{1+\mathbf{n}'\cdot\mathbf{n}}{2}\right)^{2s}. \tag{3.10}$$

A quantum spin Hamiltonian $\hat{H} = \hat{H}(\hat{\mathbf{s}})$ is a function of spin algebra generators (3.2). Its spin coherent-state (covariant) symbol is defined as an expectation value

$$H_{cov}(\bar{z},z) = \langle z|\hat{H}|z\rangle \tag{3.11}$$

in the spin coherent state (3.1). In particular,

$$\langle z|\hat{s}_+|z\rangle = s\frac{2\bar{z}}{1+|z|^2}, \quad \langle z|\hat{s}_-|z\rangle = s\frac{2z}{1+|z|^2}, \quad \langle z|\hat{s}_3|z\rangle = -s\frac{1-|z|^2}{1+|z|^2}, \tag{3.12}$$

which is equivalent to $\langle \mathbf{n}|\hat{\mathbf{s}}|\mathbf{n}\rangle = s\mathbf{n}$.

Then, for a Hamiltonian linear in spin operators

$$\hat{H} = \mathbf{C}(t)\cdot\hat{\mathbf{s}} = [2A(t)\hat{s}_3 + f(t)\hat{s}_+ + \bar{f}(t)\hat{s}_-], \tag{3.13}$$

where $\mathbf{C}(t) \equiv (2\mathrm{Re}\, f(t), -2\mathrm{Im}\, f(t), 2A(t))$, we obtain

$$H_{cov} = -2sA(t)\frac{1-|z|^2}{1+|z|^2} + 2s\frac{f(t)z + \bar{f}(t)z}{1+|z|^2} = s\mathbf{C}(t)\cdot\mathbf{n}. \tag{3.14}$$

3.1.2 Spin coherent-state propagator

In order to express the spin coherent-state propagator

$$K^s(\bar{z}_f, z_i; T) = \langle z_f|Te^{-i\int_0^T \hat{H}(t)dt}|z_i\rangle \tag{3.15}$$

in terms of path integral, we divide the time interval T into N small intervals $\tau = T/N$ with $N \to \infty$, and define $t_k = k\tau$, $z_k = z(t_k)$, $0 \le k \le N$.

The time-discrete expression for the propagator (3.15) reads

$$K^s(\bar{z}_f, z_i; T) = \lim_{N\to\infty}\int\prod_{k=0}^{N} d\mu_s(\bar{z}_k, z_k)\langle z_f|z_N\rangle\langle z_0|z_i\rangle\prod_{k=1}^{N}\langle z_k|e^{-i\tau\hat{H}(t_k)}|z_{k-1}\rangle. \tag{3.16}$$

Making the following observations

$$\begin{aligned} \langle z_k|e^{-i\tau H(t_k)}|z_{k-1}\rangle &= \langle z_k|z_{k-1}\rangle\{\exp\{-i\tau H(\bar{z}_k, z_{k-1}; t_k)\} + O(\tau^2)\}, && (3.17)\\ \ln\langle z_k|z_{k-1}\rangle &= s\frac{\bar{\delta}_k z_{k-1} - \bar{z}_k\delta_k}{1+\bar{z}_k z_{k-1}} + O(\delta^2), \quad \delta_k = z_k - z_{k-1}, && (3.18) \end{aligned}$$

where

$$H(\bar{z}_k, z_{k-1}; t_k) = \frac{\langle z_k|\hat{H}(t_k)|z_{k-1}\rangle}{\langle z_k|z_{k-1}\rangle}, \tag{3.19}$$

and discarding terms of orders $O(\tau^2)$ and $O(\delta^2)$, we obtain

$$\begin{aligned} K^s(\bar{z}_f, z_i; T) &= \lim_{N\to\infty}\int_{z_0=z_i}^{\bar{z}_N=\bar{z}_f}\prod_{k=1}^{N-1} d\mu_s(\bar{z}_k, z_k)\langle z_f|z_{N-1}\rangle\langle z_1|z_i\rangle \\ &\times \prod_{k=2}^{N-1}\langle z_k|z_{k-1}\rangle\exp\left\{-i\tau\sum_{k=1}^{N} H(\bar{z}_k, z_{k-1}; t_k)\right\} \\ &= \lim_{N\to\infty}\int_{z_0=z_i}^{\bar{z}_N=\bar{z}_f}\prod_{k=1}^{N-1} d\mu_s(\bar{z}_k, z_k)\langle z_f|z_{N-1}\rangle\langle z_1|z_i\rangle \\ &\times \exp\left\{s\sum_{k=2}^{N-1}\frac{\bar{\delta}_k z_{k-1} - \bar{z}_k\delta_k}{1+\bar{z}_k z_{k-1}} - i\tau\sum_{k=1}^{N} H(\bar{z}_k, z_{k-1}; t_k)\right\}. \end{aligned} \tag{3.20}$$

The latter expression can be symbolically written in the continuous limit as

$$K^s(\bar{z}_f, z_i; T) = \int \mathcal{D}\mu_s(\bar{z}, z) \exp\{i\Phi_s\}, \tag{3.21}$$

where $\Phi_s = \mathcal{R}_s + \Gamma_s$ is a sum of the action function and the boundary term

$$\mathcal{R}_s = \int_0^T \left[s\frac{zd\bar{z} - \bar{z}dz}{i(1+|z|^2)} - H_{cov}(\bar{z}, z)dt \right], \tag{3.22}$$

$$\Gamma_s = s \ln \left[\frac{(1+\bar{z}_f z(T))(1+\bar{z}(0)z_i)}{(1+|z_f|^2)(1+|z_i|^2)} \right], \tag{3.23}$$

respectively.

We note that, like in Sec. 2.2, we should keep in mind the shift of arguments of $\bar{z}(t)$ and $z(t)$ in the discretized expression (3.20) when passing to the respective continuous limit (3.21). It makes us consider those variables as independent, and therefore distinguish between $\bar{z}$ and z^*. For a discussion of this point in the case of spin coherent-state propagator, we refer to [56, 86, 40].

Imposing the periodic boundary condition $z_i = z_f$ in (3.20) and integrating over $d\mu_s(\bar{z}_N, z_0 = z_N)$, we obtain an expression for the trace of the propagator

$$Z^s(T) = \mathrm{Tr}[K^s] = \lim_{N\to\infty} \oint \prod_{k=1}^N d\mu_s(\bar{z}_k, z_k) \exp(i\mathcal{R}_s^{(N)}), \tag{3.24}$$

where

$$\mathcal{R}_s^{(N)} = \sum_{k=1}^N \left(s\frac{\bar{\delta}_k z_{k-1} - \bar{z}_k \delta_k}{i(1+\bar{z}_k z_{k-1})} - \tau H(\bar{z}_k, z_{k-1}; t_k) \right). \tag{3.25}$$

In the continuous limit we get

$$Z^s(T) = \oint \mathcal{D}\mu_s(\bar{z}, z) \exp\{i\mathcal{R}_s\}, \tag{3.26}$$

where $\mathcal{R}_s$ (3.22) is calculated along closed loops, and the boundary term Γ_s (3.23) is not present.

3.1.3 Propagator for the Hamiltonian linear in spin

In this section we consider a spin in the external field $\mathbf{C}(t)$ described by the Hamiltonian (3.13). For such a problem, an exact expression for the propagator (3.15) can be obtained by exploiting the SU(2) covariance property. In [35, 56] it has been proved possible to apply the SU(2) projective (canonical) transformations to the path integration variables $\bar{z}$ and z in (3.20). For the Hamiltonian (3.13) the expression (3.20) can then be simplified to give

$$K^s(\bar{z}_f, z_i; T) = \frac{[\bar{a}(T) - \bar{b}(T)\, z_i + b(T)\bar{z}_f + a(T)\, \bar{z}_f z_i]^{2s}}{(1+|z_f|^2)^s(1+|z_i|^2)^s}, \tag{3.27}$$

where the coefficients $a(T)$, $b(T)$ in (3.27) are found from the equation

$$\frac{d}{dt}\begin{pmatrix} a & b \\ -\bar{b} & \bar{a} \end{pmatrix} = -i\begin{pmatrix} A(t) & f(t) \\ \bar{f}(t) & -A(t) \end{pmatrix}\begin{pmatrix} a & b \\ -\bar{b} & \bar{a} \end{pmatrix} \tag{3.28}$$

with the initial conditions $a(0) = 1$, $b(0) = 0$. One can observe that the determinant of the matrix

$$U(t) = \begin{pmatrix} a(t) & b(t) \\ -\bar{b}(t) & \bar{a}(t) \end{pmatrix} \tag{3.29}$$

equals 1 at any t, and therefore $U(t)$ belongs to the group SU(2).

Since

$$\begin{pmatrix} A(t) & f(t) \\ \bar{f}(t) & -A(t) \end{pmatrix} = \frac{1}{2}\mathbf{C}(t)\cdot\boldsymbol{\sigma}, \tag{3.30}$$

where $\boldsymbol{\sigma}$ is a vector of Pauli matrices, we can rewrite (3.28) in the matrix form

$$\frac{d}{dt}U(t) = -\frac{i}{2}(\mathbf{C}(t)\cdot\boldsymbol{\sigma})U(t), \quad U(0) = I_2. \tag{3.31}$$

Note that this equation coincides with the equation for a spin-$\frac{1}{2}$ propagator in the standard $|s, m_s\rangle$ basis.

3.1.4 Trace of the propagator for the Hamiltonian linear in spin

In this section we present calculations of the trace of the propagator (3.27).

Let us first introduce the convenient represention for $U(t)$

$$U(t) = \exp[i\mathbf{m}(t)\cdot\boldsymbol{\sigma}\eta(t)/2] = \cos\frac{\eta(t)}{2} + i(\mathbf{m}(t)\cdot\boldsymbol{\sigma})\sin\frac{\eta(t)}{2}, \tag{3.32}$$

where $|\mathbf{m}(t)| = 1$. Comparing (3.29) and (3.32) we deduce that

$$a(t) = \cos\frac{\eta(t)}{2} + im_3(t)\sin\frac{\eta(t)}{2}, \quad b(t) = i[m_1(t) - im_2(t)]\sin\frac{\eta(t)}{2}. \tag{3.33}$$

Let us consider the equation for the spin-s propagator in the external magnetic field $\mathbf{C}(t)$ [cf. (3.31)]

$$\frac{d}{dt}U^s = -i(\mathbf{C}(t)\cdot\mathbf{J}^s)U^s, \quad U^s(0) = \hat{I}_{2s+1}, \tag{3.34}$$

where $\mathbf{J}^s = (J_1^s, J_2^s, J_3^s)$ are the generators of the $(2s+1)$-dimensional irreducible representation of SU(2).

In general, its solution at $t = T$ can be written in the form

$$U^s(T) = \exp[i\mathbf{m}(T)\cdot\mathbf{J}^s\eta(T)], \tag{3.35}$$

as well as $U(T) \equiv U^{1/2}(T) = \exp[i\mathbf{m}(T)\cdot\boldsymbol{\sigma}\eta(T)/2]$ for (3.31), where $-\eta(T)$ has the meaning of the rotation angle around the $\mathbf{m}(T)$ axis.

We can find the trace of spin propagator $Z^s(T)$ as $\mathrm{tr}[U^s(T)]$. (Note that we distinguish between the matrix trace "tr" and the functional trace "Tr".) Choosing $\mathbf{e}_3 = \mathbf{m}(T)$ as a quantization axis, we obtain after simple calculations

$$Z^s(T) = \mathrm{tr}\left[e^{iJ_3^s\eta(T)}\right] = \sum_{m_s=-s}^{s} e^{im_s\eta(T)} = \frac{\sin[(s+1/2)\eta(T)]}{\sin[\eta(T)/2]}. \tag{3.36}$$

For $s = \frac{1}{2}$ we have

$$Z^{1/2}(T) = 2\cos[\eta(T)/2]. \tag{3.37}$$

On the other hand,

$$Z^{1/2}(T) = \mathrm{tr}[U(T)] = 2\mathrm{Re}[a(T)]. \tag{3.38}$$

Due to the identity [43]

$$\frac{\sin[(s+1/2)\eta(T)]}{\sin[\eta(T)/2]} = C_{2s}^1\left(\cos[\eta(T)/2]\right), \tag{3.39}$$

where C_{2s}^1 is the Gegenbauer polynomial, we find that

$$Z^s(T) = C_{2s}^1\left(\mathrm{Re}[a(T)]\right). \tag{3.40}$$

Alternatively, we can find $Z^s(T)$ equating the functional trace of the spin propagator in spin coherent-state representation (3.27)

$$Z^s(T) = \mathrm{Tr}\left[K^s\right] = \int d\mu_s(\bar{z}', z')\, K^s(\bar{z}_f = \bar{z}', z_i = z'; T), \tag{3.41}$$

where $d\mu_s(\bar{z}', z')$ is given by (3.7) and

$$K^s(\bar{z}', z'; T) = \left[\frac{\bar{a}(T) - \bar{b}(T)z' + b(T)\bar{z}' + a(T)|z'|^2}{1+|z'|^2}\right]^{2s}. \tag{3.42}$$

After the stereographic projection $(\bar{z}', z') \to \mathbf{n}'$, which is defined in (3.4), and simple transformations we can cast (3.42) into the form

$$K^s(\mathbf{n}'; T) = \left(\cos\frac{\eta(T)}{2} + i\mathbf{n}'\cdot\mathbf{m}(T)\sin\frac{\eta(T)}{2}\right)^{2s}. \tag{3.43}$$

Since the measure (3.7) is invariant under rotations, we can choose the axis $\mathbf{e}_3$ along $\mathbf{m}(T)$. Then

$$Z^s(T) = \int d\mu_s(\mathbf{n}')K^s(\mathbf{n}'; T) = \int d\mu_s(\mathbf{n}')\left(\cos\frac{\eta(T)}{2} + in_3'\sin\frac{\eta(T)}{2}\right)^{2s}. \tag{3.44}$$

Making the following transformations in (3.44)

$$\begin{aligned} Z^s(T) &= \frac{2s+1}{2}\int_0^{\pi}\left(\cos\frac{\eta(T)}{2} + i\cos\theta'\sin\frac{\eta(T)}{2}\right)^{2s}\sin\theta' d\theta' \\ &= \frac{2s+1}{2}\int_{-1}^{1}\left(\cos\frac{\eta(T)}{2} + ix\sin\frac{\eta(T)}{2}\right)^{2s} dx \\ &= \frac{1}{2i\sin[\eta(T)/2]}\left(\cos\frac{\eta(T)}{2} + ix\sin\frac{\eta(T)}{2}\right)^{2s+1}\Bigg|_{x=-1}^{x=1}, \end{aligned}$$

we obtain the final result

$$Z^s(T) = \frac{\sin[(s+1/2)\eta(T)]}{\sin[\eta(T)/2]}, \tag{3.45}$$

which evidently coincides with (3.36).

Since $\eta(T)$ is found from $\cos[\eta(T)/2] = \mathrm{Re}[a(T)]$, we have to determine $U(t)$ from (3.31). Such a calculation provides a lot of redundant information about $\mathbf{m}(t)$ and $\eta(t)$ at every t, while we just need to know $\eta(T)$. Therefore, it is desirable to obtain the expression for $\eta(T)$ itself by another, reduced, consideration. In doing so, we will closely follow the discussion in [16] and re-derive the respective result in our notations.

Without loss of generality we again choose the basis in which $\mathbf{e}_3 = \mathbf{m}(T)$. One can decompose $U(t)$ (3.29) at every t into the matrix product

$$U(t) = \begin{pmatrix} \cos[\theta(t)/2]\, e^{-i\phi(t)} & -\sin[\theta(t)/2] \\ \sin[\theta(t)/2] & \cos[\theta(t)/2]\, e^{i\phi(t)} \end{pmatrix} \begin{pmatrix} e^{i\psi(t)} & 0 \\ 0 & e^{-i\psi(t)} \end{pmatrix} \equiv U_1(t)U_0(t). \tag{3.46}$$

where $a = \cos(\theta/2)\, e^{i(\psi-\phi)}$ and $b = -\sin(\theta/2)\, e^{-i\psi}$. Note that

$$U(\theta,\phi,\psi) = \mathcal{D}^{1/2}(\phi,\theta,\phi-2\psi), \tag{3.47}$$

where $\mathcal{D}^s$ is defined in Appendix C.

Decomposition (3.46) corresponds to the choice of a certain section in the principal U(1) Hopf bundle over $\mathbb{S}^2$, ψ being a fiber coordinate. Imposing the time periodicity on $U_1(t)$ and recalling that $U(0) = I_2$, we establish that

$$\psi(T) - \psi(0) = \eta(T)/2. \tag{3.48}$$

Note that the decomposition (3.46) is not well-defined at $t = 0$, i.e., when $\theta = 0$. Hence, the initial value $\psi(0)$ is not determined. (Still, $\eta(T)$ can be found unambiguously.) Although not essential for our purposes, the problem can be fixed if we choose a different decomposition near $\theta = 0$, related to the former by a gauge transformation [16, 95].

We define the projection of the Hopf bundle $(\theta,\phi,\psi) \in \mathbb{S}^3 \longrightarrow (\theta,\phi) \in \mathbb{S}^2$ by

$$\mathbf{n}\cdot\boldsymbol{\sigma} = U\sigma_3 U^\dagger = U_1\sigma_3 U_1^\dagger, \tag{3.49}$$

which is equivalent to $n_1 + in_2 = \sin\theta\exp(i\phi)$, $n_3 = \cos\theta$. One can find equations for $\mathbf{n}(t)$ and $\psi(t)$ from (3.31). Thus, one should calculate

$$\dot{\mathbf{n}} = \frac{1}{2}\mathrm{tr}\left[\boldsymbol{\sigma}\frac{d}{dt}\left(U\sigma_3 U^\dagger\right)\right] \tag{3.50}$$

to recover the equation

$$\dot{\mathbf{n}} = \mathbf{C}\times\mathbf{n}, \quad \mathbf{n}(0) = \mathbf{n}(T). \tag{3.51}$$

After the stereographic projection (3.4) it becomes

$$\dot{z} = -i[2Az + f - \bar{f}z^2], \quad z(0) = z(T). \tag{3.52}$$

To derive an equation for ψ, one should calculate

$$\dot{\psi} - \frac{1}{2}(1+\cos\theta)\dot{\phi} = -\frac{i}{2}\mathrm{tr}\left[\sigma_3 U^\dagger \frac{d}{dt}U\right] \tag{3.53}$$

taking into account (3.46) and (3.52). In the language of the fiber bundle theory, it corresponds to the pull-back of the canonical connection form [*r.h.s.* of (3.53)] onto the section defined by (3.46). The result of the calculation is

$$\dot{\psi} = \frac{1}{2i}\frac{z\dot{\bar{z}} - \bar{z}\dot{z}}{1+|z|^2} - \frac{1}{2}\mathbf{C}\cdot\mathbf{n}(\bar{z},z) = A - \frac{1}{2}(\bar{f}z + f\bar{z}). \tag{3.54}$$

Integrating it we find

$$\begin{aligned}\eta(T) &= 2[\psi(T)-\psi(0)] = \int_0^T dt\left[\frac{z\dot{\bar{z}} - \bar{z}\dot{z}}{i(1+|z|^2)} - \mathbf{C}\cdot\mathbf{n}(\bar{z},z)\right] \\ &= \int_0^T dt\,[2A - (\bar{f}z + f\bar{z})],\end{aligned} \tag{3.55}$$

where $z(t)$ and $\bar{z}(t)$ are implicitly given by the Riccati-type equation (3.52).

In two particular cases we can find explicitly $z(t)$ and $\bar{z}(t)$ from (3.52) and bring the expression (3.55) to the closed form.

In the case of the rotating magnetic field $\mathbf{C}(t) = c\Omega\cdot(\sin\theta\cos\Omega t, \sin\theta\sin\Omega t, \cos\theta)$ with constant c, Ω, and θ, we look for the solution of (3.52) in the form

$$z = -|z|\exp(-i\Omega t), \tag{3.56}$$

where $|z|$ is constant given by the quadratic equation

$$|z|^2 - 2\frac{1-c\cos\theta}{c\sin\theta}|z| - 1 = 0. \tag{3.57}$$

We choose one of the two roots

$$|z|_\pm = \frac{1-c\cos\theta}{c\sin\theta} \pm \sqrt{\frac{(1-c\cos\theta)^2}{c^2\sin^2\theta}+1} \tag{3.58}$$

and calculate $\eta(T)$ with $\Omega = 2\pi/T$ and $|\mathbf{C}| = 2\pi c/T$:

$$\eta(T) = 2\pi\left(1+\sqrt{(1-c\cos\theta)^2 + c^2\sin^2\theta}\right). \tag{3.59}$$

In the case of Zeeman Hamiltonian (constant magnetic field)

$$\hat{H}_Z = |\mathbf{C}|\hat{s}_3 \tag{3.60}$$

the trace of propagator equals

$$Z_Z^s(T) = \frac{\sin[(s+1/2)|\mathbf{C}|T]}{\sin[|\mathbf{C}|T/2]}. \tag{3.61}$$

We note that the constant magnetic field can be also regarded as a subcase of the rotating magnetic field in the limit $\theta \to 0$.

3.2 Jordan-Schwinger representation

In the Jordan-Schwinger representation [51, 83] the spin operators $\hat{\mathbf{s}}$ are expressed in terms of bosonic operators $\hat{a}$, $\hat{a}^\dagger$ and $\hat{b}$, $\hat{b}^\dagger$:

$$\hat{\mathbf{s}} = \frac{1}{2}(\hat{a}^\dagger, \hat{b}^\dagger)\ \boldsymbol{\sigma} \begin{pmatrix} \hat{a} \\ \hat{b} \end{pmatrix}. \tag{3.62}$$

One can check that the commutation relations (3.2) are fulfilled, and the following identity holds

$$\hat{\mathbf{s}}^2 = \frac{\hat{a}^\dagger\hat{a} + \hat{b}^\dagger\hat{b}}{2}\left(\frac{\hat{a}^\dagger\hat{a} + \hat{b}^\dagger\hat{b}}{2} + 1\right). \tag{3.63}$$

The latter relation imposes the constraint

$$\hat{a}^\dagger\hat{a} + \hat{b}^\dagger\hat{b} - 2s = 0, \tag{3.64}$$

which fixes the subspace, corresponding to the spin-s representation, in the Fock space with the basis

$$|(n_a, n_b)\rangle = \frac{(\hat{a}^\dagger)^{n_a}(\hat{b}^\dagger)^{n_b}}{\sqrt{n_a!\, n_b!}}|(0,0)\rangle. \tag{3.65}$$

Coherent states $|(\alpha,\beta)\rangle = |\alpha\rangle|\beta\rangle$ are the common eigenstates of both annihilation operators $\hat{a}$ and $\hat{b}$ [cf. (2.22), $\hbar = 1$]:

$$\hat{a}|(\alpha,\beta)\rangle = \alpha|(\alpha,\beta)\rangle, \quad \hat{b}|(\alpha,\beta)\rangle = \beta|(\alpha,\beta)\rangle. \tag{3.66}$$

The expansion of $|(\alpha,\beta)\rangle$ in the basis of Fock states reads

$$\begin{aligned} |(\alpha,\beta)\rangle &= e^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)} e^{\alpha\hat{a}^\dagger + \beta\hat{b}^\dagger}|(0,0)\rangle \\ &= e^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)} \sum_s \sum_{m_s=-s}^{s} \frac{\alpha^{s+m_s}\beta^{s-m_s}}{\sqrt{(s+m_s)!\,(s-m_s)!}}|s, m_s\rangle, \end{aligned} \tag{3.67}$$

where we have made the identification $|s, m_s\rangle \equiv |(s+m_s, s-m_s)\rangle$.

For the coherent states (3.67) there holds the resolution of unity [cf. (2.25)]

$$\int \frac{d^2\alpha}{\pi}\frac{d^2\beta}{\pi}|(\alpha,\beta)\rangle\langle(\alpha,\beta)| = \hat{I}. \tag{3.68}$$

The constraint (3.64) is realized by a projection operator in the Fock space

$$\hat{P}_s = \lim_{\epsilon\to+0}\int_0^{2\pi}\frac{d\lambda}{2\pi}e^{i\lambda(\hat{a}^\dagger\hat{a}+\hat{b}^\dagger\hat{b}-2s)-\epsilon(\hat{a}^\dagger\hat{a}+\hat{b}^\dagger\hat{b})}. \tag{3.69}$$

Due to (3.68) it can be rewritten [39] in the form

$$\begin{aligned} \hat{P}_s &= \int\frac{d^2\alpha d^2\beta}{\pi^2}\frac{d^2\alpha' d^2\beta'}{\pi^2}|(\alpha,\beta)\rangle\langle(\alpha',\beta')|\int_0^{2\pi}\frac{d\lambda}{2\pi}\langle(\alpha,\beta)|e^{i\lambda(\hat{a}^\dagger\hat{a}+\hat{b}^\dagger\hat{b}-2s)}|(\alpha',\beta')\rangle \\ &= \frac{1}{(2s)!}\int\frac{d^2\alpha d^2\beta}{\pi^2}|(\alpha,\beta)\rangle\langle(0,0)|(\bar{\alpha}\hat{a}+\bar{\beta}\hat{b})^{2s}e^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)}, \end{aligned} \tag{3.70}$$

rigorous ϵ-prescription of (3.69) being omitted.

Making change of variables

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \zeta \begin{pmatrix} z \\ 1 \end{pmatrix}, \quad d^2\alpha d^2\beta = |\zeta|^2 d^2\zeta d^2 z, \tag{3.71}$$

and integrating with respect to ζ, we find

$$\begin{aligned} \hat{P}_s &= \frac{1}{(2s)!}\int \frac{|\zeta|^2 d^2\zeta d^2 z}{\pi^2} e^{\zeta(z\hat{a}^\dagger+\hat{b}^\dagger)}|(0,0)\rangle\langle(0,0)|\{\bar{\zeta}(\bar{z}\hat{a}+\hat{b})\}^{2s} e^{-|\zeta|^2(1+|z|^2)} \\ &= \frac{2s+1}{\pi}\int \frac{d^2 z}{(1+|z|^2)^2} \frac{(z\hat{a}^\dagger+\hat{b}^\dagger)^{2s}}{\sqrt{(2s)!}\,(1+|z|^2)^s}|(0,0)\rangle\langle(0,0)|\frac{(\bar{z}\hat{a}+\hat{b})^{2s}}{\sqrt{(2s)!}\,(1+|z|^2)^s} \\ &= \sum_{m,n=0}^{\infty}\frac{2s+1}{\pi}\int \frac{d^2 z}{(1+|z|^2)^2}\frac{1}{(1+|z|^2)^{2s}}\frac{(\zeta\hat{a}^\dagger\hat{b})^m}{m!}|(0,2s)\rangle\langle(0,2s)|\frac{(\bar{\zeta}\hat{a}\hat{b}^\dagger)^n}{n!} \\ &= \frac{2s+1}{\pi}\int \frac{d^2 z}{(1+|z|^2)^2}|z\rangle\langle z| \equiv \hat{I}_{2s+1}. \end{aligned} \tag{3.72}$$

Thus, the expressions for the projection operator $\hat{P}_s$ in the Fock space and the identity operator $\hat{I}_{2s+1}$ in the spin-s representation (3.8) coincide. This establishes the equivalence of the Jordan-Schwinger and the spin coherent-state representations.

One can construct a path-integral expression for the spin propagator in the Jordan-Schwinger representation [17]. Imposing the periodic boundary conditions, one gets its trace, which amounts to

$$Z^s(T) = \lim_{N\to\infty}\prod_{k=1}^{N}\frac{d^2\alpha_k d^2\beta_k}{\pi^2}\langle(\alpha_k,\beta_k)|e^{-i\tau\hat{H}(t_k)}\hat{P}_s|(\alpha_{k-1},\beta_{k-1})\rangle. \tag{3.73}$$

We note that in this expression the constraint (3.64) is taken into account by including the projection operator $\hat{P}_s$ at each time instant.

3.3 Moyal representation for spin

In Appendix A.1 the Wigner-Weyl calculus [93, 94], which establishes the correspondence between quantum operators $\hat{H}(\hat{\mathbf{q}}, \hat{\mathbf{p}})$ and their phase-space symbols, is discussed. The list of properties, which the Wigner-Weyl symbols possess, is also quoted there. These properties appear to be necessary and sufficient to establish the Wigner-Weyl correspondence.

In Appendix A.2 one of the listed properties is generalized. This leads to generalization of the definition of the respective phase-space symbols. In fact, one can then introduce a continuous family of symbols, which includes the Wigner-Weyl and the coherent-state symbols (defined in Sec. 2.2) as particular cases.

In the case of spin operators $\hat{H}(\hat{\mathbf{s}})$ the similar set of properties has been fomulated by Stratonovich [87]. In [90] the Stratonovich-Weyl correspondence has been constructed on the basis of these properties. Such a phase-space representation of quantum spin systems has been called the Moyal representation for spin, and the Moyal-like formula [cf. (A.7)] for the symbol of the product of two spin operators has been also derived in [90].

Later on, the generalization of the Stratonovich postulates has been proposed in [20], and a continuous family of symbols interpolating between the Stratonovich-Weyl and the spin coherent-state symbols (defined in Sec. 3.1) has been constructed [54].

In this section we review the Stratonovich-Weyl correspondence and its generalization, so that to make transparent the analogy between the Wigner-Weyl and Stratonovich-Weyl symbol calculi. We also discuss the application of the latter to the path-integral representation of the spin propagator.

3.3.1 Stratonovich-Weyl calculus

The Stratonovich-Weyl correspondence is established by the formula

$$A_W(\mathbf{n}) = \mathrm{tr}[\hat{A}\hat{\Delta}^s(\mathbf{n})], \tag{3.74}$$

where $\hat{\Delta}^s(\mathbf{n})$ is the operator kernel [cf. (A.1)]. The following properties (Stratonovich postulates) [87] are imposed on the phase-space symbol $A_W(\mathbf{n})$, which is defined on the unit sphere $\mathbf{n} \in \mathbb{S}^2$:

0) linearity, i.e. $\hat{A} \longrightarrow A_W(\mathbf{n})$ is a one-to-one map;

i) reality
$$(\hat{A}^\dagger)_W(\mathbf{n}) = A_W^*(\mathbf{n}); \tag{3.75}$$

ii) standartization
$$\mathrm{tr}\hat{A} = \int_{\mathbb{S}^2} d\mu_s(\mathbf{n}) A_W(\mathbf{n}), \tag{3.76}$$
where $d\mu_s(\mathbf{n})$ is given by (3.7);

iii) traciality
$$\mathrm{tr}[\hat{A}\hat{B}] = \int_{\mathbb{S}^2} d\mu_s(\mathbf{n}) A_W(\mathbf{n}) B_W(\mathbf{n}); \tag{3.77}$$

iv) covariance

$$\left(\mathcal{D}^s(g)\hat{A}\mathcal{D}^s(g^{-1})\right)_W(\mathbf{n}) = A_W(O^{-1}(g)\mathbf{n}), \tag{3.78}$$

where $\mathcal{D}^s(g)$ denotes a matrix of the $(2s+1)$-dimensional SU(2) representation, O denotes a 3×3 matrix of adjoint (orthogonal) representation (Appendix C).

The properties (i-iv) can be translated to the operator kernel $\hat{\Delta}^s(\mathbf{n})$:

i')

$$\hat{\Delta}^s(\mathbf{n}) = \left[\hat{\Delta}^s(\mathbf{n})\right]^\dagger; \tag{3.79}$$

ii')

$$\hat{I}_{2s+1} = \int_{\mathbb{S}^2} d\mu_s(\mathbf{n})\hat{\Delta}^s(\mathbf{n}); \tag{3.80}$$

iii')

$$\hat{\Delta}^s(\mathbf{m}) = \int_{\mathbb{S}^2} d\mu_s(\mathbf{n})\mathrm{tr}[\hat{\Delta}^s(\mathbf{m})\hat{\Delta}^s(\mathbf{n})]\hat{\Delta}^s(\mathbf{n}); \tag{3.81}$$

iv')

$$\hat{\Delta}^s(O(g)\mathbf{n}) = \mathcal{D}^s(g)\hat{\Delta}^s(\mathbf{n})\mathcal{D}^s(g^{-1}). \tag{3.82}$$

The function

$$\delta^s(\mathbf{m},\mathbf{n}) = \mathrm{tr}[\hat{\Delta}^s(\mathbf{m})\hat{\Delta}^s(\mathbf{n})] \tag{3.83}$$

is called the reproducing kernel. It plays the role of δ-function on $\mathbb{S}^2$, since it relates symbols with different arguments

$$A_W(\mathbf{m}) = \int_{\mathbb{S}^2} d\mu_s(\mathbf{n})\delta^s(\mathbf{m},\mathbf{n})A_W(\mathbf{n}). \tag{3.84}$$

As a consequence of (3.81), one can establish the inverse mapping

$$\hat{A} = \int_{\mathbb{S}^2} d\mu_s(\mathbf{n})A_W(\mathbf{n})\hat{\Delta}^s(\mathbf{n}) \tag{3.85}$$

with the same operator kernel as in (3.74).

It has been shown in [90] that kernel $\hat{\Delta}^s(\mathbf{n})$ exists, and its definition is not unique. The problem of finding a Stratonovich-Weyl correspondence has exactly 2^{2s} solutions. They are given by

$$\hat{\Delta}^s(\mathbf{n}) = \sum_{p,q=-s}^{s} Z^s_{pq}(\mathbf{n})|s,p\rangle\langle s,q| \tag{3.86}$$

with matrix elements

$$Z^s_{pq}(\mathbf{n}) = \sum_{l=0}^{2s}\sum_{m=-l}^{l}\varepsilon^s_l\sqrt{\frac{4\pi}{2s+1}}(-1)^{s-p}\left\langle \begin{matrix} s & s \\ p & -q \end{matrix} \middle| \begin{matrix} l \\ -m \end{matrix}\right\rangle Y_{lm}(\mathbf{n}), \tag{3.87}$$

where $Y_{lm}(\mathbf{n})$ are the spherical harmonics. For $l=0$ the value of $\varepsilon^s_l=+1$ is fixed by the standartization condition, while for $l=1,\dots,2s$ the value of $\varepsilon^s_l=\pm 1$ is determined up to a sign. This causes the ambiguity in the definition of the Stratonovich-Weyl symbol, the number of possible versions being equal 2^{2s}.

We remark that arbitrary function $f(\mathbf{n})$ on $\mathbb{S}^2$ can be expanded in a series of spherical harmonics

$$f(\mathbf{n}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} f_{lm} Y_{lm}(\mathbf{n}) \tag{3.88}$$

with integer l running to infinity. The expansion of the symbol (3.74) terminates, as follows from (3.87), at the maximal value of $l = 2s$. Then, if we would take an arbitrary function and construct the respective operator according to (3.85), the harmonics with l higher than $2s$ will be neglected. Thus, in the spin-s representation the correspondence between spin operators and phase-space functions holds modulo these higher harmonics.

The explicit expression for the reproducing kernel (3.83) reads

$$\delta^s(\mathbf{m},\mathbf{n}) = \sum_{l=0}^{2s} \sum_{m=-l}^{l} Y_{lm}(\mathbf{m}) Y^*_{lm}(\mathbf{n}) = \sum_{l=0}^{2s} \frac{2l+1}{4\pi} P_l(\mathbf{m}\cdot\mathbf{n}), \tag{3.89}$$

where P_l are the Legendre polynomials. Note that there holds the identity

$$\sum_{m=-l}^{l} Y_{lm}(\mathbf{m}) Y^*_{lm}(\mathbf{n}) = \frac{2l+1}{4\pi} P_l(\mathbf{m}\cdot\mathbf{n}). \tag{3.90}$$

The operator kernel $\hat{\Delta}^s$ can be expressed in terms of the spin coherent states (3.1)

$$\hat{\Delta}^s(\mathbf{n}) = \sum_{l=0}^{2s} (\varepsilon_l^s b_l^s)^{-1} \frac{2l+1}{2s+1} \int_{\mathbb{S}^2} d\mu_s(\mathbf{m}) P_l(\mathbf{n}\cdot\mathbf{m}) |\mathbf{m}\rangle\langle\mathbf{m}|, \tag{3.91}$$

where

$$b_l^s = \left\langle \begin{array}{cc} s & l \\ s & 0 \end{array} \middle| \begin{array}{c} s \\ s \end{array} \right\rangle = \frac{(2s)!\sqrt{2s+1}}{\sqrt{(2s+l+1)!(2s-l)!}}. \tag{3.92}$$

One can easily establish the relations of the respective Stratonovich-Weyl symbol to the Berezin's covariant and contravariant symbols [6]:

$$\begin{aligned}
A_W(\mathbf{n}) &= \sum_{l=0}^{2s} (\varepsilon_l^s b_l^s)^{-1} \frac{2l+1}{2s+1} \int_{\mathbb{S}^2} d\mu_s(\mathbf{m}) P_l(\mathbf{n}\cdot\mathbf{m}) A_{cov}(\mathbf{m}), &(3.93)\\
A_{cov}(\mathbf{n}) &= \sum_{l=0}^{2s} (\varepsilon_l^s b_l^s)^{+1} \frac{2l+1}{2s+1} \int_{\mathbb{S}^2} d\mu_s(\mathbf{m}) P_l(\mathbf{n}\cdot\mathbf{m}) A_W(\mathbf{m}), &(3.94)\\
A_W(\mathbf{n}) &= \sum_{l=0}^{2s} (\varepsilon_l^s b_l^s)^{+1} \frac{2l+1}{2s+1} \int_{\mathbb{S}^2} d\mu_s(\mathbf{m}) P_l(\mathbf{n}\cdot\mathbf{m}) A_{ctr}(\mathbf{m}), &(3.95)\\
A_{ctr}(\mathbf{n}) &= \sum_{l=0}^{2s} (\varepsilon_l^s b_l^s)^{-1} \frac{2l+1}{2s+1} \int_{\mathbb{S}^2} d\mu_s(\mathbf{m}) P_l(\mathbf{n}\cdot\mathbf{m}) A_W(\mathbf{m}). &(3.96)
\end{aligned}$$

We recall that the covariant symbol $A_{cov}(\mathbf{n})$ coincides with the spin coherent-state symbol (3.11), and the contravariant symbol $A_{ctr}(\mathbf{n})$ is implicitly given by

$$\hat{A} = \int d\mu_s(\mathbf{n}) A_{ctr}(\mathbf{n}) |\mathbf{n}\rangle\langle\mathbf{n}|. \tag{3.97}$$

We also remark that the derivation of the expressions (3.94)-(3.96) implies the use of the orthogonality condition of the Legendre polynomials

$$\frac{2l+1}{2s+1}\int_{\mathbb{S}^2} d\mu_s(\mathbf{n}) P_l(\mathbf{m}\cdot\mathbf{n}) P_{l'}(\mathbf{n}\cdot\mathbf{k}) = \delta_{ll'} P_l(\mathbf{m}\cdot\mathbf{k}), \tag{3.98}$$

and the relations between the covariant and contravariant symbols

$$A_{ctr}(\mathbf{n}) = \sum_{l=0}^{2s} (b_l^s)^{-2} \frac{2l+1}{2s+1} \int_{\mathbb{S}^2} d\mu_s(\mathbf{m}) P_l(\mathbf{n}\cdot\mathbf{m}) A_{cov}(\mathbf{m}), \tag{3.99}$$

$$A_{cov}(\mathbf{n}) = \sum_{l=0}^{2s} (b_l^s)^{+2} \frac{2l+1}{2s+1} \int_{\mathbb{S}^2} d\mu_s(\mathbf{m}) P_l(\mathbf{n}\cdot\mathbf{m}) A_{ctr}(\mathbf{m}). \tag{3.100}$$

Note that (3.99) provides an explicit formula for the calculation of contravariant symbols.

Berezin's symbols A_{cov} and A_{ctr} do not possess the tracial property

$$\int_{\mathbb{S}^2} d\mu_s(\mathbf{n}) A_{cov}(\mathbf{n}) B_{cov}(\mathbf{n}) \neq \mathrm{tr}[\hat{A}\hat{B}] \neq \int_{\mathbb{S}^2} d\mu_s(\mathbf{n}) A_{ctr}(\mathbf{n}) B_{ctr}(\mathbf{n}), \tag{3.101}$$

which means that with either class the expectation values cannot be calculated as phase-space averages. For instance, if $\hat{A} = \hat{B} = \hat{s}_3$, then $A_{cov} = s\cos\theta$, $A_{ctr} = (s+1)\cos\theta$, and the three terms in (3.101) are in the proportion $s^2 : s(s+1) : (s+1)^2$. There holds even a stronger relation for operators $\hat{A} \neq \hat{I}_{2s+1}$ and $\hat{B} \neq \hat{I}_{2s+1}$

$$\int_{\mathbb{S}^2} d\mu_s(\mathbf{n}) A_{cov}(\mathbf{n}) B_{cov}(\mathbf{n}) < \mathrm{tr}[\hat{A}\hat{B}] < \int_{\mathbb{S}^2} d\mu_s(\mathbf{n}) A_{ctr}(\mathbf{n}) B_{ctr}(\mathbf{n}), \tag{3.102}$$

which is known as Berezin-Lieb inequality [7, 64].

However, another observation made by Berezin [7]

$$\int_{\mathbb{S}^2} d\mu_s(\mathbf{n}) A_{cov}(\mathbf{n}) B_{ctr}(\mathbf{n}) = \mathrm{tr}[\hat{A}\hat{B}] = \int_{\mathbb{S}^2} d\mu_s(\mathbf{n}) A_{ctr}(\mathbf{n}) B_{cov}(\mathbf{n}) \tag{3.103}$$

allows for the generalization of the tracial condition and construction of a wider class of symbols continuously interpolating between covariant, Weyl and contravariant symbols.

3.3.2 Generalized Stratonovich-Weyl calculus

In [20] the generalized Stratonovich-Weyl calculus referring to the generalized coherent states [77] has been developed. The Cahill-Glauber [22] and Stratonovich-Weyl symbol calculi referring to the Heisenberg-Weyl and SU(2) groups, respectively, appear as particular cases in such a consideration. The details of the Cahill-Glauber construction of a family of symbols continuously interpolating between covariant, Weyl and contravariant symbols for the Heisenberg-Weyl group can be found in Appendix A.2. For the SU(2) (spin) group the generalized Stratonovich-Weyl symbols have been recently presented in [54]. We briefly outline the main results below, giving the explicit formulae for the generalized operator kernels and for the respective symbols.

We can define a λ-symbol $A^{(\lambda)}(\mathbf{n})$ through the generalized operator kernel $\hat{\Delta}^s_\lambda(\mathbf{n})$ with $\lambda \in [0,1]$ similarly to (3.74):

$$A^{(\lambda)}(\mathbf{n}) = \mathrm{tr}[\hat{A}\hat{\Delta}^s_\lambda(\mathbf{n})]. \tag{3.104}$$

To specify the generalized opretor kernel $\hat{\Delta}^s_\lambda(\mathbf{n})$, we impose the postulates of reality, standartization and covariance on $\hat{\Delta}^s_\lambda(\mathbf{n})$, which are the same as for $\hat{\Delta}^s(\mathbf{n})$ (Sec. 3.3.1). The tracial condition is generalized to be

$$\hat{\Delta}^s_\lambda(\mathbf{m}) = \int_{\mathbb{S}^2} d\mu_s(\mathbf{n})\mathrm{tr}[\hat{\Delta}^s_\lambda(\mathbf{m})\hat{\Delta}^s_{1-\lambda}(\mathbf{n})]\hat{\Delta}^s_\lambda(\mathbf{n}). \tag{3.105}$$

Obviously, for $\lambda = \frac{1}{2}$ we recover the original tracial condition (3.81), and therefore $\hat{\Delta}^s_{1/2} \equiv \hat{\Delta}^s$ and $A^{(1/2)} \equiv A_W$ are reproduced.

The reproducing kernel corresponding to (3.105) is given by

$$\delta^s(\mathbf{m},\mathbf{n}) = \mathrm{tr}[\hat{\Delta}^s_\lambda(\mathbf{m})\hat{\Delta}^s_{1-\lambda}(\mathbf{n})]. \tag{3.106}$$

From (3.105) it also follows the representation of the operator $\hat{A}$ in terms of the kernel basis

$$\hat{A} = \int_{\mathbb{S}^2} d\mu_s(\mathbf{n})A^{(\lambda)}(\mathbf{n})\hat{\Delta}^s_{1-\lambda}(\mathbf{n}). \tag{3.107}$$

We emphasize that, unlike to (3.104), it uses $\hat{\Delta}^s_{1-\lambda}$, which is conjugated to $\hat{\Delta}^s_\lambda$ by the new tracial condition (3.105).

An explicit formula for λ-kernel reads

$$\hat{\Delta}^s_\lambda(\mathbf{n}) = \sum_{l=0}^{2s}(\varepsilon^s_l b^s_l)^{-2\lambda}\frac{2l+1}{2s+1}\int_{\mathbb{S}^2} d\mu_s(\mathbf{m})P_l(\mathbf{n}\cdot\mathbf{m})\hat{\Delta}^s_0(\mathbf{m}), \tag{3.108}$$

where

$$\hat{\Delta}^s_0(\mathbf{m}) = |\mathbf{m}\rangle\langle\mathbf{m}|, \tag{3.109}$$

and all ε^s_l must be taken equal to $+1$ in order to satisfy the reality condition for every λ.

Using the definition (3.108), the identity

$$|\langle\mathbf{m}|\mathbf{n}\rangle|^2 = \left(\frac{1+\mathbf{m}\cdot\mathbf{n}}{2}\right)^{2s} = \sum_{l=0}^{2s}(b^s_l)^{+2}\frac{2l+1}{2s+1}P_l(\mathbf{m}\cdot\mathbf{n}), \tag{3.110}$$

and the relation (3.98), we can easily check that the reproducing kernel (3.106) does not depend on λ and coincides with (3.89). Due to its reproducing property, we recover the identity in (3.108) at $\lambda = 0$.

For $\lambda = 1$ we get

$$\hat{\Delta}_1^s(\mathbf{n}) = \sum_{l=0}^{2s} (b_l^s)^{-2} \frac{2l+1}{2s+1} \int_{\mathbb{S}^2} d\mu_s(\mathbf{m}) P_l(\mathbf{n}\cdot\mathbf{m}) \hat{\Delta}_0^s(\mathbf{m}). \tag{3.111}$$

A more general relation between arbitrary λ- and λ'-kernels reads

$$\hat{\Delta}_\lambda^s(\mathbf{n}) = \sum_{l=0}^{2s} (b_l^s)^{-2(\lambda-\lambda')} \frac{2l+1}{2s+1} \int_{\mathbb{S}^2} d\mu_s(\mathbf{m}) P_l(\mathbf{n}\cdot\mathbf{m}) \hat{\Delta}_{\lambda'}^s(\mathbf{m}). \tag{3.112}$$

From (3.104) and (3.108) we obtain an expression for λ-symbol

$$A^{(\lambda)}(\mathbf{n}) = \sum_{l=0}^{2s} (b_l^s)^{-2\lambda} \frac{2l+1}{2s+1} \int_{\mathbb{S}^2} d\mu_s(\mathbf{m}) P_l(\mathbf{n}\cdot\mathbf{m}) A^{(0)}(\mathbf{m}), \tag{3.113}$$

where $A^{(0)}$ and $A^{(1)}$ are idetified with A_{cov} and A_{ctr}, respectively. A general relation between λ- and λ'-symbols

$$A^{(\lambda)}(\mathbf{n}) = \sum_{l=0}^{2s} (b_l^s)^{-2(\lambda-\lambda')} \frac{2l+1}{2s+1} \int_{\mathbb{S}^2} d\mu_s(\mathbf{m}) P_l(\mathbf{n}\cdot\mathbf{m}) A^{(\lambda')}(\mathbf{m}) \tag{3.114}$$

follows from (3.112).

We note that the generalized tracial condition (3.105) can be equivalently formulated in the form

$$\mathrm{tr}[\hat{A}\hat{B}] = \int_{\mathbb{S}^2} d\mu_s(\mathbf{n}) A^{(\lambda)}(\mathbf{n}) B^{(1-\lambda)}(\mathbf{n}), \tag{3.115}$$

which reproduces (3.103) at $\lambda = 0$ and $\lambda = 1$.

In the semiclassical limit $s \to \infty$ the relation between spin covariant and contravariant symbols reads [58]

$$A_{cov}(\bar{z}, z) = \left[1 + \frac{1}{2s}\Delta_{\mathbb{S}^2} + O\left(\frac{1}{s^2}\right)\right] A_{ctr}(\bar{z}, z), \tag{3.116}$$

where

$$\Delta_{\mathbb{S}^2} = (1+\bar{z}z)^2 \frac{\partial^2}{\partial z \partial \bar{z}} \equiv \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \tag{3.117}$$

is the Laplace operator on $\mathbb{S}^2$, and the relation between complex variable z and unit vector $\mathbf{n}$ is given by (3.5).

The expression (3.116) can also be generalized to arbitrary λ

$$A^{(0)}(\mathbf{n}) = \left[1 + \frac{\lambda}{2s}\Delta_{\mathbb{S}^2} + O\left(\frac{1}{s^2}\right)\right] A^{(\lambda)}(\mathbf{n}). \tag{3.118}$$

The relation between λ- and λ'-symbols in the semiclassical limit $s \to \infty$ is straitforward

$$A^{(\lambda')}(\mathbf{n}) = \left[1 + \frac{\lambda-\lambda'}{2s}\Delta_{\mathbb{S}^2} + O\left(\frac{1}{s^2}\right)\right] A^{(\lambda)}(\mathbf{n}). \tag{3.119}$$

Considering $\lambda' = \frac{1}{2}$ and $\lambda = 0, 1$, we can regard the Stratonovich-Weyl symbol A_W, like in the case of the Heisenberg-Weyl group, as an intermediate symbol, which is just "halfway" between A_{cov} and A_{ctr}.

3.3.3 Phase-space representation of the quantum spin evolution

Equations for the quantum evolution operator and for the density operator $\hat{\rho} = |\psi\rangle\langle\psi|$ are given by

$$\begin{aligned}\frac{d\hat{K}}{dt} &= -i\hat{H}\hat{K}, \quad \hat{K}(0) = \hat{I}_{2s+1}, &(3.120)\\ \frac{d\hat{\rho}}{dt} &= -i[\hat{H},\hat{\rho}], \quad \hat{\rho}(0) = \hat{\rho}_0, &(3.121)\end{aligned}$$

respectively.

In this section we consider the phase-space representation of these equations. For simplicity, we restrict ourselves to the case of $\lambda = \frac{1}{2}$, corresponding to the Stratonovich-Weyl symbol. A similar consideration can be carried out for any symbol introduced in Sec. 3.3.2, and some related remarks will be made in this section as well.

The Stratonovich-Weyl symbol $(\hat{A}\hat{B})_W(\mathbf{n})$ of the product of two operators is given by the twisted (Moyal-like) product $(A_W \times B_W)(\mathbf{n})$ of their respective symbols:

$$\begin{aligned}(A_W \times B_W)(\mathbf{n}) &= \int_{\mathbb{S}^2}\int_{\mathbb{S}^2} d\mu_s(\mathbf{m})d\mu_s(\mathbf{k})A_W(\mathbf{m})B_W(\mathbf{k})L^s(\mathbf{n},\mathbf{m},\mathbf{k}), &(3.122)\\ L^s(\mathbf{n},\mathbf{m},\mathbf{k}) &= \mathrm{tr}[\hat{\Delta}^s(\mathbf{n})\hat{\Delta}^s(\mathbf{m})\hat{\Delta}^s(\mathbf{k})]. &(3.123)\end{aligned}$$

It is worth mentioning that explicit formulae of the Moyal-like product for generalized Stratonovich-Weyl symbols with arbitrary λ have been presented in [54].

The phase-space counterpart of the Eq. (3.120) is

$$\frac{\partial}{\partial t}K^s_W(\mathbf{n};t) = -i(H_W(t) \times K^s_W(t))(\mathbf{n}), \quad K^s_W(\mathbf{n};0) = 1. \tag{3.124}$$

$K^s_W(\mathbf{n};t)$ is called the twisted exponential, and it represents the Stratonovich-Weyl symbol of the evolution operator $\hat{K}$. In other words, it is the spin propagator in the Stratonovich-Weyl representation.

Time evolution of the Stratonovich-Weyl symbol of the density operator is then expressed through K^s_W according to

$$\rho_W(\mathbf{n};t) = K^s_W(\mathbf{n};t) \times \rho_0 \times K^{s*}_W(\mathbf{n};t), \quad \rho_W(\mathbf{n};0) = \rho_0(\mathbf{n}). \tag{3.125}$$

In the differential form we obtain the respective evolution equation [cf. (3.121)]

$$\frac{\partial \rho_W}{\partial t} = -i[H_W, \rho_W]_\times \equiv -i(H_W \times \rho_W - \rho_W \times H_W). \tag{3.126}$$

For the Hamiltonians linear in spin operators (3.13) one can show that

$$[H_W, \rho_W]_\times = -i\frac{1}{\sqrt{s(s+1)}}\sum_{i,j,k}\epsilon_{ijk}\frac{\partial H_W}{\partial n_i}\frac{\partial \rho_W}{\partial n_j}n_k, \tag{3.127}$$

and find the solution of (3.126) in the form

$$\rho_W(\mathbf{n};t) = \rho_0(\mathbf{n}_t). \tag{3.128}$$

Hereby

$$\mathbf{n}_t = O^{-1}(g(t))\mathbf{n} \tag{3.129}$$

and

$$g(t) = \mathrm{Texp}\left(-\frac{i}{2}\boldsymbol{\sigma}\cdot\int_0^t \mathbf{C}(t')dt'\right). \tag{3.130}$$

The formula (3.128) means that for the Hamiltonians linear in spin the initial distribution $\rho_0(\mathbf{n})$ is not deformed during the time evolution, it is just rotated around some axis by some angle. We note that $g(t)$ (3.130) satisfies the Eq. (3.31).

For such Hamiltonians the expression for $K_W^s(\mathbf{n};t)$ can be also obtained in the closed form. If then to take its trace, one should in principle recover (3.45). In particular, it has been confirmed in [90] for Zeeman Hamiltonian (3.60) with spin value $s=\frac{1}{2}$ by the direct calculation.

Due to the generalized Lie-Trotter formula (2.51) we can write a solution of the operator equation (3.120) in the path-integral representation for arbitrary spin Hamiltonian (in general, nonlinear in spin operators)

$$\begin{aligned}
\hat{K}(T) &= \lim_{N\to\infty}\int\prod_{k=1}^{N}[d\mu_s(\mathbf{n}_k)]\exp[-i\tau\sum_{k=1}^{N}H^{(\lambda)}(\mathbf{n}_k;t_k)] \\
&\times [\hat{\Delta}^s_{1-\lambda}(\mathbf{n}_N)\hat{\Delta}^s_{1-\lambda}(\mathbf{n}_{N-1})\dots\hat{\Delta}^s_{1-\lambda}(\mathbf{n}_1)] \\
&= \int d\mu_s(\mathbf{n}_N)K^{(\lambda)}(\mathbf{n}_N)\hat{\Delta}^s_{1-\lambda}(\mathbf{n}_N).
\end{aligned} \tag{3.131}$$

where $t_k = k\tau$, $\tau = T/N$, and $\mathbf{n}_N = \mathbf{n}_f$. For $\lambda=\frac{1}{2}$ the symbol $K_W(\mathbf{n}_f)\equiv K_W(\mathbf{n};T)$ is a solution of the equation (3.124) at $t=T$.

A calculation of $Z^s(T) = \mathrm{tr}[\hat{K}(T)]$ assumes taking the trace in (3.131) of an infinite product of operator kernels defined in different points on a sphere $\mathbb{S}^2$. For $\lambda = 1$ it becomes easier to fold this product due to the projective property of $\hat{\Delta}_0(\mathbf{n}) = |\mathbf{n}\rangle\langle\mathbf{n}|$, and thus we arrive at the expression containing contravariant symbols, similarly to that used in [13]. As for the evaluation of the spin propagator within arbitrary λ-quantization scheme, we expect that it might represent an interesting subject for a further theoretical study.

3.4 Trace of propagator for spin-orbit interaction using spin coherent states

Let us now consider a quantum Hamiltonian with spin-orbit interaction

$$\widehat{H} = \widehat{H}_0 + \widehat{H}_s = \widehat{H}_0(\hat{\mathbf{q}}, \hat{\mathbf{p}}) + \hbar\,\hat{\mathbf{s}} \cdot \widehat{\mathbf{C}}(\hat{\mathbf{q}}, \hat{\mathbf{p}})\,, \tag{3.132}$$

where $\hat{\mathbf{s}} = (\hat{s}_1, \hat{s}_2, \hat{s}_3)$, and $\widehat{\mathbf{C}} = (\widehat{C}_1, \widehat{C}_2, \widehat{C}_3)$ is a vector function of the coordinate and momentum operators $\hat{\mathbf{q}}$, $\hat{\mathbf{p}}$. Thereby we assume the most general form of spin-orbit interaction linear in spin. We write the expression for the respective quantum propagator in terms of a path integral in both the orbital variables $\mathbf{q}, \mathbf{p}$ and the spin variables $\bar{z}, z$. Imposing periodic boundary conditions on the propagation and thus integrating over closed paths, we arrive at the expression for the trace of propagator [cf. (2.8) and (3.26)]:

$$Z(T) = \int \mathcal{D}\mathbf{q}\mathcal{D}\mathbf{p}\, \mathcal{D}\mu_s(\bar{z}, z)\, \exp\left\{\frac{i}{\hbar}\mathcal{R}[\mathbf{q}, \mathbf{p}, \bar{z}, z; T]\right\}. \tag{3.133}$$

The Hamilton principal action function now includes the spin-action term:

$$\mathcal{R}[\mathbf{q}, \mathbf{p}, \bar{z}, z; T] = \oint_0^T \left[\frac{1}{2}(\mathbf{p}\cdot\dot{\mathbf{q}} - \mathbf{q}\cdot\dot{\mathbf{p}}) + \hbar s\,\frac{z\dot{\bar{z}} - \bar{z}\dot{z}}{i(1+|z|^2)} - H(\mathbf{q}, \mathbf{p}, \bar{z}, z)\right] dt\,. \tag{3.134}$$

The path integration in (3.133) is taken over the $2(d+1)$-dimensional extended phase space, and the notation

$$\mathcal{D}\mathbf{q}\mathcal{D}\mathbf{p}\mathcal{D}\mu_s(\bar{z}, z) = \lim_{N\to\infty} \prod_{k=1}^{N} \frac{d\mathbf{q}_k d\mathbf{p}_k}{(2\pi\hbar)^d}\, d\mu_s(\bar{z}_k, z_k) \tag{3.135}$$

is introduced.

The c-number Hamiltonian $H(\mathbf{q}, \mathbf{p}, \bar{z}, z)$ appearing in the integrand of (3.134) is

$$H(\mathbf{q}, \mathbf{p}, \bar{z}, z) = H_0(\mathbf{q}, \mathbf{p}) + H_s(\mathbf{q}, \mathbf{p}, \bar{z}, z) = H_0(\mathbf{q}, \mathbf{p}) + \hbar s\mathbf{n}(\bar{z}, z) \cdot \mathbf{C}(\mathbf{q}, \mathbf{p})\,, \tag{3.136}$$

where $H_0(\mathbf{q}, \mathbf{p})$ and $\mathbf{C}(\mathbf{q}, \mathbf{p})$ are the Wigner-Weyl symbols of the operators $\widehat{H}_0$ and $\widehat{\mathbf{C}}$, and $s\mathbf{n} = \langle z|\hat{\mathbf{s}}|z\rangle$ is the spin coherent-state symbol. We recall that one should always keep in mind the discretization corresponding to the choice of the symbols when passing to the continuous limit (see discussion in Secs. 2.2 and 3.1).

The expression (3.133) serves as a starting point for the generalization of the Gutzwiller's Trace Formula to systems with spin-orbit interaction, which will be considered in the next chapter. One can also write down similar expressions for $Z(T)$ exploiting the Jordan-Schwinger (Sec. 3.2) and the Moyal (Sec. 3.3) representations for spin, and develop semiclassical approximations in their framework. Some related references will be quoted in the next chapter as well.

Chapter 4

Semiclassics with spin

In this chapter we consider the semiclassical approaches to spin sysytems and systems with spin-orbit interaction. We begin with the useful review of the semiclassical results for spin systems in the external time-dependent field (Sec. 4.1). In Sec. 4.2 we formulate the semiclassical theory of spin-orbit interaction in the extended phase space using the spin coherent-state representation, which has been recently presented in [78]. We also represent the earlier semiclassical approaches of Refs. [16] and [66, 67] to the limits of weak (Sec. 4.3) and strong (Sec. 4.4) coupling, respectively, in terms of path integrals. The relationship between the different approaches is discussed in Sec. 4.5.

4.1 Semiclassical spin coherent-state propagator

In this section we consider a semiclassical approximation for a propagator of a spin particle with a time-dependent Hamiltonian. For instance, the quantum spin evolution may be described by the Hamiltonian (3.13), which is linear in spin operators. However, we shall assume in this section a rather general denendence $\hat{H}(\hat{\mathbf{s}}, t)$ on spin operators, e.g. polinomial in $\hat{\mathbf{s}}$ with arbitrary time-dependent coefficients.

For spin systems the semiclassical limit is defined as the limit of the large spin value s. An asymptotic expression for the spin coherent-state propagator (3.15) as $s \to \infty$ is given by [56, 92]

$$K_{sc}(\bar{z}_f, z_i, T) = \left(i \frac{(1+\bar{z}_f z_{cl}(T))(1+\bar{z}_{cl}(0) z_i)}{2s} \frac{\partial^2 \mathcal{R}_{cl}}{\partial z_i \partial \bar{z}_f} \right)^{1/2} e^{i\mathcal{R}_{cl}(\bar{z}_f, z_i, T) + i\varphi_{\mathrm{SK}}}. \tag{4.1}$$

The validity of this formula has been proven in [86]. It has been also shown that the degree of its accuracy, assuming errors of at most $O(1/s)$, is uniform in T.

The leading contribution to the phase of K_{sc} is given by the classical action function and by the suitable boundary terms

$$\begin{aligned} \mathcal{R}_{cl}(\bar{z}_f, z_i, T) &= -is\{\ln[(1+\bar{z}_f z_{cl}(T))(1+\bar{z}_{cl}(0) z_i)] - \ln[(1+|z_f|^2)(1+|z_i|^2)]\} \\ &+ \int_0^T \left\{ -is \frac{\dot{\bar{z}}_{cl} z_{cl} - \bar{z}_{cl} \dot{z}_{cl}}{1+\bar{z}_{cl} z_{cl}} - H(\bar{z}_{cl}, z_{cl}) \right\} dt. \end{aligned} \tag{4.2}$$

Classical trajectories $z_{cl}(t), \bar{z}_{cl}(t)$ are found from the classical equations of motion

$$\dot{z} = -i \frac{(1+\bar{z}z)^2}{2s} \frac{\partial H}{\partial \bar{z}}, \quad z(0) = z_i, \tag{4.3}$$

$$\dot{\bar{z}} \;=\; i\frac{(1+\bar{z}z)^2}{2s}\frac{\partial H}{\partial z}, \quad \bar{z}(T) = z_f. \tag{4.4}$$

These equations follow from the variational principle $\delta\Phi_s = 0$, which coincides with the stationary phase condition for the quantum propagator (3.21). As it has been already discussed before, variables z and $\bar{z}$ should be considered as independent in order to satisfy the boundary conditions.

The Solari-Kochetov phase $\varphi_{\mathrm{SK}} \sim O(s^0)$ is the quantum correction which must be taken into account in (4.1). It equals

$$\varphi_{\mathrm{SK}} = \frac{1}{2}\int_0^T B(t)dt. \tag{4.5}$$

It is expressed through the B-term [cf. (2.44)]

$$B(t) = \frac{1}{2}\left(\frac{\partial}{\partial\bar{z}}\frac{(1+\bar{z}z)^2}{2s}\frac{\partial H}{\partial z} + \frac{\partial}{\partial z}\frac{(1+\bar{z}z)^2}{2s}\frac{\partial H}{\partial\bar{z}}\right)\Big|_{z=z_{cl},\bar{z}=\bar{z}_{cl}}, \tag{4.6}$$

which is evaluated along the classical path. Originally the phase correction (4.5) has been obtained by Solari [85] through a careful calculation of the path integral in the discrete-time approximation. Kochetov [56] derived it independently considering the continuous version of the spin coherent-state path integral in the semiclassical limit. A discrete-time evaluation similar to that of Solari has been carried out by Vieira and Sacramento [92] who have also reproduced the same result. Being purely of a kinematic nature, this phase plays the role of a normalization [56]. Complementary points of view on its origin can be found in [41] and in Appendix B.3.

For the semiclassical trace calculation we can ignore the difference between $\bar{z}$ and z^*, and solve equations (4.3)-(4.4) with the periodic boundary conditions considering z and $\bar{z}$ as complex conjugated to each other (see discussion in Sec. 2.2). Like in the case of the flat coherent-state semiclassics, the very inclusion of φ_{SK} compensates the neglect of the shift of the discretized arguments (and the difference between $\bar{z}$ and z^* as well) in the continuous limit.

In [57] it has been shown that the trace of the semiclassical propagator (4.1) for the Hamiltonian linear in spin (3.13) coincides with the exact quantum-mechanical formula (3.45). The expression for η (3.55), implicitly defined by the solutions of the Riccati-type equations (3.52), has been reproduced semiclassically as well. The coincidence of the results for the trace of propagator obtained in quantum-mechanical and semiclassical treatments represents the specific feature of the Hamiltonians linear in spin, which distinguishes them among the others. Note that in this particular case the Solari-Kochetov phase

$$\varphi_{\mathrm{SK}} = \int_0^T dt\left\{A(t) - \frac{1}{2}[\bar{f}(t)z_{cl}(t) + f(t)\bar{z}_{cl}(t)]\right\} \tag{4.7}$$

equals to $\frac{1}{2}\eta$, and its account in the semiclassical trace calculation is crucial to achieve the consistency with the result of quantum computation.

We remark that in [57] the partition function of the Heisenberg ferromagnet has been considered. The latter becomes mathematically equivalent to the trace of spin propagator after the association of inverse temperature in the quantum-statistical problem with imaginary time in the quantum-mechanical problem (the so-called Wick rotation).

4.2 Semiclassics in the extended phase space

In Chapter 2 we have presented the derivation of the spinless Trace Formula starting from the trace of quantum propagator. Here we apply the same scheme to the spin-dependent $Z(T)$ (3.133) with the c-number Hamiltonian (3.136) responsible for the classical dynamics.

We define the semiclassical limit assuming the standard semiclassical requirements of large action $\mathcal{R}, \mathcal{S} \gg \hbar$ and large spin angular momentum, i.e.,

$$S \equiv \hbar s \gg \hbar. \tag{4.8}$$

It is also inferred that the energy of spin-orbit interaction in (3.136) is comparable to the orbital part of the energy: $|H_s| \sim |H_0|$. The above conditions can be formally rewritten as an asymptotic limit $\hbar \to 0$, $s \to \infty$ with $\hbar s = \text{const}$.

In such a limit, both the orbital and spin degrees of freedom can be treated semiclassically [78]. The first step is to obtain the classical equations of motion from the variational principle $\delta\mathcal{R}[\mathbf{q}, \mathbf{p}, \bar{z}, z] = 0$. They have the form

$$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}, \quad \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}}, \tag{4.9}$$

$$\dot{\bar{z}} = i\frac{(1+|z|^2)^2}{2S}\frac{\partial H}{\partial z}, \quad \dot{z} = -i\frac{(1+|z|^2)^2}{2S}\frac{\partial H}{\partial \bar{z}}. \tag{4.10}$$

In the two last equations we consider z and $\bar{z}$ as being complex conjugated to each other. Then, we equivalently represent Eqs. (4.10) in the form

$$\dot{\mathbf{n}} = \mathbf{C} \times \mathbf{n}, \tag{4.11}$$

where $\mathbf{n}$ is given by (3.4). We can also rewrite (4.10) in terms of real variables $v = \operatorname{Im}\bar{z} = -\operatorname{Im} z$ and $u = \operatorname{Re}\bar{z} = \operatorname{Re} z$ as

$$\dot{v} = \frac{(1+|z|^2)^2}{4S}\frac{\partial H}{\partial u}, \quad \dot{u} = -\frac{(1+|z|^2)^2}{4S}\frac{\partial H}{\partial v}. \tag{4.12}$$

We note that the equations of motion (4.9), (4.12) can be formulated in terms of the generalized Poisson bracket

$$\dot{F} = \{F, H\} = \frac{\partial F}{\partial \mathbf{q}}\frac{\partial H}{\partial \mathbf{p}} - \frac{\partial F}{\partial \mathbf{p}}\frac{\partial H}{\partial \mathbf{q}} + \frac{(1+u^2+v^2)^2}{4S}\left(\frac{\partial F}{\partial v}\frac{\partial H}{\partial u} - \frac{\partial F}{\partial u}\frac{\partial H}{\partial v}\right) \tag{4.13}$$

for any function F of the extended phase-space coordinates. We emphasize that these equations describe the coupled dynamics of spin and orbital degrees of freedom and collectively determine the periodic orbits in the extended phase space $(\mathbf{q}, \mathbf{p}, v, u)$, and they have to be solved with the periodic boundary conditions

$$\mathbf{q}(0) = \mathbf{q}(T), \quad \mathbf{p}(0) = \mathbf{p}(T), \quad v(0) = v(T), \quad u(0) = u(T). \tag{4.14}$$

According to (3.134), the action along a periodic orbit is

$$\mathcal{S}_{po}(E) = \oint_0^{T(E)} \left[\frac{1}{2}(\mathbf{p}\cdot\dot{\mathbf{q}} - \mathbf{q}\cdot\dot{\mathbf{p}}) + 2S\,\frac{u\dot{v} - v\dot{u}}{1+u^2+v^2}\right] dt. \tag{4.15}$$

The functional of the second variations $\mathcal{R}_{po}^{(2)}[\boldsymbol{\eta}, T]$ is still given by (2.15) with

$$\boldsymbol{\eta} = (\boldsymbol{\lambda}, \nu, \boldsymbol{\rho}, \xi) = \frac{1}{\sqrt{\hbar}} \left(\delta\mathbf{q}, \frac{2\sqrt{S}\,\delta v}{1+u^2+v^2}, \delta\mathbf{p}, \frac{2\sqrt{S}\,\delta u}{1+u^2+v^2} \right), \tag{4.16}$$

as well as the $2(d+1)$-dimensional unit symplectic matrix $\mathcal{J}$ and the second variation of the classical Hamiltonian (3.136)

$$\begin{aligned} H^{(2)} &= \frac{1}{2}\sum_{i,j}\left[\lambda_i\lambda_j\frac{\partial^2 H}{\partial q_i \partial q_j} + 2\lambda_i\rho_j\frac{\partial^2 H}{\partial q_i \partial p_j} + \rho_i\rho_j\frac{\partial^2 H}{\partial p_i \partial p_j}\right] \\ &\quad + \frac{1}{2}(\nu^2+\xi^2)\,(-u\,C_1 - v\,C_2 + C_3) \\ &\quad + \sqrt{S}\,\frac{(1+|z|^2)}{2}\left(\nu\frac{\partial \mathbf{n}}{\partial v} + \xi\frac{\partial \mathbf{n}}{\partial u}\right)\cdot\sum_j\left(\lambda_j\frac{\partial \mathbf{C}}{\partial q_j} + \rho_j\frac{\partial \mathbf{C}}{\partial p_j}\right). \end{aligned} \tag{4.17}$$

The stability matrices and the Maslov indices are determined by the linearized dynamics $\dot{\boldsymbol{\eta}} = \mathcal{J}\,\partial H^{(2)}/\partial\boldsymbol{\eta}$ (Appendix B.1).

The Solari-Kochetov phase (4.5) emerges as a normalization factor in the semiclassical evaluation of $Z(T)$ (3.133). Since $\varphi_{\rm SK} \sim O(\hbar^0)$, it survives the Fourier-Laplace transform from T to E without affecting the stationary-phase condition and thus enters the semiclassical expression for the oscillating density of states:

$$\delta g_{sc}(E) = \sum_{po}\mathcal{A}_{po}(E)\cos\left(\frac{1}{\hbar}\mathcal{S}_{po}(E) + \varphi_{{\rm SK},po}(E) - \frac{\pi}{2}\sigma_{po}\right). \tag{4.18}$$

Except for the extra-phase correction, the Trace Formula for systems with spin-orbit interaction appears in the standard form (2.3). The difference to the spinless case is that all elements in (4.18) (periodic orbits, their actions, periods, and stabilities) are to be found from the dynamics in the extended phase space.

We would like to remark that other continuous representations for spin—Jordan-Schwinger (Sec. 3.2) and Moyal (Sec. 3.3)—have been also applied to the semiclassical description of systems with both orbital (boson) and spin (pseudo-spin) degrees of freedom in the extended phase space. In [89] the Jordan-Schwinger mapping has been used for the semiclassical description of nonadiabatic quantum dynamics on coupled potential-energy surfaces. In [15] the Moyal representation for spin has been exploited for a formulation of quantum ergodicity for Pauli Hamiltonians with arbitrary spin. However, the Trace Formula for the density of states in the form (4.18) has not been derived so far within these alternative approaches.

4.3 Weak coupling limit (WCL)

In certain physical situations the energy of spin-orbit interaction is small: $|H_s| \ll |H_0|$, i.e., the system is in the weak-coupling regime. In addition to the standard semiclassical requirement $\mathcal{R}/\hbar \gg 1$, we imply that $S \equiv \hbar s$ is the small quantity. Formally, it can be expressed as an asymptotic limit $\hbar \to 0$ at arbitrary finite s. It means that the influence of the spin-orbit interaction is considered as the next-order $\hbar$-correction to the *unperturbed* dynamics governed by the Hamiltonian $H_0(\mathbf{q}, \mathbf{p})$.

The Trace Formula in the weak-coupling limit (WCL) can be derived from (3.133) by applying the stationary-phase condition to the orbital part of the action function, integration over the spin variables being exact. It means that at the first stage we should neglect the spin-orbit interaction, and find classical periodic solutions $\mathbf{q}^{(0)}(t)$, $\mathbf{p}^{(0)}(t)$ from $H_0(\mathbf{q}, \mathbf{p})$. Then we should solve exactly the quantum-mechanical problem for spin in the "external" time-dependent field $\mathbf{C}^{(0)}(t) = \mathbf{C}(\mathbf{q}^{(0)}(t), \mathbf{p}^{(0)}(t))$. The respective consideration is presented in Sec. 4.3.1.

However, for the Hamiltonians linear in spin one can obtain the same result from (4.18) by making perturbation theory in the parameter S, even though the smallness of S contradicts to (4.8). In other words, this implies an expansion of all classical ingredients in (4.18) in series of $\hbar$ at finite s. The relevance of such a derivation of the WCL Trace Formula, which is outlined in Sec. 4.3.2, relies on the specific feature of the Hamiltonians linear in spin which has been discussed in Sec. 4.1.

4.3.1 WCL with quantum-mechanical treatment of spin

In this treatment of the WCL it is convenient to separate the terms that explicitly contain $\hbar$ in the Hamilton principal action function (3.134). Representing

$$\mathcal{R}[\mathbf{q}, \mathbf{p}, \bar{z}, z; T] = \mathcal{R}_0[\mathbf{q}, \mathbf{p}; T] + \hbar s \mathcal{R}_1[\mathbf{q}, \mathbf{p}, \bar{z}, z; T], \tag{4.19}$$

where the unperturbed part $\mathcal{R}_0$ is given by (2.10) with the Hamiltonian $H_0(\mathbf{q}, \mathbf{p})$ and

$$\mathcal{R}_1[\mathbf{q}, \mathbf{p}, \bar{z}, z; T] = \oint_0^T \Big[\frac{z\dot{\bar{z}} - \bar{z}\dot{z}}{i(1+|z|^2)} - \mathbf{n}(\bar{z}, z) \cdot \mathbf{C}(\mathbf{q}, \mathbf{p})\Big] dt\,, \tag{4.20}$$

we can rewrite (3.133) in the form

$$Z(T) = \int \mathcal{D}\mathbf{q}\mathcal{D}\mathbf{p}\mathcal{M}_s[\mathbf{q}, \mathbf{p}; T] \exp\left\{\frac{i}{\hbar}\mathcal{R}_0[\mathbf{q}, \mathbf{p}; T]\right\} \tag{4.21}$$

with

$$\mathcal{M}_s[\mathbf{q}, \mathbf{p}; T] = \int \mathcal{D}\mu_s(\bar{z}, z) \exp\left\{is\mathcal{R}_1[\mathbf{q}, \mathbf{p}, \bar{z}, z; T]\right\}. \tag{4.22}$$

Now we can evaluate $Z(T)$ in the stationary-phase approximation in variables $\mathbf{q}$ and $\mathbf{p}$. Since $s\mathcal{R}_1 \ll \mathcal{R}_0/\hbar$ in the case under consideration, $\mathcal{M}_s[\mathbf{q}, \mathbf{p}; T]$ is a slowly varying functional of $\mathbf{q}$ and $\mathbf{p}$, and need not be taken into account when evaluating the stationary-phase condition. Applying the results of Sec. 2, we obtain the semiclassical approximation of the trace of propagator (3.133) in the WCL as a sum over the *unperturbed* periodic orbits (determined entirely by H_0)

$$Z_{sc}(T) = \sum_{po} \mathcal{M}_{po}(T)\, \mathcal{A}_{po}^{(0)}(T) \exp\left\{i\mathcal{R}_{po}^{(0)}/\hbar - \nu_{po}^{(0)}\pi/2\right\}, \tag{4.23}$$

where $\mathcal{A}_{po}^{(0)}$, $\nu_{po}^{(0)}$, $\mathcal{R}_{po}^{(0)} \equiv \mathcal{R}_0[\mathbf{q}_{po}^{(0)}, \mathbf{p}_{po}^{(0)}; T]$, and the modulation factor $\mathcal{M}_{po}(T) \equiv \mathcal{M}_s[\mathbf{q}_{po}^{(0)}, \mathbf{p}_{po}^{(0)}; T]$ are evaluated for the unperturbed trajectory. Performing the Fourier-Laplace transform (2.11) (also in the stationary-phase approximation) we arrive at the Trace Formula in the weak-coupling limit

$$\delta g_{sc}^{\mathrm{WCL}} = \sum_{po} \mathcal{M}_{po}(E)\, \mathcal{A}_{po}^{(0)}(E) \cos\left\{i\mathcal{S}_{po}^{(0)}/\hbar - \sigma_{po}^{(0)}\pi/2\right\}, \tag{4.24}$$

which differs from the unperturbed Trace Formula for H_0 only by the presence of the modulation factor $\mathcal{M}_{po}(E) \equiv \mathcal{M}_{po}(T^{(0)}(E))$ with $T^{(0)}(E) = d\mathcal{S}_{po}^{(0)}/dE$.

For the Hamiltonian linear in spin, the modulation factor is determined in Sec. 3.1.3 by a direct evaluation of the path integral (4.22). The problem is effectively reduced to the calculation of the trace of spin propagator in the time-dependent external field $\mathbf{C}(\mathbf{q}^{(0)}(t), \mathbf{p}^{(0)}(t)) \equiv (2\,\mathrm{Re} f^{(0)}(t), -2\,\mathrm{Im} f^{(0)}(t), 2A^{(0)}(t))$, determined by the path $(\mathbf{q}^{(0)}(t), \mathbf{p}^{(0)}(t))$. Then, for a periodic orbit one finds

$$\mathcal{M}_{po}(E) = \frac{\sin[(s+1/2)\,\eta(E)]}{\sin[\eta(E)/2]} \tag{4.25}$$

with

$$\eta(E) = \int_0^{T^{(0)}} dt\, \{2A^{(0)}(t) - [\bar{f}^{(0)}(t) z + f^{(0)}(t)\bar{z}]\}. \tag{4.26}$$

$\bar{z}(t)$ and $z(t)$ are to be found from the first-order differential equation

$$\dot{z} = -i[2A^{(0)}(t) z + f^{(0)}(t) - \bar{f}^{(0)}(t) z^2], \quad z(0) = z(T), \tag{4.27}$$

which is simply the precession equation $\dot{\mathbf{n}} = \mathbf{C}^{(0)} \times \mathbf{n}$, $\mathbf{n}(0) = \mathbf{n}(T)$ for the classical spin vector $\mathbf{n}$ [Eq. (3.4)]. This equation is angle-preserving, i.e., it rotates the Bloch sphere without deforming it. Thus, the orientations of the Bloch sphere at $t = 0$ and $t = T$ are related by a rotation about some axis. The angle of rotation is $-\eta(E)$ (Sec. 3.1.3). The choice of initial condition $\mathbf{n}(0)$ along this axis corresponds to a periodic solution (cf. [96]). Thus, (4.27) has two periodic solutions, whose $\eta(E)$ have opposite signs. Nevertheless, $\mathcal{M}_{po}(E)$ is well-defined. Note that $\eta(E)$ is equal to the part $\mathcal{R}_1[\mathbf{q}_{po}^{(0)}, \mathbf{p}_{po}^{(0)}, \bar{z}, z; T^{(0)}]$ of the Hamilton principal action function calculated along the periodic $\bar{z}(t)$ and $z(t)$. Although we are able to give a classical interpretation to the ingredients of $\mathcal{M}_{po}(E)$, no stationary-phase approximation was used in its derivation.

In the absence of spin-orbit interaction or external magnetic fied one finds $\mathcal{M}_{po}(E) = 2s+1$, i.e., the unperturbed Trace Formula is multiplied by the spin degeneracy factor.

For $s = 1/2$ the modulation factor $\mathcal{M}_{po}(E)$ was derived in [16] by a different method, which, as ours, treats the spin degrees of freedom on the quantum-mechanical level.

Note that the representation of terms in the WCL Trace Formula as a product of the unperturbed part and the modulation factor [Eq. (4.24)] remains valid even when the Hamiltonian is nonlinear in spin. However, the simple expression for the modulation factor (4.25) is specific to the Hamiltonian linear in spin.

4.3.2 WCL from the extended phase space dynamics

In [96] it has been shown how to obtain the WCL Trace Formula from the extended phase dynamics by performing the formal perturbative expansions in a series of $\hbar$ of the equations of motion (4.9), (4.12) and of equations for small linear variations $\boldsymbol{\eta}$ (4.16). Although that consideration has been carried out for $s = \frac{1}{2}$, its generalization for the arbitrary s is straightforward. Since s is finite, $S \equiv \hbar s$ can be equivalently used as a perturbation parameter in the approach of [96].

Making such expansion one finds two types of periodic solutions, which have opposite orientations of $\mathbf{n}(t)$. Their actions $\mathcal{S}^{\pm} = \mathcal{S}^{(0)} \pm \hbar\delta S$ differ in the next-to-leading order in $\hbar$ by $2\delta\mathcal{S} = (2s+1)\eta$, the Solari-Kochetov phase correction $\varphi^{\pm}_{\rm SK} = \pm\frac{1}{2}\eta$ being included. In the leading order of $\hbar$ the stability prefactors can be factorized into the orbital and spin parts, the stability angle of the spin block being equal η. Thus, the Trace Formula reads

$$\delta g(E) = \sum_{po} \frac{\mathcal{A}^{(0)}}{2|\sin\frac{\eta}{2}|} \sum_{\pm} \cos\left[\frac{1}{\hbar}(\mathcal{S}^{(0)} \pm \hbar\delta\mathcal{S}) - \frac{\pi}{2}(\sigma^{(0)} + \sigma^{\pm})\right], \qquad (4.28)$$

where the first sum is over the unperturbed periodic orbits, which assume no account of spin-orbit interaction, and the second sum takes care of the contribution of the two spin orientations. The orbital part of the stability prefactor is given by the stability prefactor $\mathcal{A}^{(0)}$ of the unperturbed system, while the spin part of the prefactor is $(2|\sin\frac{\eta}{2}|)^{-1}$. $\mathcal{S}^{(0)}$ and $\sigma^{(0)}$ are the unperturbed action and the Maslov index, respectively; $\sigma^{\pm}$ are the additional Maslov indices due to spin. With respect to the prescription for the calculation of the latter [cf. (B.24)]

$$\sigma^{\pm} = 1 + 2\left[\pm\frac{\eta}{2\pi}\right], \qquad (4.29)$$

where $[x]$ denotes the integer part of x, one can cast the *r.h.s.* of (4.28) into the form

$$\sum_{po} \frac{\mathcal{A}^{(0)}}{2|\sin\frac{\eta}{2}|} \sum_{\pm} \cos\left[\Phi^{(0)} \pm \left(\delta\mathcal{S} - \frac{\pi}{2}\right)\right] = \sum_{po} \frac{\sin(s+\frac{1}{2})\eta}{\sin\frac{\eta}{2}} \mathcal{A}^{(0)} \cos\Phi^{(0)}, \qquad (4.30)$$

where $\Phi^{(0)} = (1/\hbar)\mathcal{S}^{(0)} - (\pi/2)\sigma^{(0)}$.

Though this approach is less rigorous than that of Sec. 4.3.1, nevertheless, it yields the result which is equivalent to (4.24). This agreement is important, since it underscores the necessity of inclusion of the Solari-Kochetov phase which makes the semiclassical results consistent with those obtained in quantum calculations.

4.4 Adiabatic and strong coupling limits (SCL)

4.4.1 Multicomponent WKB approach to SCL

Adiabatic limit is defined by the requirement

$$|\mathbf{C}(\mathbf{q},\mathbf{p})| \gg T_{\rm orb}^{-1}, \tag{4.31}$$

where $T_{\rm orb}$ is the period of the orbital motion. Since $|\mathbf{C}|$ is the frequency of precession of the classical spin about the instantaneous magnetic field $\mathbf{C}$, Eq. (4.31) means that the spin motion is much faster than the orbital motion. The results of this section will be most useful in the strong-coupling limit (SCL) $|H_s| \sim |H_0|$ or $|\mathbf{C}| \sim |H_0|/\hbar$, where (4.31) is automatically satisfied. For the spin-orbit Hamiltonian (3.132) one absorbs $\hbar$ into the $\overline{|\mathbf{C}|} = \hbar|\mathbf{C}|$. The fact that this corresponds to a double limit $\hbar \to 0$ and $|\mathbf{C}| \to \infty$, with $\overline{|\mathbf{C}|}$ kept fixed, justifies the name "strong coupling" limit (cf. [16]).

Littlejohn and Flynn developed the semiclassical theory of the multicomponent wave equations in [66]. It was suggested to perform the diagonalization of the Wigner-Weyl symbol of the Hamiltonian matrix operator making perturbative expansions in $\hbar$. The leading contribution to the diagonalized symbol of the quantum Hamiltonian contains $2s+1$ classical Hamiltonians

$$\lambda_0^{(m)}(\mathbf{q},\mathbf{p}) = H_0(\mathbf{q},\mathbf{p}) + m\hbar|\mathbf{C}(\mathbf{q},\mathbf{p})| = H_0(\mathbf{q},\mathbf{p}) + m\overline{|\mathbf{C}|}(\mathbf{q},\mathbf{p}). \tag{4.32}$$

They create $2s+1$ classes of dynamics for $m = -s,\ldots,s$. Each of them can be studied separately by the standard semiclassical methods. Therefore, this approach bears the name of the multicomponent WKB approximation. Periodic orbits of all the Hamiltonians (4.32) must be superposed in a final Trace Formula. Such a Trace Formula has, however, not been derived explicitly so far. Littlejohn and Flynn [66, 67] argued that a non-canonical transformation of the phase-space variables $\mathbf{q},\mathbf{p}$ would be necessary to calculate the stability amplitudes. Frisk and Guhr [37] surmised, based upon the Fourier transforms of quantum spectra, that this is not necessary, provided that the actions $\mathcal{S}_{po}^{(m)}$ of the periodic orbits generated by the Hamiltonians $\lambda_0^{(m)}$ be corrected by two phases accumulated along the periodic orbits:

$$\frac{1}{\hbar}\mathcal{S}_{po}^{(m)} \to \frac{1}{\hbar}\mathcal{S}_{po}^{(m)} + \delta\Phi^{(m)}, \qquad \delta\Phi^{(m_s)} = -\oint_{po}(\lambda_{\rm B}^{(m)} + \lambda_{\rm NN}^{(m)})dt. \tag{4.33}$$

The phase velocities $\lambda_{\rm B}^{(m)}$, $\lambda_{\rm NN}^{(m)}$, which have been called the "Berry" and the "no-name" terms [66], arise as first-order $\hbar$ corrections in the semiclassical expansion of the symbol of the Hamiltonian matrix operator. They are given by

$$\lambda_{\rm B}^{(m)} = -i\sum_\alpha \bar{\tau}_\alpha^{(m)}\{\tau_\alpha^{(m)}, \lambda_0^{(m)}\}, \tag{4.34}$$

and

$$\lambda_{\rm NN}^{(m)} = -\frac{i}{2}\sum_{\alpha,\beta}(D_{\alpha\beta} - \lambda_0^{(m)}\delta_{\alpha\beta})\{\bar{\tau}_\alpha^{(m)}, \tau_\beta^{(m)}\}, \tag{4.35}$$

where the Poisson bracket $\{\cdot,\cdot\}$ is given by (A.9), and the summation over Greek indices is carried out from $-s$ up to s. Hereby

$$D_{\alpha\beta} = H_0\delta_{\alpha\beta} + \hbar|\mathbf{C}|(\mathbf{n}_C\cdot\mathbf{J}^s)_{\alpha\beta}, \quad \mathbf{n}_C = \mathbf{C}/|\mathbf{C}|. \tag{4.36}$$

We identify $\tau_\alpha^{(\gamma)} \equiv U^s_{\alpha\gamma}$ and $\bar{\tau}_\alpha^{(\gamma)} \equiv (U^{s\dagger})_{\gamma\alpha}$, where $\tau_\alpha^{(\gamma)}$ are the eigenvectors of the eigenproblem

$$(\mathbf{n}_C\cdot\mathbf{J}^s)\tau_\alpha^{(\gamma)} = \gamma\tau_\alpha^{(\gamma)}. \tag{4.37}$$

The latter is equivalent to the matrix relation $(\mathbf{n}_C\cdot\mathbf{J}^s)U^s = U^sJ_3^s$ which leads to

$$\mathbf{n}_C\cdot\mathbf{J}^s = U^sJ_3^sU^{s\dagger}. \tag{4.38}$$

In what follows we put $m\equiv\gamma$ and assume no summation carried over this index. Thus, we have $(J_3^s)_{\gamma\gamma} = m$.

Clearly, in the SCL the spin affects the classical dynamics, albeit only in an adiabatic, polarized fashion. Moreover, there is a serious limitation to the procedure outlined above. Whenever $\mathbf{C}=0$ at a given point in (or in a subspace of) phase space, the $2s+1$ Hamiltonians (4.32) become degenerate and singularities arise, both in the classical equations of motion and in the calculation of the phase corrections (4.34), (4.35) and the stabilities of the periodic orbits. Such points are called the "mode conversion" (MC) points. A similar situation occurs in the chemistry of molecular reactions when two or more adiabatic surfaces intersect. The MC poses a difficult problem in semiclassical physics and chemistry, that has not been satisfactorily solved so far for systems with more than one spatial dimension (see [68] for a discussion of the MC problem in one dimension).

Generally speaking, the multicomponent WKB approach and the formulae (4.34) and (4.35) are not restricted to problems with spin—they are valid for any multicomponent wave operator. However, when we deal with the matrices of SU(2) representations, these formulae can be further specified. In [67] it has been done for a particular type of spin-orbit interaction with $\mathbf{C}\sim\mathbf{L}$, where $\mathbf{L}=\mathbf{q}\times\mathbf{p}$ is the orbital angular momentum. In this section we generalize the consideration of [67] to the general type of spin-orbit interaction, as introduced in (3.132).

First of all, we need to choose certain gauge for U^s in (4.38). U^s is defined up to the U(1) gauge transformation: $U^s\to U^se^{iJ_3^s\psi}$. We choose for our calculations the so-called south standard gauge (SSG), which amounts to fixing U^s in the form

$$U^s = e^{-i\phi_CJ_3^s}e^{-i\theta_CJ_2^s}e^{-i\phi_CJ_3^s} = \mathcal{D}^s(\phi_C,\theta_C,\phi_C) \tag{4.39}$$

[cf. Appendix C]. In particular, for $s=\frac{1}{2}$ we have

$$U^{1/2} = \begin{pmatrix} e^{-\frac{i}{2}\phi_C} & 0 \\ 0 & e^{\frac{i}{2}\phi_C}\end{pmatrix}\begin{pmatrix}\cos\frac{\theta_C}{2} & -\sin\frac{\theta_C}{2} \\ \sin\frac{\theta_C}{2} & \cos\frac{\theta_C}{2}\end{pmatrix}\begin{pmatrix} e^{-\frac{i}{2}\phi_C} & 0 \\ 0 & e^{\frac{i}{2}\phi_C}\end{pmatrix} \tag{4.40}$$

$$= \begin{pmatrix}\cos\frac{\theta_C}{2}e^{-i\phi_C} & -\sin\frac{\theta_C}{2} \\ \sin\frac{\theta_C}{2} & \cos\frac{\theta_C}{2}e^{i\phi_C}\end{pmatrix}. \tag{4.41}$$

It is easy to check that

$$\mathbf{n}_C\cdot\mathbf{J}^{1/2} \equiv \frac{1}{2}(\mathbf{n}_C\cdot\boldsymbol{\sigma}) = \frac{1}{2}\begin{pmatrix}\cos\theta_C & \sin\theta e^{-i\phi_C} \\ \sin\theta_Ce^{i\phi_C} & \cos\theta_C\end{pmatrix}, \tag{4.42}$$

which is equivalent to $\mathbf{n}_C = (\sin\theta_C \cos\phi_C, \sin\theta_C \sin\phi_C, \cos\theta_C)$.

We can establish the following properties of U^s (4.39)

$$\frac{\partial U^s}{\partial \theta_C} = -iU^s B_\theta, \qquad \frac{\partial U^s}{\partial \phi_C} = -iU^s B_\phi, \tag{4.43}$$

where

$$\begin{aligned} B_\theta &= e^{iJ_3^s\phi_C} J_2^s e^{-iJ_3^s\phi_C} = J_1^s \sin\phi_C + J_2^s \cos\phi_C, & (4.44) \\ B_\phi &= J_3^s + U^{s\dagger} J_3^s U^s = J_3^s(1+\cos\theta_C) - (J_1^s\cos\phi_C - J_2^s \sin\phi_C)\sin\theta_C. & (4.45) \end{aligned}$$

Berry's term (4.34) equals

$$\begin{aligned} \lambda_{\mathrm{B}}^{(\gamma)} &= -i\sum_\alpha (U^{s\dagger})_{\gamma\alpha}\{U^s_{\alpha\gamma}, \lambda_0^{(\gamma)}\} = -(B_\phi)_{\gamma\gamma}\{\phi_C, \lambda_0^{(\gamma)}\} - (B_\theta)_{\gamma\gamma}\{\theta_C, \lambda_0^{(\gamma)}\} \\ &= -(J_3^s)_{\gamma\gamma}(1+\cos\theta_C)\{\phi_C, \lambda_0^{(\gamma)}\}, & (4.46) \end{aligned}$$

and therefore

$$\lambda_{\mathrm{B}}^{(m)} = -m(1+\cos\theta_C)\{\phi_C, \lambda_0^{(\gamma)}\} = -m(1+\cos\theta_C)\dot{\phi}_C. \tag{4.47}$$

For the calculation of the no-name term, we first need to find

$$\{\bar{\tau}_\alpha^{(\gamma)}, \tau_\beta^{(\gamma)}\} = A_{\alpha\beta}^{(\gamma)}\{\theta_C, \phi_C\}, \tag{4.48}$$

where

$$A_{\alpha\beta}^{(\gamma)} = \frac{\partial (U^{s\dagger})_{\gamma\alpha}}{\partial\theta_C}\frac{\partial U^s_{\beta\gamma}}{\partial\phi_C} - \frac{\partial (U^{s\dagger})_{\gamma\alpha}}{\partial\phi_C}\frac{\partial U^s_{\beta\gamma}}{\partial\theta_C} = (B_\theta U^{s\dagger})_{\gamma\alpha}(U^s B_\phi)_{\beta\gamma} - (B_\phi U^{s\dagger})_{\gamma\alpha}(U^s B_\theta)_{\beta\gamma}. \tag{4.49}$$

Taking into account that $U^{s\dagger}(\mathbf{n}_C\cdot\mathbf{J}^s)U^s = J_3^s$ [cf. (4.38)] and $(\mathbf{J}^s)^2 = s(s+1)$, we find after some algebra

$$\begin{aligned} \sum_{\alpha,\beta}(\mathbf{n}_C\cdot\mathbf{J}^s)_{\alpha\beta}A_{\alpha\beta}^{(\gamma)} &= B_\theta J_3^s B_\phi - B_\phi J_3^s B_\theta = -i\sin\theta_C((\mathbf{J}^s)^2 - 2(J_3^s)^2)_{\gamma\gamma}, & (4.50) \\ \sum_{\alpha,\beta}\delta_{\alpha\beta}A_{\alpha\beta}^{(\gamma)} &= ([B_\theta, B_\phi])_{\gamma\gamma} = i\sin\theta_C(J_3^s)_{\gamma\gamma}, & (4.51) \end{aligned}$$

and therefore

$$\sum_{\alpha,\beta}((\mathbf{n}_C\cdot\mathbf{J}^s)_{\alpha\beta} - (J_3^s)_{\gamma\gamma}\delta_{\alpha\beta})A_{\alpha\beta}^{(\gamma)} = -i\sin\theta_C(s(s+1)-m^2). \tag{4.52}$$

Collecting all the contributions, we obtain

$$\lambda_{\mathrm{NN}}^{(m)} = \frac{\hbar|\mathbf{C}|}{2}(m^2 - s(s+1))\sin\theta_C\{\theta_C, \phi_C\}. \tag{4.53}$$

Using the formula

$$\sin\theta_C\{\theta_C,\phi_C\} = \sum_j \mathbf{n}_C\cdot\left(\frac{\partial\mathbf{n}_C}{\partial q_j}\times\frac{\partial\mathbf{n}_C}{\partial p_j}\right), \tag{4.54}$$

we can rewrite (4.53) in the form

$$\lambda_{\mathrm{NN}}^{(m)} = \frac{\hbar(m^2 - s(s+1))}{2|\mathbf{C}|^2} \sum_j \mathbf{C} \cdot \left(\frac{\partial \mathbf{C}}{\partial q_j} \times \frac{\partial \mathbf{C}}{\partial p_j} \right). \tag{4.55}$$

For $\mathbf{C} = (1/\hbar) f(|\mathbf{q}|) \mathbf{q} \times \mathbf{p} = (1/\hbar) f(|\mathbf{q}|) \mathbf{L}$, we can find that $\sin\theta_C \{\theta_C, \phi_C\} = 1/|\mathbf{L}|$, provided the angular momentum $\mathbf{L}$ is conserved. Plugging it into (4.53), we recover results of [67].

4.4.2 Path integral approach to SCL

We can also derive the Trace Formula in the adiabatic limit with an exact integration over the spin degrees of freedom in the path integral.

We start with the representation (4.21) for the trace of the propagator and write the prefactor in the form (Sec. 3.1.3)

$$\mathcal{M}_s[\mathbf{q}, \mathbf{p}; T] = \frac{\sin\{(s + 1/2)\, \eta\, [\mathbf{q}, \mathbf{p}; T]\}}{\sin\{\eta\, [\mathbf{q}, \mathbf{p}; T]/2\}} = \sum_{m=-s}^{s} \exp\{im\eta\, [\mathbf{q}, \mathbf{p}; T]\}. \tag{4.56}$$

Then $Z(T)$ becomes a sum over polarizations

$$Z(T) = \sum_{m=-s}^{s} \int \mathcal{D}\mathbf{q}\mathcal{D}\mathbf{p} \exp\left\{ i\mathcal{R}_0[\mathbf{q}, \mathbf{p}; T]/\hbar + im\eta\, [\mathbf{q}, \mathbf{p}; T] \right\}, \tag{4.57}$$

where the path integrals will be calculated by the stationary phase. The functional $\eta\, [\mathbf{q}, \mathbf{p}; T]$ is given by [cf. (4.26)]

$$\eta\, [\mathbf{q}, \mathbf{p}; T] = \int_0^T dt \left\{ 2A - [\bar{f} z + f \bar{z}] \right\} \tag{4.58}$$

with $f = |\mathbf{C}| \sin\theta_C e^{-i\phi_C}$ and $A = (|\mathbf{C}|/2) \cos\theta_C$ in terms of the polar angles θ_C, ϕ_C of the vector $\mathbf{C}$. The trajectory $z(t)$ is one of the two periodic solutions of the equation

$$\dot{\mathbf{n}} = \mathbf{C} \times \mathbf{n}, \quad |\mathbf{n}| = 1, \tag{4.59}$$

which can be solved approximately in the adiabatic limit. We look for the solution in the form $\mathbf{n} = \mathbf{n}^{(0)} + \mathbf{n}^{(1)}$, where $\mathbf{n}^{(0)} \parallel \mathbf{C}$ and $\mathbf{n}^{(1)} \perp \mathbf{C}$. Assuming $\mathbf{n}^{(1)} \sim \mathbf{n}^{(0)}/(|\mathbf{C}|\, T_{\mathrm{orb}}) \ll \mathbf{n}^{(0)}$, we obtain

$$\mathbf{n}^{(0)} = \pm \frac{\mathbf{C}}{|\mathbf{C}|}, \quad \mathbf{n}^{(1)} = \mp \frac{\mathbf{n}^{(0)} \times \dot{\mathbf{n}}^{(0)}}{|\mathbf{C}|}. \tag{4.60}$$

Then (4.58) gives us the phase

$$m\, \eta\, [\mathbf{q}, \mathbf{p}; T] = -m \int_0^T |\mathbf{C}|\, dt + \varphi_{\mathrm{B}}^{(m)} + O(1/|\mathbf{C}|\, T_{\mathrm{orb}}). \tag{4.61}$$

Here the second term is the Berry phase

$$\varphi_{\mathrm{B}}^{(m)} = m \int_0^T (1 + \cos\theta_C)\, \dot{\phi}_C\, dt. \tag{4.62}$$

When the path integrals (4.57) for $Z(T)$ are evaluated by stationary phase, the Berry phase $\varphi_{\mathrm{B}}^{(m)} \sim O(\hbar^0)$ does not play a role in the determination of the stationary-phase point. In the SCL, i.e., when $|\mathbf{C}| \sim |H_0|/\hbar$, the first term of (4.61) must be varied together with $\mathcal{R}_0/\hbar$ in order to derive the stationary-phase condition. Then after the standard procedure (Chapter 2) we obtain the Trace Formula

$$\delta g_{sc}^{\mathrm{SCL}} = \sum_{m=-s}^{s} \delta g_{sc}^{(m)}, \tag{4.63}$$

where the density of states $\delta g_{sc}^{(m)}$ in each polarization is given by (2.3) with the classical dynamics controlled by the effective Hamiltonian

$$H_{\mathrm{eff}}^{(m)}(\mathbf{q},\mathbf{p}) = H_0(\mathbf{q},\mathbf{p}) + m\hbar|\mathbf{C}(\mathbf{q},\mathbf{p})| \tag{4.64}$$

and the Berry phase added.

Actually, this result is valid only if $\mathbf{C}(\mathbf{q},\mathbf{p})$ depends on either q_j or p_j, but not both, for each $j = 1,\ldots,d$. In the latter case such symbolic manipulations with path integrals do not seem to be valid, and, as a result, the "no-name" term found by Littlejohn and Flynn [66] is missing. The problem of recovering this term in the path-integral approach has been known for some time and was already mentioned in [66]. Making some heuristic assumptions, Fukui [38] reproduced the no-name term for the Jaynes-Cummings model in a framework similar to ours. It is not yet clear, whether his approach can be generalized to a wider class of Hamiltonians. We suppose that this term would emerge if the proper consideration is given to the discretized path integral, and the time-shift in arguments of the canonically conjugated variables is carefully taken into account in the respective continuous limit.

We note that the expression (4.61) becomes invalid if the adiabatic condition (4.31) breaks down anywhere along the periodic orbit. In particular, this occurs in the mode-conversion points defined by $\mathbf{C}(\mathbf{q},\mathbf{p}) = 0$.

In the above consideration of the adiabatic limit we have treated spin quantum-mechanically, since we have performed the integration over spin variables exactly. Now let us consider the same limit semiclassically in the extended phase space.

As it was shown in Appendix B of [79], in the adiabatic regime the classical system described by the Hamiltonian H (3.136) possesses an adiabatic invariant—the angle between the instantaneous magnetic field $\mathbf{C}$ and the classical spin vector $\mathbf{n}$. It means that the time derivative of $\mathcal{I} \equiv \mathbf{n}\cdot\mathbf{n}_C$ averaged over the fast spin motion approximately equals to zero.

Having an approximate integral of motion $\mathcal{I}$ has two consequences. First, in the adiabatic limit the fast spin precession about $\mathbf{C}$ can be separated from the orbital motion. The latter is then described by the polarized Hamiltonian

$$H_{\mathcal{I}}(\mathbf{q},\mathbf{p}) = H_0(\mathbf{q},\mathbf{p}) + \hbar s\mathcal{I}|\mathbf{C}(\mathbf{q},\mathbf{p})| \tag{4.65}$$

with $\mathcal{I}$ as a parameter. Second, the number of periodic orbits in the extended phase space is very large. They should not be considered any longer as isolated, but as appearing in one-parameteric (quasi-)continuous families instead. Therefore, we should use the Trace Formula for systems with continuous symmetries [26] rather than that for systems with isolated orbits. The proper resummation of all periodic orbits emerging in the extended phase space in the adiabatic limit [79] leads to the re-quantization condition $\mathcal{I} = m/s$, $m = -s, \ldots, s$ and to the expression for the density of states

$$\delta g_{sc}^{\mathrm{SCL}}(E) = \frac{1}{\pi\hbar} \sum_{m=-s}^{s} \sum_{po} \frac{T_{ppo}^{(m)} \cos\left(\frac{1}{\hbar} S_{po}^{(m)} + \varphi_{\mathrm{B}}^{(m)} - \frac{\pi}{2}\sigma_{po}^{(m)}\right)}{\left|\det\left(\widetilde{M}_{po}^{(m)} - I_{2(d-1)}\right)\right|^{1/2}}, \tag{4.66}$$

which is given by the sum over the periodic orbits of polarized Hamiltonians (4.64) and thus coincides with (4.63). The Berry phase

$$\varphi_{\mathrm{B}}^{(m)} = m \oint_{0}^{T_{po}^{(m)}} (1 + \cos\theta_C)\, \dot{\phi}_C \, dt, \tag{4.67}$$

derived in this consideration, is equivalent to (4.62).

Thus, we make the conclusion that the sum over quantized polarizations can be obtained from the classical-spin dynamics, where any polarization is allowed. However, in such a derivation the problem of the missing no-name term remains as well.

4.5 Applicability conditions

The path-integral representation for the trace of propagator (3.133) is a good starting point for further semiclassical approximations. One can define the limits of large spin (Sec. 4.2), and of weak (Sec. 4.3) and strong (Sec. 4.4) coupling. In the two last limits spin is considered quantum mechanically (in effective external field or in adiabatic approximation), which assumes an exact integration over spin variables in (3.133), while an integration over orbital variables is performed by the stationary-phase method. The path-integral approach reproduces earlier results of [16] and [67] for the limits of weak and strong[1] coupling, respectively.

But as we have seen before, the semiclassical approach of Sec. 4.2, which treats both spin and orbital degrees of freedom by the stationary-phase method, can be succesfully used even beyond the formal limit of large spin (4.8), provided that the Hamiltonian is linear in spin. The respective justifying arguments were presented in [79]. The main idea is based on the fact that the results of a quantum-mechanical and a semiclassical description of spin systems in external time-dependent field coincide (see Sec. 4.1). When we couple spin and orbital degrees of freedom and consider dynamics in the extended phase space, we, in general, violate this remarkable property.

However, in the weak coupling limit this does not show up in the Trace Formula within the required accuracy. The results of Sec. 4.3.2 validate the application of the semiclassical approach of Sec. 4.2 in this limit even for small s.

In the strong coupling limit one can realize the extended phase-space dynamics as possessing adiabatic invariant (approximate integral of motion). Then, one can regard the corresponding quasi-continuous symmetry as continuous. This implies the use of the semiclassical theory of Ref. [26] which is adapted to systems with continuous symmetries. As it was shown in Appendix B of [79], such an approach leads to the correct re-quantization of spin and also reproduces the results of the multicomponent WKB theory [66, 67].

We conclude that for the Hamiltonian linear in spin, the general semiclassical requirement of large spin $S \gg \hbar$, under which the Trace Formula (4.18) was derived, can be omitted. In fact, in many physical problems the spin angular momentum is small ($S \sim \hbar$) and the Hamiltonian is linear in spin. The Trace Formula (4.18) can be used in the limits of weak and strong coupling, since these are asymptotic limits, and their boundaries may not be strictly defined in specific numerical examples.

[1]At this stage we have to restrict ourselves to the case of $\mathbf{C}(\mathbf{q}, \mathbf{p})$ depending on either q_j or p_j, but not both, for each $j = 1, \ldots, d$, due to the problem of the "no-name" term (see Sec. 4.4).

Chapter 5

Applications

We shall now apply the semiclassical methods of Chapter 4 to two specific systems. In Sec. 5.1 we study the free two-dimensional electron gas in a homogeneous magnetic field with the Rashba Hamiltonian and the Jaynes-Cummings model, that allow analytical treatment on both quantum-mechanical and semiclassical levels. Then in Sec. 5.2 we consider a numerical example of a quantum dot with harmonic confinement and Rashba interaction. This system is a good test case for the semiclassical approach in the extended phase space, since the SCL method suffers from the mode-conversion problem, while the WCL Trace Formula completely neglects the spin-orbit interaction.

5.1 Rashba and Jaynes-Cummings (JC) models

The free two-dimensional electron gas with a Rashba spin-orbit interaction [21] in a homogeneous magnetic field $\mathbf{B} = B_0\mathbf{e}_3$ is characterized by the Hamiltonian

$$\widehat{H} = \frac{\hat{\pi}_1^2}{2m^*} + \frac{\hat{\pi}_2^2}{2m^*} + \frac{2\alpha_R}{\hbar}(\hat{\pi}_1\hat{s}_2 - \hat{\pi}_2\hat{s}_1) + g^*\mu_B B_0\hat{s}_3. \tag{5.1}$$

Using the symmetric gauge for the vector potential, the components of noncanonical momentum are given by $\hat{\pi}_1 = \hat{p}_1 - (eB_0/2c)\,\hat{q}_2$ and $\hat{\pi}_2 = \hat{p}_2 + (eB_0/2c)\,\hat{q}_1$. α_R is the Rashba constant [21, 29], m^* is the effective mass of an electron, e is the absolute value of its charge, g^* is the effective gyromagnetic ratio, $\mu_B = e\hbar/2mc$ is the Bohr magneton.

Due to the commutation relation $[\hat{\pi}_2, \hat{\pi}_1] = i\hbar eB_0/c$ we can introduce canonically conjugated operators $\hat{Q} = -\hat{\pi}_2\sqrt{c/eB_0}$ and $\hat{P} = -\hat{\pi}_1\sqrt{c/eB_0}$ satisfying $[\hat{Q}, \hat{P}] = i\hbar$. Then, the Hamiltonian (5.1) can be written as

$$\widehat{H} = \frac{\omega_c}{2}(\hat{Q}^2 + \hat{P}^2) + 2\hbar\kappa\omega_c(\hat{Q}\hat{s}_1 - \hat{P}\hat{s}_2) + \hbar\gamma\omega_c\hat{s}_3, \tag{5.2}$$

where we have introduced the new parameters[1] $\kappa = \alpha_R\sqrt{eB_0}/\hbar^2\sqrt{c}$, $\gamma = g^*m^*/2m$, and the cyclotron frequency $\omega_c = eB_0/m^*c$.

For the model in question the value of spin in (5.2) equals $s = \frac{1}{2}$. With this spin value the Hamiltonian (5.2) can be applied to the other physical system, namely, to

[1] This definition of κ is applicable only within Sec. 5.1.

the Jaynes-Cummings (JC) model in the so-called rotating wave approximation (RWA) [50], which describes the simplest possible interaction between a bosonic mode and a two-level system (see [44] for the review). The conventional form of the JC, or Rabi, Hamiltonian is

$$\widehat{H}_{\rm JC} = \hbar\omega_c \hat{a}^\dagger \hat{a} + \lambda(\hat{a}\hat{s}_+ + \hat{a}^\dagger \hat{s}_-) + \hbar\gamma\omega_c \hat{s}_3, \tag{5.3}$$

where $\hat{a} = (\hat{Q} + i\hat{P})/\sqrt{2\hbar}$, $a^\dagger = (\hat{Q} - i\hat{P})/\sqrt{2\hbar}$ describe a bosonic mode of frequency ω_c, spin-$\frac{1}{2}$ operators $\hat{\mathbf{s}}$ descibe a two-level system with level-splitting $\hbar\gamma\omega_c$, and $\lambda = \sqrt{2}\hbar^{3/2}\kappa\omega_c$ is a coupling strength. To establish the full correspondence between (5.2) and (5.3), we should also subtract $\hbar\omega_c/2$ from *r.h.s.* of (5.2).

It is remarkable that for $s = \frac{1}{2}$ the quantum-mechanical energy spectrum of (5.2) is known analytically [21]:

$$E_0 = \hbar\omega_c(1-\gamma)/2\,, \quad E_k^\pm = \hbar\omega_c\left(k \pm \sqrt{(1-\gamma)^2/4 + 2k\hbar\kappa^2}\right), \quad k = 1,2,3,\ldots \tag{5.4}$$

Using Poisson summation, it can be identically transformed to an exact quantum-mechanical Trace Formula [3]. The smooth part is $\widetilde{g}(E) = 2/\hbar\omega_c$ and the oscillating part becomes

$$\begin{aligned} \delta g(E) &= \frac{2}{\hbar\omega_c}\sum_\pm \left(1 \pm \frac{\hbar\kappa^2}{\sqrt{(1-\gamma)^2/4 + 2E\kappa^2/\omega_c + \hbar^2\kappa^4}}\right) \\ &\times \sum_{r=1}^\infty \cos\left[r2\pi\left(\frac{E}{\hbar\omega_c} + \hbar\kappa^2 \pm \sqrt{(1-\gamma)^2/4 + 2E\kappa^2/\omega_c + \hbar^2\kappa^4}\right)\right]. \end{aligned} \tag{5.5}$$

In [3] there have been calculated the oscillating parts of the level density in the WCL and SCL for $s = \frac{1}{2}$ and $\gamma = 0$:

$$\delta g_{sc}^{\rm WCL}(E) = \frac{2}{\hbar\omega_c}\sum_\pm\sum_{r=1}^\infty \cos\left[r\,2\pi\left(\frac{E}{\hbar\omega_c} \pm \sqrt{1/4 + 2E\,\kappa^2/\omega_c}\right)\right], \tag{5.6}$$

$$\begin{aligned} \delta g_{sc}^{\rm SCL}(E) &= \frac{2}{\hbar\omega_c}\sum_\pm\left(1 \pm \frac{\hbar\kappa^2}{\sqrt{2E\,\kappa^2/\omega_c + \hbar^2\kappa^4}}\right) \\ &\times \sum_{r=1}^\infty \cos\left[r\,2\pi\left(\frac{E}{\hbar\omega_c} + \hbar\,\kappa^2 \pm \sqrt{2E\,\kappa^2/\omega_c + \hbar^2\kappa^4}\right)\right]. \end{aligned} \tag{5.7}$$

The relation of these semiclassical formulae to the asymptotic limits of the exact expression (5.5) has been also discussed.

In Sec. 5.1.1 we shall re-derive the results (5.6) and (5.7) for $\gamma \neq 0$, and extend the discussion of [3] about the asymptotics of (5.5).

For higher values of s the Hamiltonians (5.2) and (5.3) also have physical applications. After replacing λ by $\tilde{\lambda}/\sqrt{2s}$, the Hamiltonian (5.3) coincides with the Dicke Hamiltonian (DH) [33] describing a collection of N two-level atoms interacting with a single bosonic mode via a dipole interaction with an atom-field coupling strength $\tilde{\lambda}$:

$$\widehat{H}_{\rm DH} = \hbar\omega_c \hat{a}^\dagger \hat{a} + \frac{\tilde{\lambda}}{\sqrt{2s}}(\hat{a}\hat{s}_+ + \hat{a}^\dagger \hat{s}_-) + \hbar\gamma\omega_c \hat{s}_3. \tag{5.8}$$

The collective behavior of the atomic ensemble is modelled by the operators $\hat{\mathbf{s}}$ of (pseudo-)spin $s = N/2$. The thermodynamic limit of $N \to \infty$ is thus equivalent to making the value of (pseudo-)spin tend to infinity $s \to \infty$. Like the JC model (5.3), the Dicke model is usually considered in RWA, which assumes the book-keeping of the rotating terms $\hat{a}\hat{s}_+$ and $\hat{a}^\dagger \hat{s}_-$ only (anti-rotating terms $\hat{a}^\dagger \hat{s}_+$ and $\hat{a}\hat{s}_-$ are neglected).

However, the analytical expression for the spectrum of (5.2) for $s > \frac{1}{2}$ is not known. As a consequence, the exact formula for the oscillating part of the denisty of states is restricted to the case $s = \frac{1}{2}$. The respective semiclassical expessions in either WCL or SCL have been also derived for just this spin value. Although the reconstruction of the full quantum spectrum does not seem to be an easy task, the generalization of (5.6) and (5.7) to higher spins is possible.

To illustrate the semiclassical methods discussed in the previous chapter, we shall derive $\delta g_{sc}^{\mathrm{WCL}}$ and $\delta g_{sc}^{\mathrm{SCL}}$ for arbitrary s and γ:
—using the WCL approach of Sec. 4.3.1;
—working in the extended phase space in the WCL, as formulated in Sec. 4.3.2;
—using multicomponent WKB approach to SCL, according to Sec. 4.4.1.

5.1.1 Interpretations of WCL and SCL for JC model

In [3] there have been discussed the relations between the Trace Formulae obtained by the Poisson summation of the exact spectrum (5.5) and by the semiclassical methods in the limits of weak (5.6) and strong (5.7) coupling. The question how to derive the latter expressions from (5.5) by making the formal asymptotic expansions has been also addressed. In order to extend the discussion of [3], we introduce for convenience the following dimesionless parameters

$$\epsilon = \hbar\kappa\sqrt{\frac{\omega_c}{E}}, \qquad \beta = \kappa\sqrt{\frac{E}{\omega_c}}. \tag{5.9}$$

We then rewrite the exact Trace Formula (5.5) in the new notations

$$\delta g(E) = \frac{2}{\hbar\omega_c}\sum_{\pm}\left(1 \pm \frac{\epsilon}{G}\right)\sum_{r=1}^{\infty}\cos\left[r2\pi\left(\frac{\beta}{\epsilon} + \beta\epsilon \pm \beta A\right)\right], \tag{5.10}$$

where

$$G = \sqrt{\frac{(1-\gamma)^2}{4\beta^2} + 2 + \epsilon^2}. \tag{5.11}$$

In the WCL we can identify two small dimensionless parameters proportional to $\hbar$: $\hbar\omega_c/E \ll 1$ (validity of semiclassics) and $\hbar\kappa^2 \ll 1$ (weak coupling). They are related to ϵ and β of (5.9) by the obvious expressions

$$\frac{\hbar\omega_c}{E} = \frac{\epsilon}{\beta}, \qquad \hbar\kappa^2 = \beta\epsilon. \tag{5.12}$$

We impose that in the WCL $\hbar\omega_c/E \sim \hbar\kappa^2 \ll 1$, meaning that in the double limit $E \to \infty$, $\kappa \to 0$ the combination $E\kappa^2/\omega_c$ is kept constant. It corresponds to the formal limit $\hbar \to 0$. Since ϵ is proportional to $\hbar$, and β is not, we can state the WCL as $\epsilon \to 0$, $\beta = \text{const} = O(\epsilon^0)$, $\gamma = \text{const} = O(\epsilon^0)$. We then obtain the WCL Trace Formula

$$\delta g_{sc}^{\mathrm{WCL}}(E) = \frac{2}{\hbar\omega_c} \sum_{\pm} \sum_{r=1}^{\infty} \cos\left[r\, 2\pi \left(\frac{\beta}{\epsilon} \pm \sqrt{\frac{(1-\gamma)^2}{4} + 2\beta^2} \right) \right] \tag{5.13}$$

by neglecting higher order ϵ-terms in (5.10) and (5.11). Obviously, (5.13) coincides with (5.6) after the change of parameters (5.9).

For a specification of the SCL, it is suggested to absorb $\hbar$ into the coupling constant (Sec. 4.4.1). Thus, we define

$$\bar{\kappa} = \hbar\kappa. \tag{5.14}$$

We also need to introduce

$$\bar{\gamma} = \frac{\gamma}{\beta}. \tag{5.15}$$

In the SCL we have to formally consider that $\bar{\kappa}$ and $\bar{\gamma}$ are of the order $O(\hbar^0)$, and realize this limit as $\hbar \to 0$. Since $1/\beta$ is proportional to $\hbar$, and ϵ is not, we define SCL as $\beta \to \infty$, $\epsilon = \text{const} = O(\beta^0)$, $\bar{\gamma} = \text{const} = O(\beta^0)$. In these notations the SCL Trace Formula (5.7) reads

$$\delta g_{sc}^{\mathrm{SCL}}(E) = \frac{2}{\hbar\omega_c} \sum_{\pm} \left(1 \pm \frac{\epsilon}{G'}\right) \sum_{r=1}^{\infty} \cos\left[r\, 2\pi\beta \left(\frac{1}{\epsilon} + \epsilon \pm G' \right) \mp \frac{r\pi\bar{\gamma}}{2G'} \right], \tag{5.16}$$

where

$$G' = \sqrt{\frac{\bar{\gamma}^2}{4} + 2 + \epsilon^2}. \tag{5.17}$$

It is obvious that making an expansion of G (5.11) in a series of $1/\beta$

$$G = \sqrt{\frac{1}{4\beta^2} - \frac{\bar{\gamma}}{2\beta} + \frac{\bar{\gamma}^2}{4} + 2 + \epsilon^2} = G' - \frac{\bar{\gamma}}{4\beta G'} + O(\beta^{-2}), \tag{5.18}$$

and neglecting higher order $(1/\beta)$-terms, we recover (5.16) from (5.10).

Thus, we conclude that ϵ and $1/\beta$ introduced in (5.9) play the role of the formal asymptotic parameters for the limits of the weak and strong coupling, respectively. Though the above consideration has been carried out for the integrable JC model (5.3), the definition of these asymptotic limits can be straitforwardly generalized to any system with spin-orbit interaction, where $\mathbf{C}$ appears as a linear function of $\mathbf{q}$ and/or $\mathbf{p}$.

5.1.2 WCL regime

In this section we derive the WCL Trace Formula for the JC model (5.3) with arbitrary s using the method of Sec. 4.3.1.

According to (3.136) the phase-space symbol of the Hamiltonian (5.2) is

$$H = \frac{\omega_c}{2}(Q^2 + P^2) + 2\hbar s\kappa\omega_c(Qn_1 - Pn_2) + \hbar s\gamma\omega_c n_3. \tag{5.19}$$

It is suitable to introduce the complex variables $\alpha = (Q + iP)/\sqrt{2}$ and $n = n_1 + in_2$, and to rewrite the Hamiltonian (5.19) in the form

$$H = \omega_c \bar{\alpha}\alpha + \sqrt{2}\hbar s\kappa\omega_c(\alpha n + \bar{\alpha}\bar{n}) + \hbar s\gamma\omega_c n_3. \tag{5.20}$$

The unperturbed Trace Formula for the system without spin degrees of freedom, corresponding to $\widehat{H}_0 = \hat{\boldsymbol{\pi}}^2/2m^*$, is that of a one-dimensional harmonic oscillator with the cyclotron frequency ω_c. It reads [18]

$$\delta g^{(0)}(E) = \frac{2}{\hbar\omega_c}\sum_{r=1}^{\infty}(-1)^r \cos\left(r\frac{2\pi E}{\hbar\omega_c}\right). \tag{5.21}$$

The modulation factor is given by (4.25)-(4.26), where we should use

$$A^{(0)} = \gamma\omega_c/2, \quad f^{(0)} = \kappa\sqrt{2E\omega_c}\exp(-i\omega_c t). \tag{5.22}$$

For such "external" field, we can find η_r (for the rth repetition) from (3.59). It equals

$$\eta_r(E) = 2\pi r(1 + 2g), \tag{5.23}$$

where

$$g = \sqrt{\frac{(1-\gamma)^2}{4} + \frac{2E\kappa^2}{\omega_c}}. \tag{5.24}$$

According to (4.24), the WCL Trace Formula is

$$\delta g_{sc}^{\mathrm{WCL}}(E) = \frac{2}{\hbar\omega_c}\sum_{r=1}^{\infty}(-1)^{r(2s+1)}\frac{\sin[(2s+1)2\pi rg]}{\sin[2\pi rg]}\cos\left(r\frac{2\pi E}{\hbar\omega_c}\right). \tag{5.25}$$

For spin $s = \frac{1}{2}$ it yields

$$\delta g_{sc}^{\mathrm{WCL}}(E) = \frac{2}{\hbar\omega_c}\sum_{r=1}^{\infty} 2\cos[2\pi rg]\cos\left(r\frac{2\pi E}{\hbar\omega_c}\right) = \frac{2}{\hbar\omega_c}\sum_{\pm}\sum_{r=1}^{\infty}\cos\left[r2\pi\left(\frac{E}{\hbar\omega_c} \pm g\right)\right], \tag{5.26}$$

which coincides with (5.13) and agrees with (5.6) at $\gamma = 0$.

5.1.3 WCL in the extended phase space

Now we will reproduce (5.25) by carrying out the procedure outlined in Sec. 4.3.2.

The classical dynamics of the system is described by the equations of motion (4.9), (4.11), which now have the form

$$\begin{aligned} \dot{\alpha} &= -i\omega_c(\alpha + \sqrt{2}\hbar s\kappa\bar{n}), \\ \dot{n} &= i\omega_c(\gamma n - 2\sqrt{2}\kappa n_3\bar{\alpha}), \\ \dot{n}_3 &= -i\sqrt{2}\kappa\omega_c(n\alpha - \bar{n}\bar{\alpha}). \end{aligned} \tag{5.27}$$

Along with the energy conservation $H = E$ there is another conserved quantity $|\alpha|^2 + \hbar s n_3 = \text{const}$. It means that the system (5.19) is classically integrable. Its general analytic solution has been given in [1]. Here, however, we are interested in the *periodic* solutions, which infer the knowledge of certain initial conditions. Let us make an ansatz for the particular isolated periodic orbits with $n_3 = \text{const}$:

$$\alpha = |\alpha| e^{-i\Omega t}, \quad n = -\xi |n| e^{i\Omega t} \qquad (\xi = \pm 1) \tag{5.28}$$

with constant parameters Ω, $|\alpha|$ and $|n|$. Plugging (5.28) into (5.27) we obtain the relations between them:

$$\begin{aligned} \Omega &= \omega_c(1 - \sqrt{2}\xi\hbar s\kappa |n|/|\alpha|), \\ \Omega &= \omega_c(\gamma + 2\sqrt{2}\xi\kappa n_3 |\alpha|/|n|), \\ E &= \omega_c(|\alpha|^2 + \hbar s\gamma n_3 - 2\sqrt{2}\xi\hbar s\kappa|\alpha||n|). \end{aligned} \tag{5.29}$$

For the rth repetition of the orbits (5.28) we can calculate the action

$$\begin{aligned} \mathcal{S}_r^\xi(E) &= \oint_0^{T(E)} dt \left(\frac{\alpha\dot{\bar\alpha} - \bar\alpha\dot\alpha}{2i} + \hbar s \frac{z\dot{\bar z} - \bar z \dot z}{i(1+|z|^2)} \right) = 2\pi r(|\alpha|^2 + \hbar s n_3) + 2\pi r \hbar s \\ &= 2\pi r \left(\frac{E}{\omega_c} + \hbar s (1-\gamma) n_3 + 2\sqrt{2}\xi\hbar s\kappa|\alpha||n| \right) + 2\pi r\hbar s, \end{aligned} \tag{5.30}$$

and the stability angle

$$\Lambda_r^\xi = r\frac{4\pi\kappa\omega_c}{\Omega}\sqrt{\frac{\hbar^2 s^2 |n|^2}{2|\alpha|^2} + \frac{2|\alpha|^2}{|n|^2} - 2\hbar s n_3} + 2\pi r. \tag{5.31}$$

It seems to be difficult to solve the algebraic equations (5.29) with respect to Ω, $|\alpha|$, and $|n|$. Moreover, for rather large κ there might appear other periodic orbits with more complicated shapes. Up to now we have not used the WCL conditions in our calculations. In particular, the expressions for the action and the stability angle are valid for any values of parameters. We gain considerable simplifications in the WCL, that corresponds to the formal expansion in a series of $\hbar$: $|\alpha| = |\alpha|^{(0)} + \hbar|\alpha|^{(1)} + \ldots$, etc. Then we can find that, for instance,

$$|\alpha|^{(0)} = \sqrt{E/\omega_c}, \quad \Omega^{(0)} = \omega_c, \tag{5.32}$$

$$n_3^{(0)} = \xi(1-\gamma)/2g, \quad |n|^{(0)} = \kappa\sqrt{2E}/g\sqrt{\omega_c}. \tag{5.33}$$

We conclude that, in the leading order, the orbital motion is unaffected by spin and for the two periodic orbits we have $\mathbf{n}^{\xi=1}(t) = -\mathbf{n}^{\xi=-1}(t)$, i.e., the spins are opposite at any time. Moreover, we know from the general considerations [96] that in the WCL only two periodic orbits are possible for the Hamiltonian (5.20), and they are given by (5.28). For these orbits we can calculate the action $\mathcal{S}_r^\xi = (2\pi r E/\omega_c) + \xi\,\hbar\, s\,\eta_r(E) + O(\hbar^2)$ and the stability angle $\Lambda_r^\xi = \eta_r(E) + O(\hbar)$ using (5.30) and (5.31), respectively. As was discussed in Sec. 4.2, the Solari-Kochetov extra phase $\varphi_{\mathrm{SK},r}^\xi$, which in the WCL is equal to $\frac{1}{2}\xi\,\eta_r(E)$, should be added to the Trace Formula. Thus, the total phase is (up to the Maslov indices)

$$\Phi_r^\xi = \frac{\mathcal{S}_\xi^r}{\hbar} + \varphi_{\mathrm{SK},r}^\xi = \frac{2\pi r E}{\hbar\omega_c} + (2s+1)2\pi r\xi\,(2g+1) + O(\hbar). \tag{5.34}$$

Then we find the oscillating part of the level density

$$\delta g_{sc}^{\mathrm{WCL}}(E) = \frac{1}{\hbar\pi} \sum_{\xi=\pm 1} \sum_{r=1}^{\infty} \frac{T^{(0)}}{2|\sin\frac{1}{2}\Lambda_r^{(0)}|} \cos\left(\Phi_r^{\xi} - \sigma_r^{\xi}\frac{\pi}{2}\right), \tag{5.35}$$

where $T^{(0)} = 2\pi/\omega_c$ is the period of the primitive orbit in the unperturbed dynamics. Adding the appropriate Maslov indices according to (4.29), and summing up $\xi = \pm 1$, we recover (5.25).

5.1.4 SCL regime

In this section we apply the results of Sec. 4.4.1 in order to generalize the SCL Trace Formula (5.7) to arbitrary value of s and $\gamma \neq 0$.

For each polarized Hamiltonian (4.32) we assume the conservation of energy

$$\lambda_0^{(m)} = E_0^{(m)} + 2\hbar m_s \omega_c \sqrt{\frac{\gamma^2}{4} + \frac{2\kappa^2 E_0^{(m)}}{\omega_c}} = E, \tag{5.36}$$

where the quantity

$$E_0^{(m)} = \frac{\omega_c}{2}(Q^2 + P^2) \tag{5.37}$$

is conserved in each polarization as well. We can express the frequencies and classical actions of the periodic orbits found from the Hamiltonians (5.36) through $E_0^{(m)}$ (cf. [3]):

$$\omega^{(m)} = \omega_c \left(1 + \frac{2\hbar m\kappa^2}{\sqrt{\gamma^2/4 + 2\kappa^2 E_0^{(m)}/\omega_c}}\right), \tag{5.38}$$

$$\mathcal{S}^{(m)} = 2\pi E_0^{(m)}/\omega_c, \tag{5.39}$$

respectively.

Below we quote the list of useful formulae which express the quantities characterizing the classical dynamics in each polarization through the energy E, parameters of the system, and polarization index m:

$$E_0^{(m)} = E + 4\hbar^2 m^2 \kappa^2 \omega_c - 2\hbar m \omega_c \sqrt{\frac{\gamma^2}{4} + \frac{2\kappa^2 E}{\omega_c} + 4\hbar^2 m^2 \kappa^4}, \tag{5.40}$$

$$\frac{|\mathbf{C}|^{(m)}}{2\omega_c} = \sqrt{\frac{\gamma^2}{4} + \frac{2\kappa^2 E}{\omega_c} + 4\hbar^2 m^2 \kappa^4} - 2\hbar m \kappa^2, \tag{5.41}$$

$$\mathcal{S}^{(m)} = 2\pi \left(\frac{E}{\omega_c} + 4\hbar^2 m^2 \kappa^2 - 2\hbar m \sqrt{\frac{\gamma^2}{4} + \frac{2\kappa^2 E}{\omega_c} + 4\hbar^2 m^2 \kappa^4}\right), \tag{5.42}$$

$$T^{(m)} = \frac{2\pi}{\omega_c}\left(1 - \frac{2\hbar m \kappa^2}{\sqrt{\gamma^2/4 + 2\kappa^2 E/\omega_c + 4\hbar^2 m^2 \kappa^4}}\right), \tag{5.43}$$

$$\frac{T^{(m)}}{|\mathbf{C}|^{(m)}} = \frac{\pi}{\omega_c^2} \frac{1}{\sqrt{\gamma^2/4 + 2\kappa^2 E/\omega_c + 4\hbar^2 m^2 \kappa^4}}. \tag{5.44}$$

For the calculation of the phase corrections according to (4.47) and (4.53), we need to find

$$\cos\theta_C \equiv (\mathbf{n}_C)_3 = \frac{\gamma/2}{\sqrt{\gamma^2/4 + 2\kappa^2 E_0/\omega_c}} = \frac{\gamma\omega_c}{|\mathbf{C}|}, \tag{5.45}$$

$$\sin\theta_C\{\theta_C,\phi_C\} = \{\phi_C, E_0\}\frac{d(\mathbf{n}_C)_3}{dE_0} = \{\phi_C,\lambda_0\}\left(\frac{d\lambda_0}{dE_0}\right)^{-1}\frac{d(\mathbf{n}_C)_3}{dE_0}, \tag{5.46}$$

where we omit m to simplify notations. From the relations (5.37) and

$$\tan\phi_C = -\frac{P}{Q} \tag{5.47}$$

we can easily find that $\{\phi_C, E_0\} = \omega_c$. It is also straightforward that

$$\frac{d\lambda_0}{dE_0} = \frac{\omega}{\omega_c}, \quad \frac{d(\mathbf{n}_C)_3}{dE_0} = \frac{\gamma\omega_c}{\hbar m|\mathbf{C}|^2}\left(1 - \frac{d\lambda_0}{dE_0}\right) = \frac{\gamma(\omega_c - \omega)}{\hbar m|\mathbf{C}|^2}. \tag{5.48}$$

After simple transformations we can express the phase corrections (with restored m)

$$\delta\Phi^{(m)} = -\left(\lambda_{\mathrm{B}}^{(m)} + \lambda_{\mathrm{NN}}^{(m)}\right)T^{(m)} \tag{5.49}$$

in terms of

$$\lambda_{\mathrm{B}}^{(m)} = -m\omega^{(m)}\left(1 + \frac{\gamma\omega_c}{|\mathbf{C}|^{(m)}}\right), \tag{5.50}$$

$$\lambda_{\mathrm{NN}}^{(m)} = (m^2 - s(s+1))\frac{\gamma\omega_c(\omega_c - \omega^{(m)})}{2m|\mathbf{C}|^{(m)}}, \tag{5.51}$$

and $T^{(m)}$ given by (5.43). It is evident that $\lambda_{\mathrm{NN}}^{(m)} = 0$ for $\gamma = 0$.

As it was noticed in [3], the Maslov indices for periodic orbits in each polarization m are the same as for the one-dimensional harmonic oscillator. Thus, we obtain the Trace Formula

$$\delta g_{sc}^{\mathrm{SCL}}(E) = \frac{1}{\hbar\pi}\sum_{m=-s}^{s} T^{(m)}\sum_{r=1}^{\infty}\cos\left(r\frac{S^{(m)}}{\hbar} + r\delta\Phi^{(m)} - r\pi\right), \tag{5.52}$$

which is a generalization of (5.7) for arbitrary s and $\gamma \neq 0$.

For $s = \frac{1}{2}$ $(m = \mp\frac{1}{2})$

$$T^{\mp} = \frac{2\pi}{\omega_c}\left(1 \pm \frac{\hbar\kappa^2}{\sqrt{\gamma^2/4 + 2\kappa^2 E/\omega_c + \hbar^2\kappa^4}}\right), \tag{5.53}$$

$$\mathcal{S}^{\mp} = 2\pi\left(\frac{E}{\omega_c} + \hbar^2\kappa^2 \pm \hbar\sqrt{\frac{\gamma^2}{4} + \frac{2\kappa^2 E}{\omega_c} + \hbar^2\kappa^4}\right), \tag{5.54}$$

$$\delta\Phi^{\mp} = \mp\pi\left(1 + \frac{\gamma/2}{\sqrt{\gamma^2/4 + 2\kappa^2 E/\omega_c + \hbar^2\kappa^4}}\right). \tag{5.55}$$

Taking $\gamma = 0$ we recover (5.7).

5.2 Quantum dot with the Rashba interaction

In this section we consider a two-dimensional electron gas in a semiconductor heterostructure, laterally confined to a quantum dot by a harmonic potential. We assume that its Hamiltonian

$$\hat{H} = \frac{\hat{p}_1^2}{2m^*} + \frac{\hat{p}_2^2}{2m^*} + \frac{m^*\,\Omega_1^2\,\hat{q}_1^2}{2} + \frac{m^*\,\Omega_2^2\,\hat{q}_2^2}{2} + 2\kappa\hbar\,(\hat{s}_2\hat{p}_1 - \hat{s}_1\hat{p}_2) \tag{5.56}$$

includes a spin-orbit interaction of Rashba type [21], where[2] $\kappa = \alpha_R/\hbar^2$. The c-number Hamiltonian (3.136) in this case is

$$H = \frac{p_1^2}{2m^*} + \frac{p_2^2}{2m^*} + \frac{m^*\Omega_1^2 q_1^2}{2} + \frac{m^*\Omega_2^2 q_2^2}{2} + 2S\kappa(n_2p_1 - n_1p_2). \tag{5.57}$$

We will treat this system within the semiclassical approach in the extended phase space (Sec. 4.2). As discussed in [3], the WCL Trace Formula fails to account for the spin-orbit interaction. Indeed, without spin-orbit coupling the only periodic orbits of the system are the two self-retracting librations along the principal axes (we assume Ω_1/Ω_2 to be irrational). The effective magnetic field $\mathbf{C}(\mathbf{p}) = 2\kappa\mathbf{e}_3 \times \mathbf{p}$ changes its sign together with $\mathbf{p}$. Hence the spin precession generated by a libration is self-retracting as well, making the rotation angle for the Bloch sphere $\eta(E)$ vanish. Then the modulation factor $\mathcal{M}_{po}(E) = 2s+1$ for both orbits is trivial. Thus, the WCL Trace Formula is that of the two-dimensional anisotropic harmonic oscillator [18] multiplied by the spin degeneracy factor $(2s+1)$:

$$\begin{aligned}\delta g_{sc}^{\mathrm{WCL}}(E) &= \frac{2s+1}{\hbar\Omega_1}\sum_{k=1}^{\infty}\frac{(-1)^k}{\sin\left(k\pi\frac{\Omega_1}{\Omega_2}\right)}\sin\left(k\frac{2\pi E}{\hbar\Omega_1}\right)\\ &+ \frac{2s+1}{\hbar\Omega_2}\sum_{k=1}^{\infty}\frac{(-1)^k}{\sin\left(k\pi\frac{\Omega_2}{\Omega_1}\right)}\sin\left(k\frac{2\pi E}{\hbar\Omega_2}\right).\end{aligned} \tag{5.58}$$

In the SCL the two pendulating orbits are still present and contain the mode-conversion points [3], where the interaction term vanishes. Thus the SCL approach in its original form cannot be applied either. Although one can fix it to some extent by an *ad hoc* procedure [37], it would be only natural for us to resort to our extended phase-space semiclassics, that does not suffer from the mode conversion problem and is not restricted to weak or strong spin-orbit coupling.

The classical dynamics is described by the equations of motion (4.9) and (4.12) that now become

$$\dot{q}_1 = \frac{p_1}{m^*} + \frac{4S\kappa v}{1+u^2+v^2} = \frac{p_1}{m^*} + 2S\kappa n_2, \tag{5.59}$$

$$\dot{q}_2 = \frac{p_2}{m^*} - \frac{4S\kappa u}{1+u^2+v^2} = \frac{p_2}{m^*} - 2S\kappa n_1, \tag{5.60}$$

$$\dot{v} = -\kappa(1+u^2+v^2)p_2 + 2\kappa u(up_2 - vp_1), \tag{5.61}$$

$$\dot{p}_1 = -m^*\Omega_1^2 q_1, \tag{5.62}$$

$$\dot{p}_2 = -m^*\Omega_2^2 q_2, \tag{5.63}$$

$$\dot{u} = -\kappa(1+u^2+v^2)p_1 - 2\kappa v(up_2 - vp_1). \tag{5.64}$$

[2] This definition of κ is applicable only within Sec. 5.2

Equations (5.61) and (5.64) are equivalent to (4.11), or,

$$\dot{n}_1 = 2\kappa p_1 n_3, \quad \dot{n}_2 = 2\kappa p_2 n_3, \quad \dot{n}_3 = -2\kappa(p_1 n_1 + p_2 n_2). \tag{5.65}$$

For a numerical study, it is convenient to describe the system in dimensionless quantities. Let us choose a characteristic frequency Ω_0 and define the dimensionless $\omega_1 = \Omega_1/\Omega_0$ and $\omega_2 = \Omega_2/\Omega_0$ (note that there is a degree of arbitrariness in the choice of Ω_0). Then we can construct the following scaled variables:

$$\tilde{\mathbf{q}} = \mathbf{q}\sqrt{\frac{m^*\Omega_0}{2S}}, \quad \tilde{\mathbf{p}} = \mathbf{p}\frac{1}{\sqrt{2Sm^*\Omega_0}}, \quad \tilde{\kappa} = \kappa\sqrt{\frac{2Sm^*}{\Omega_0}}, \tag{5.66}$$

$$(\tilde{E}, \tilde{H}) = \frac{1}{2S\Omega_0}(E, H), \quad \tilde{t} = \Omega_0 t, \quad (\tilde{\mathcal{S}}, \tilde{\mathcal{R}}) = \frac{1}{2S}(\mathcal{S}, \mathcal{R}). \tag{5.67}$$

The Hamiltonian in the scaled coordinates has the form

$$\tilde{H} = \frac{\tilde{p}_1^2}{2} + \frac{\tilde{p}_2^2}{2} + \frac{\omega_1^2\tilde{q}_1^2}{2} + \frac{\omega_2^2\tilde{q}_2^2}{2} + 2\tilde{\kappa}\frac{v\tilde{p}_1 - u\tilde{p}_2}{1 + u^2 + v^2}. \tag{5.68}$$

With the scaled action (4.15)

$$\tilde{\mathcal{S}} = \oint \left[\frac{1}{2}(\tilde{\mathbf{p}} \cdot d\tilde{\mathbf{q}} - \tilde{\mathbf{q}} \cdot d\tilde{\mathbf{p}}) + \frac{udv - vdu}{1 + u^2 + v^2}\right] \tag{5.69}$$

the applicability condition of the semiclassical approach now reads $\tilde{\mathcal{S}} \gg 1/2s$.

The equations of motion for the tilded variables are

$$\begin{aligned}
\dot{\tilde{q}}_1 &= \tilde{p}_1 + \tilde{\kappa} n_2, \quad \dot{\tilde{q}}_2 = \tilde{p}_2 - \tilde{\kappa} n_1, && (5.70)\\
\dot{\tilde{p}}_1 &= -\omega_1^2 \tilde{q}_1, \quad \dot{\tilde{p}}_2 = -\omega_2^2 \tilde{q}_2, && (5.71)\\
\dot{n}_1 &= 2\tilde{\kappa}\tilde{p}_1 n_3, \quad \dot{n}_2 = 2\tilde{\kappa}\tilde{p}_2 n_3, \quad \dot{n}_3 = -2\tilde{\kappa}(\tilde{p}_1 n_1 + \tilde{p}_2 n_2), && (5.72)
\end{aligned}$$

where time derivatives are taken with respect to $\tilde{t}$ as well.

Note that the system possesses certain discrete symmetries:

$$\begin{aligned}
R_{12} &: \tilde{q}_1 \to -\tilde{q}_1, \quad \tilde{q}_2 \to -\tilde{q}_2, \quad n_3 \to -n_3, \quad \tilde{t} \to -\tilde{t} && (5.73)\\
R_1 &: \tilde{q}_1 \to -\tilde{q}_1, \quad \tilde{p}_2 \to -\tilde{p}_2, \quad n_1 \to -n_1, \quad \tilde{t} \to -\tilde{t} && (5.74)\\
R_2 &: \tilde{q}_2 \to -\tilde{q}_2, \quad \tilde{p}_1 \to -\tilde{p}_1, \quad n_2 \to -n_2, \quad \tilde{t} \to -\tilde{t} && (5.75)
\end{aligned}$$

There are trivial solutions to the equations of motion—the pendulating orbits with "frozen spin":

- The pair of orbits $A_x^\pm$ pendulating along the $\tilde{q}_1$ axis with spin $n_2 = \pm 1$. The phase-space coordinates along these orbits are

$$\tilde{q}_1(\tilde{t}) = \pm\left(\sqrt{2\tilde{E} + \tilde{\kappa}^2}/\omega_1\right)\sin(\omega_1\tilde{t}), \quad \tilde{p}_1(\tilde{t}) = \mp\tilde{\kappa} \pm \sqrt{2\tilde{E} + \tilde{\kappa}^2}\cos(\omega_1\tilde{t}),$$
$$v(\tilde{t}) = \pm 1, \quad \tilde{q}_2(\tilde{t}) = \tilde{p}_2(\tilde{t}) = u(\tilde{t}) = 0. \tag{5.76}$$

  The period of the orbits is $\tilde{T}_1 = 2\pi/\omega_1$. The orbits are invariant under R_{12} and R_1 (R_2 produces the symmetry partner, i.e., maps + onto −).

- Similarly, there are a pair of orbits $A_y^{\pm}$ pendulating in the $\tilde{q}_2$ direction with spin $n_1 = \pm 1$. They are given by

$$\tilde{q}_2(\tilde{t}) = \pm\left(\sqrt{2\tilde{E} + \tilde{\kappa}^2}/\omega_2\right)\sin(\omega_2\tilde{t}), \quad \tilde{p}_2(t) = \pm\tilde{\kappa} \pm \sqrt{2\tilde{E} + \tilde{\kappa}^2}\cos(\omega_2\tilde{t}),$$
$$u(\tilde{t}) = \pm 1, \quad \tilde{q}_1(\tilde{t}) = \tilde{p}_1(\tilde{t}) = v(\tilde{t}) = 0. \tag{5.77}$$

  The period is $\tilde{T}_2 = 2\pi/\omega_2$. The orbits are invariant under R_{12} and R_2 (R_1 produces the symmetry partner).

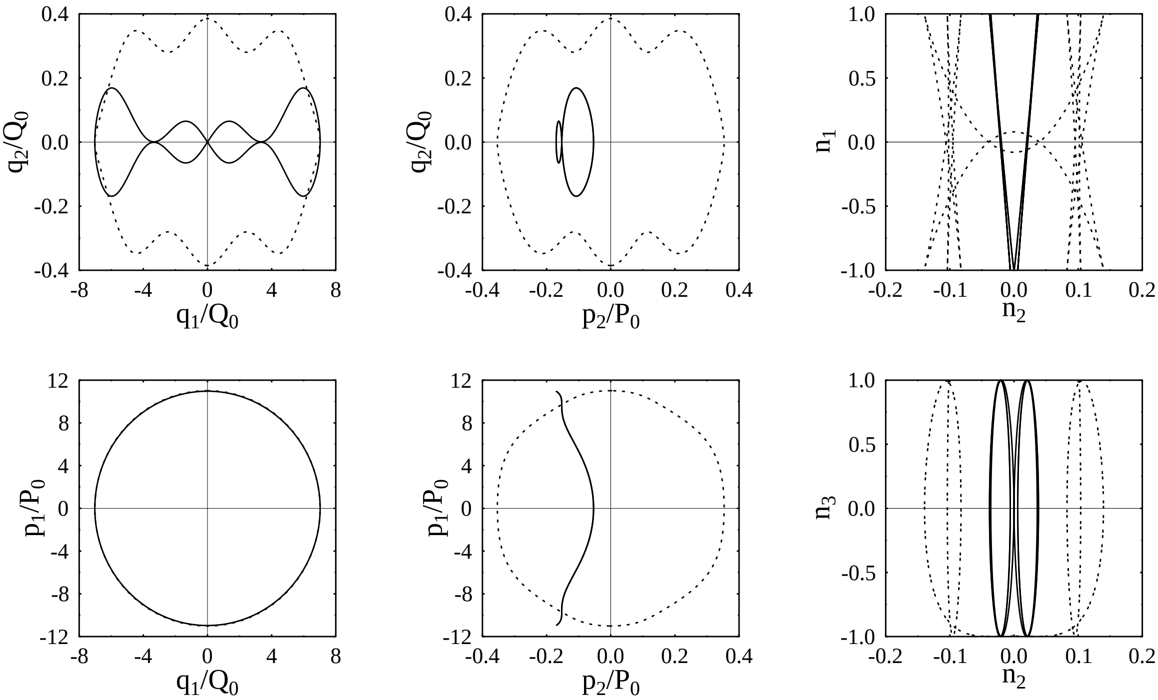

Figure 5.1: Periodic orbits D_{x1}^{+} (solid line) and D_{x2}^{+} (dotted line) for $\tilde{\kappa} = 0.67$, $\tilde{E} = 60$, represented in different cross-sections of the phase space. Here $Q_0 = \sqrt{2S/m^*\Omega_0}$, $P_0 = \sqrt{2Sm^*\Omega_0}$. Note the different scales along the axes. In the lower left plot the two orbits are almost indistinguishable. For the $\mathbf{n}(t)$ time dependence see [78].

Other types of periodic orbits can be found from the numerical solution of the equations of motion (5.70)-(5.72). In our numerical example we use $\omega_1 = 1.56$ and $\omega_2 = 1.23$. For a large range of parameters with $0 < \tilde{\kappa} \lesssim 0.75$ and $\tilde{E} \gtrsim 8$ we find the following non-trivial periodic orbits:

- Two pairs of orbits $D_{x1}^{\pm}$ and $D_{x2}^{\pm}$ oscillating around $A_x^{\pm}$ in the configuration space, with $n_2 \sim 0$ (Fig. 5.1). The spin is rotating about n_2 axis. The superscripts ($\pm$) denote the sense of rotation in the subspace $(\tilde{q}_1, \tilde{q}_2)$.

- Two pairs of orbits $D_{y1}^{\pm}$ and $D_{y2}^{\pm}$ oscillating around $A_y^{\pm}$, with $n_1 \sim 0$ (Fig. 5.2). The spin is rotating about n_1 axis.

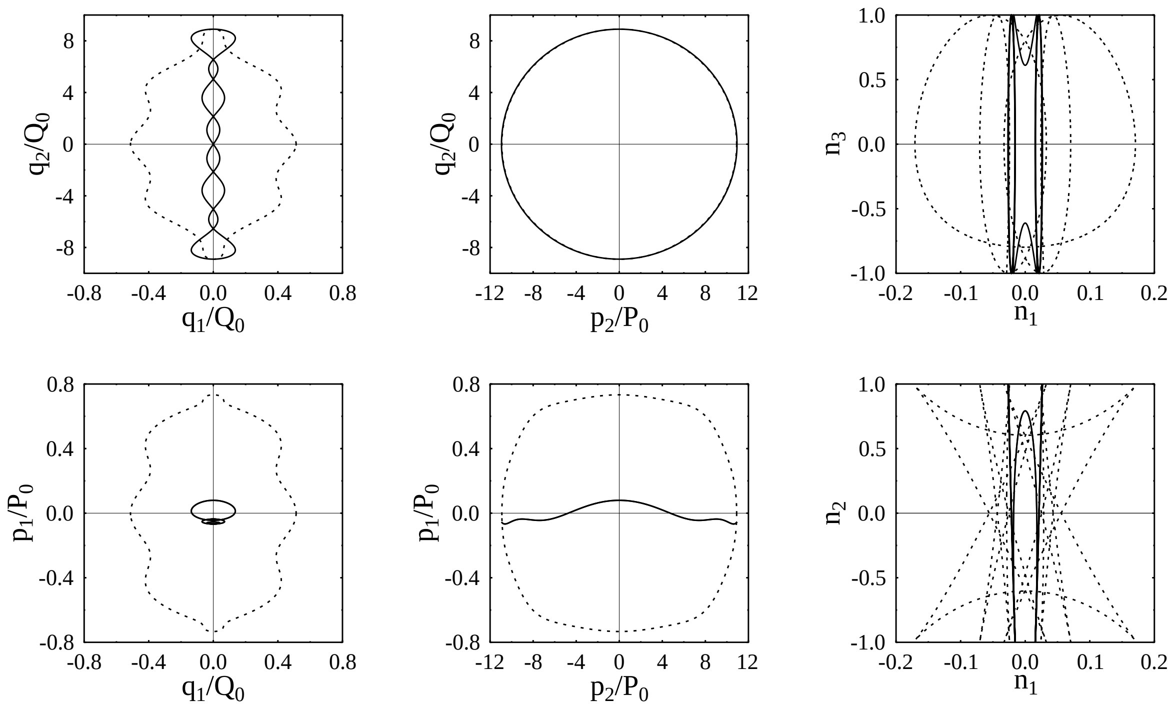

Figure 5.2: Same as in Fig. 5.1 for orbits D_{y1}^{+} (solid line) and D_{y2}^{+} (dotted line). In the upper middle plot the two orbits are almost indistinguishable.

For stronger couplings $\tilde{\kappa} \gtrsim 0.75$ or smaller energies $\tilde{E} \lesssim 8$, new orbits bifurcate from the A and D orbits. Near the bifurcations the Trace Formula would have to be modified by uniform approximations [84]. The periods of the orbits are shown in Fig. 5.3.

The spin-orbit strength $\tilde{\kappa}$ depends on the band structure [29]. For example, for an InGaAs-InAlAs quantum dot with ~ 100 confined electrons one would obtain a value of $\tilde{\kappa} \sim 0.25$. In order to have the effect of spin on the orbital motion more pronounced, we choose $\tilde{\kappa} = 0.67$ for our numerics.

The stability determinant in the Trace Formula can be calculated according to the general prescription (Sec. 4.2). The second variation of the Hamiltonian (5.68) is

$$\begin{aligned} \tilde{H}^{(2)} &= \frac{\tilde{\rho}_1^2}{2} + \frac{\tilde{\rho}_2^2}{2} + \frac{\omega_1^2\tilde{\lambda}_1^2}{2} + \frac{\omega_2^2\tilde{\lambda}_2^2}{2} \\ &+ \tilde{\kappa}(u\tilde{p}_2 - v\tilde{p}_1)(\xi^2+\nu^2) + \tilde{\kappa}\frac{2\sqrt{2}\,uv}{1+u^2+v^2}(\tilde{\rho}_2\nu - \tilde{\rho}_1\xi) \\ &+ \tilde{\kappa}\sqrt{2}\left(\frac{2u^2}{1+u^2+v^2} - 1\right)\tilde{\rho}_2\xi - \tilde{\kappa}\sqrt{2}\left(\frac{2v^2}{1+u^2+v^2} - 1\right)\tilde{\rho}_1\nu, \qquad (5.78) \end{aligned}$$

where the variables $\boldsymbol{\lambda}$ and $\boldsymbol{\rho}$ are scaled like $\mathbf{q}$ and $\mathbf{p}$, respectively. Numerically solving

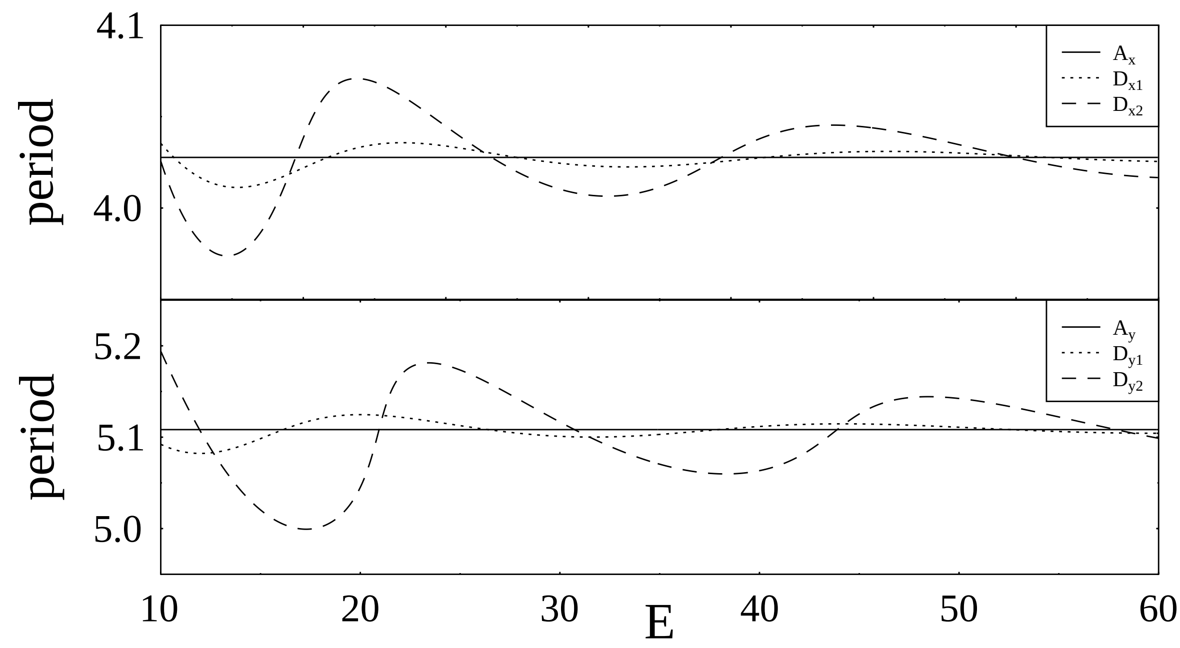

Figure 5.3: The periods of the $A^{\pm}$ and $D^{\pm}$ orbits as functions of energy for $\tilde{\kappa} = 0.67$. The periods are given in units of $1/\Omega_0$, the energy unit is $2S\Omega_0$. For the orbits $A_x^{\pm}$ and $A_y^{\pm}$ the periods are independent of energy and equal to $\tilde{T}_1 \approx 4.02768$ and $\tilde{T}_2 \approx 5.10828$, respectively.

the equations of motion for variations

$$\dot{\tilde{\lambda}}_1 = \tilde{\rho}_1 - \tilde{\kappa}\sqrt{2}\frac{2uv}{1+u^2+v^2}\xi - \tilde{\kappa}\sqrt{2}\left(\frac{2v^2}{1+u^2+v^2} - 1\right)\nu, \tag{5.79}$$

$$\dot{\tilde{\lambda}}_2 = \tilde{\rho}_2 + \tilde{\kappa}\sqrt{2}\left(\frac{2u^2}{1+u^2+v^2} - 1\right)\xi + \tilde{\kappa}\sqrt{2}\frac{2uv}{1+u^2+v^2}\nu, \tag{5.80}$$

$$\dot{\nu} = -\tilde{\kappa}\frac{2\sqrt{2}\,uv}{1+u^2+v^2}\tilde{\rho}_1 + \tilde{\kappa}\sqrt{2}\left(\frac{2u^2}{1+u^2+v^2} - 1\right)\tilde{\rho}_2 + 2\tilde{\kappa}(u\tilde{p}_2 - v\tilde{p}_1)\xi, \tag{5.81}$$

$$\dot{\tilde{\rho}}_1 = -\omega_1^2\tilde{\lambda}_1, \tag{5.82}$$

$$\dot{\tilde{\rho}}_2 = -\omega_2^2\tilde{\lambda}_2, \tag{5.83}$$

$$\dot{\xi} = \tilde{\kappa}\sqrt{2}\left(\frac{2v^2}{1+u^2+v^2} - 1\right)\tilde{\rho}_1 - \tilde{\kappa}\frac{2\sqrt{2}\,uv}{1+u^2+v^2}\tilde{\rho}_2 - 2\tilde{\kappa}(u\tilde{p}_2 - v\tilde{p}_1)\nu, \tag{5.84}$$

one determines the reduced monodromy matrix and then finds the stability determinant $\det(\widetilde{M}_{po} - I_4)$ of the periodic orbits.

After calculating the Maslov indices according to Appendix B.1 (see the Table 5.1) and the Solari-Kochetov phase by (4.5), we can compute the oscillating part of the density of states using the Trace Formula (4.18) (Fig. 5.4). Note that while the classical dynamics in the scaled variables is independent of the value of spin, the density of states will depend on S, since the unscaled action $2S\tilde{S}$ enters the phase of the Trace Formula. We choose the physically meaningful $S = \hbar/2$ in our example. To ensure

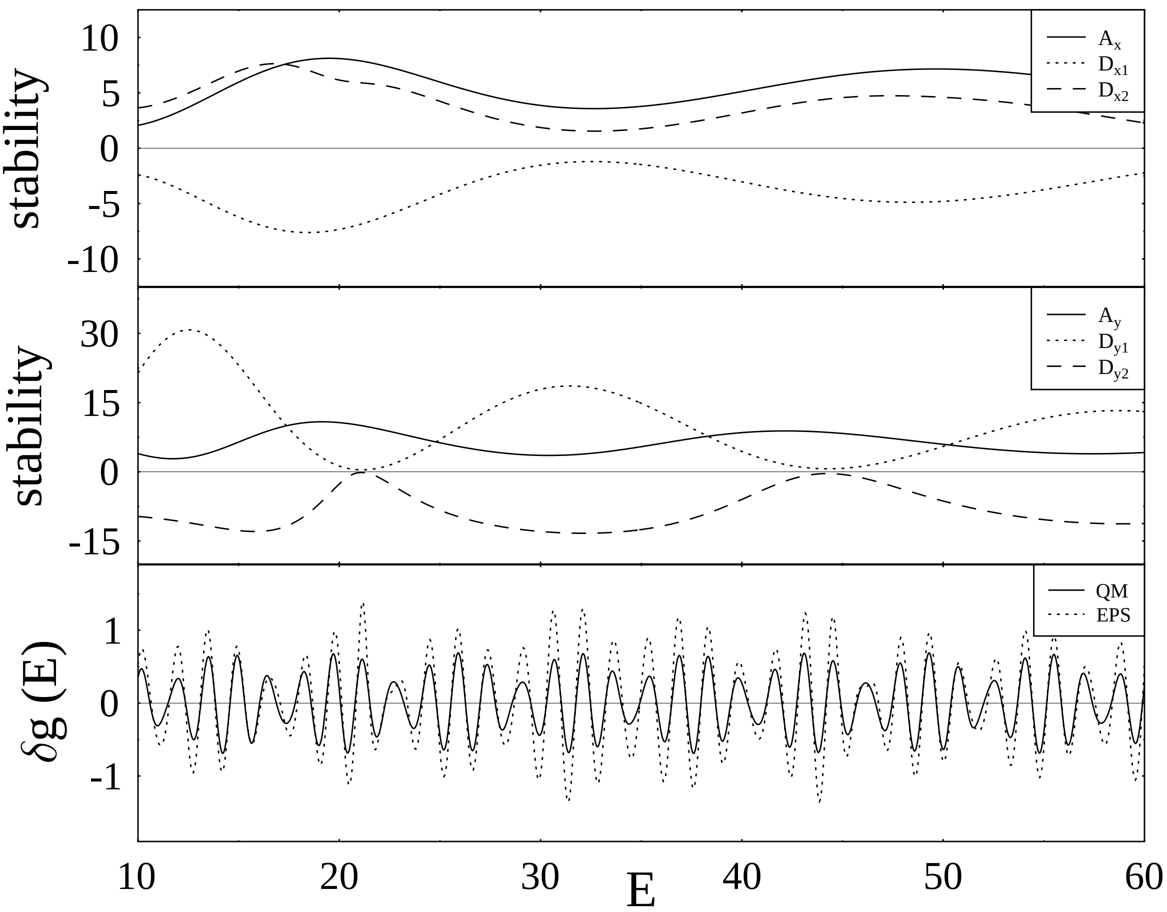

Figure 5.4: *Upper and middle panels:* the stabilities $\det(\widetilde{M}_{po} - I_4)$ of the $A^{\pm}$ and $D^{\pm}$ orbits. The curves come close to the zero level, but do not touch or cross it (avoided bifurcations). *Lower panel:* the oscillating part of density of states for $\tilde{\kappa} = 0.67$ and $S = \hbar/2$. QM: the quantum-mechanical exact diagonalization. EPS: the semiclassical calculation in the extended phase space, including only the first repetitions of the 12 primitive periodic orbits A and D (Gaussian averaging parameter $\gamma = 0.6$). The energy is measured in units of $\hbar\Omega_0$.

orbit	blocks	$\mathrm{sign}(s_1, s_2)$	m	σ_{av}	$\widetilde{m}$	$\widetilde{\sigma}_{\mathrm{av}}$	σ
$A_x^{\pm}$	ell, ell	$-\,,\,-$	1	2	3	-2	4
$D_{x1}^{\pm}$	hyp, ell	$,\,-$	2	1	3	-1	5
$D_{x2}^{\pm}$	ell, ell	$-\,,\,-$	0	2	2	-2	2
$A_y^{\pm}$	lox		3	0	3	0	6
$D_{y1}^{\pm}$	lox		2	0	2	0	4
$D_{y2}^{\pm}$	hyp, ell	$,\,+$	2	1	2	$+1$	5

Table 5.1: Stabilities, Maslov indices and their ingredients of the shortest orbits in the Rashba Hamiltonian (5.57). Notations are defined in Appendix B.1.

the convergence of the periodic orbit sum, the density of states was convoluted with a normalized Gaussian, $\exp[-(E/\gamma)^2]/\gamma\sqrt{\pi}$, i.e., it was smoothed out with the energy window $\sim \gamma$ (see [18] for details of this procedure). With the averaging parameter $\gamma = 0.6$, the first repetitions of the 12 primitive periodic orbits A and D were sufficient in the Trace Formula. The semiclassical result for the density of states is compared with the quantum-mechanical curve, obtained from a numerical diagonalization of the Hamiltonian (5.56). We observe a rather good agreement between the two, especially for the oscillation frequencies. The difference in the amplitudes can be explained by the vicinity of the bifurcations in the parameter space. Indeed, the disparity becomes larger near the avoided bifurcations, where the stabilities are extremely small (Fig. 5.4). In principle, these energy regions should be treated by a uniform approximation [84]. The matter is complicated, however, by the fact that the avoided bifurcations are non-generic and of codimension larger than 1. The theory for such bifurcations is developed only for two-dimensional systems. Our system is effectively three-dimensional. In addition to the elliptic and (inverse) hyperbolic orbits, it also has the loxodromic orbits. Thus, the extension of the standard theory of bifurcations is difficult and still needs to be developed.

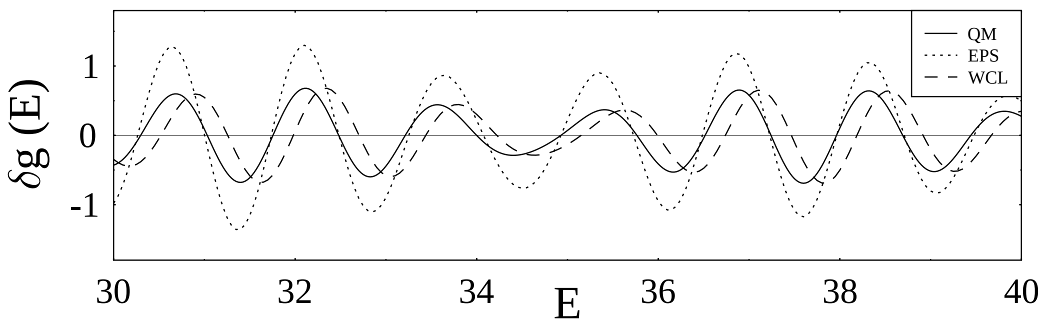

Figure 5.5: A detailed view of the lower panel of Fig. 5.4 with the WCL density of states added.

A more detailed view of $\delta g(E)$ is shown in Fig. 5.5. For comparison, we added there the density of states calculated by the WCL Trace Formula with spin $S = \hbar/2$, which, in this case, is the Trace Formula of the two-dimensional anisotropic harmonic oscillator without spin-orbit coupling [18] multiplied by the spin degeneracy factor 2 (see above). Clearly, it is shifted by phase from the exact density of states. It is worth mentioning that the dashed (WCL) curve would come very close to the exact quantum-mechanical curve if the former is shifted by $-\tilde{\kappa}^2/2$ in the scaled energy $\tilde{E}$. Note that the action of the trivial periodic orbits is $\tilde{\mathcal{S}}_i = (\pi/\omega_i)(2\tilde{E} + \tilde{\kappa}^2)$. Thus the shift can be related to the perturbative correction to the action in the extended phase space, which is of the second order in $\tilde{\kappa}$. To explain the shift, it would be interesting to develop the second-order perturbation theory in the parameter $\tilde{\kappa}$ for the Trace Formula in the extended phase space, similar to that proposed in [19]. (The first-order perturbation theory [25] should be equivalent to the WCL Trace Formula.) Apparently, the shift of the dashed curve cannot be justified within the standard WCL approach of [16]. With the increase of $\tilde{\kappa}$, the non-integrability of the system will show up, and the shape of the WCL curve (describing the integrable system) will start to deviate from the exact density of states.

Chapter 6

Conclusions and Outlook

The semiclassical description of systems with spin-orbit interaction is presented. The path-integral expression for the trace of the respective quantum propagator serves as a starting point for further semiclassical approximation of the density of states. For the construction of such expression we employ the basis of spin coherent states. Path-integral approach appears to unify the derivation of the Gutzwiller's Trace Formula for both spinless systems and systems with spin-orbit interaction.

In **Chapter 2** we review the Periodic Orbit Theory for systems without spin. The Trace Formula, which is central in this theory, expresses the oscillating part of the density of states in terms of classical quantities like classical actions, periods and stabilities of periodic orbits. The important ingredient to the Trace Formula is the so-called Maslov index which ensures the correct interference of contributions coming from different orbits. It can be obtained in a very elegant way within the path-integral approach as well. We review the respective derivation of [88], and specify some of its aspects in more detail in **Appendix B.1**. The Maslov index is often considered as a quantum phase correction, since it is small compared to the classical action. In the definite situations it might be necessary to also include phase corrections of different origin. They are directly related to the operator ordering in the quantum Hamiltonian. Especially, this often happens in the coherent-state semiclassical approximations. We discuss the nature of these phase corrections and give the prescription for their calculation.

In **Chapter 3** we review different possibilities to construct path-integral expressions for spin propagators. Among them are the spin coherent-state, Jordan-Schwinger and Stratonovich-Weyl representations. In principle, all of them can be applied to systems with spin-orbit interaction. Nevertheless, for the semiclassical approximation of the trace of propagator we choose the representation based on the spin coherent states. We develop the respective formalism in **Chapter 4**. One can define the semiclassical limit of large spin, as well as the limits of weak and strong coupling. Spin coherent-state path integrals prove especially advantageous in the large spin limit since they allow to obtain the generalization of the Gutzwiller's Trace Formula in the closed form, the necessary Solari-Kochetov phase correction being included. The origin of the latter is very similar to that occuring in the flat coherent-state semiclassics (this is discussed in **Appendix B.3**). In the weak coupling limit we generalize the Trace Formula for $s = 1/2$ known before [16] to the arbitrary value of spin. We also re-derive in the path-integral representation the results of the multicomponent WKB theory [66, 67] in the strong coupling limit (under the certain restriction, which can in principle be removed by a more accurate consideration of the discretized path integral).

In **Chapter 5** we apply the developed semiclassical methods to the specific physical systems. First, we study the free two-dimensional electron gas with the Rashba Hamiltonian in a homogeneous magnetic field. It is mathematically equivalent to the Jaynes-Cummings model of the dipole interaction of a two-level system (atom) with a single mode of electromagnetic field in the so-called rotating wave approximation. Both models are considered at the spin value $s = 1/2$ and allow for analytical treatment on both quantum-mechanical and semiclassical levels. We interpret the semiclassical limits of weak and strong coupling as formal asymptotic limits, and find the corresponding asymptotic parameters. The generalization of the semiclassical results in these limits to arbitrary value of s is proposed as well, and the physical system where it might appear useful is pointed out (the Dicke model). In **Chapter 5** we also consider an example of a quantum dot with harmonic confinement and Rashba interaction. This system is a good test case for the semiclassical approach in the extended phase space (formally defined in the large spin limit), since the SCL method suffers from the mode-conversion problem, while the WCL Trace Formula completely neglects the spin-orbit interaction. After making the numerical calculations, we observe the good phase correspondence of the semiclassical oscillating density of states with the respective quantum-mechanical curve, even though we apply the extended phase-space method beyond the formal limit of its applicability, i.e. for $s = 1/2$. We also discuss the possible ways to improve the amplitude of the semiclassical density of states, which slightly deviates from the quantum-mechanical value.

Our analytical and numerical results underscore the importance of the Solari-Kochetov phase correction in the spin coherent-state path integrals and the proper evaluation of the Maslov indices in the extended phase space.

The questions which are still open include the improvement of the semiclassical evaluation of path integrals in the case of strong spin-orbit coupling (restoration of the no-name term); generalizations of the method treating symmetry breaking and bifurcations by uniform approximations to systems with spin-orbit interaction; study of models with the Hamiltonian nonlinear in spin and driven by an external system, such as the kicked top [47].

The developed semiclassical methods can be applied to specific systems of interest in spintronics, molecular dynamics, and nuclear physics. One of the most promising perspectives is to generalize a semiclassical Landauer formula for conductance in order to take account of spin-orbit interaction, and then to explain semiclassically the phenomena of *weak antilocalization* in the spin-assisted transport through the chaotic cavities in the ballistic regime [97].

Appendix A

Phase-space picture of quantum mechanics

A.1 Wigner-Weyl calculus

It was noticed by Moyal [73] that Wigner's recipe [94] for associating a function on a phase space to a density operator on Hilbert space was essentially the inverse of Weyl's correspondence rule [93].

The Wigner-Weyl calculus (see, e.g., [5, 9, 76] for modern reviews) is based on the one-to-one linear mapping which associates to each operator $\hat{H}$ on Hilbert space a function, or Wigner-Weyl symbol, $H_W(q,p)$ which is defined on phase space (for simplicity, we restrict ourselves to a single degree of freedom: $d=1$). This mapping possesses the properties of reality (which means that $\hat{H}^\dagger \to H_W^*(q,p)$), standartization, traciality and covariance with respect to the action of the Heisenberg-Weyl group generated by $\hat{q}$ and $\hat{p}$.

The Wigner-Weyl correspondence is constructed due to the operator kernel

$$\hat{\Delta}(q,p) = \int \frac{dudv}{2\pi\hbar} \exp\left[\frac{i}{\hbar}\left(u(p-\hat{p}) + v(q-\hat{q})\right)\right], \tag{A.1}$$

which represents a continuously labelled basis for operators on Hilbert space. Each operator can be expressed as a linear combination in terms of $\hat{\Delta}$:

$$\hat{H} = \int \frac{dqdp}{2\pi\hbar} \hat{\Delta}(q,p) H_W(q,p). \tag{A.2}$$

Due to the properties of $\hat{\Delta}(q,p)$, the formula (A.2) can be inverted to give

$$H_W(q,p) = \mathrm{Tr}[\hat{H}\hat{\Delta}(q,p)] = \int dq' \langle q'|\hat{H}\hat{\Delta}(q,p)|q'\rangle. \tag{A.3}$$

It is easy to show that the Wigner-Weyl symbol equals

$$H_W(q,p) = \int dx e^{ipx/\hbar} \langle q - \frac{x}{2}|\hat{H}|q + \frac{x}{2}\rangle. \tag{A.4}$$

The standartization and tracial properties mean that

$$\begin{aligned} \mathrm{Tr}[\hat{F}] &= \int \frac{dqdp}{2\pi\hbar} F_W(q,p), && \text{(A.5)} \\ \mathrm{Tr}[\hat{F}\hat{G}] &= \int \frac{dqdp}{2\pi\hbar} F_W(q,p) G_W(q,p), && \text{(A.6)} \end{aligned}$$

respectively.

The Wigner-Weyl symbol of the product of two operators is given by the Moyal product [73] of two respective symbols. The Moyal formula can be written in the symbolic form

$$(\hat{F}\hat{G})_W = F_W * G_W = F_W \, e^{i\hbar\mathcal{L}/2} \, G_W, \tag{A.7}$$

where the operator

$$\mathcal{L} = \frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q} \tag{A.8}$$

is associated with the Poisson bracket

$$F_W \mathcal{L} G_W = \{F_W, G_W\}_{q,p} = \frac{\partial F_W}{\partial q}\frac{\partial G_W}{\partial p} - \frac{\partial F_W}{\partial p}\frac{\partial G_W}{\partial q}. \tag{A.9}$$

Expanding (A.7) into a series of $\hbar$, we obtain the leading and the next-to-leading contributions to the Moyal formula

$$(\hat{F}\hat{G})_W = F_W G_W + \frac{i\hbar}{2}\{F_W, G_W\}_{q,p} + O(\hbar^2). \tag{A.10}$$

Respectively, the leading contribution to the Weyl symbol of the commutator

$$([\hat{F},\hat{G}])_W = (\hat{F}\hat{G} - \hat{G}\hat{F})_W = F_W * G_W - G_W * F_W = i\hbar\{F_W, G_W\}_{q,p} + O(\hbar^3) \tag{A.11}$$

establishes the "correspondence principle" between commutators and Poisson brackets.

In general, the Wigner-Weyl symbol of an arbitrary operator contains terms with different powers of $\hbar$. The limit $\hbar \to 0$ of the Wigner-Weyl symbol yields the principal symbol. There exists a special class of operators whose Wigner-Weyl symbols coincide with their pricipal symbols. These operators are symmetrically, or Weyl-, ordered in $\hat{q}$ and $\hat{p}$ [72]. After the transformation (2.20) they convert into the operators symmetrically ordered in $\hat{A}$ and $\hat{A}^\dagger$. One can then define the Wigner-Weyl symbols $F_W(\bar{\alpha},\alpha)$ and $G_W(\bar{\alpha},\alpha)$ and the Poisson bracket

$$\{F_W(\bar{\alpha},\alpha), G_W(\bar{\alpha},\alpha)\}_{\bar{\alpha},\alpha} = i\left(\frac{\partial F_W}{\partial \bar{\alpha}}\frac{\partial G_W}{\partial \alpha} - \frac{\partial F_W}{\partial \alpha}\frac{\partial G_W}{\partial \bar{\alpha}}\right) \tag{A.12}$$

by making a change of variables

$$\alpha = \frac{1}{\sqrt{2}}\,(q + ip)\,, \quad \bar{\alpha} = \frac{1}{\sqrt{2}}\,(q - ip) \tag{A.13}$$

in $F_W(q,p)$ and $G_W(q,p)$ and in the Poisson bracket (A.9), respectively.

A.2 Cahill-Glauber representation

A definition of a phase-space symbol associated to a quantum operator is not unique. If the tracial condition (A.6) is replaced by a more general one (see below), one can then construct a one-parametric family of symbols [22], which continuously interpolates between covariant (2.36) and contravariant (implicitly defined by (2.50)) symbols, and includes as an element the Wigner-Weyl symbol (A.3). In particular, the so-called λ-symbol is defined by

$$H^{(\lambda)}(\bar{\alpha},\alpha) = \mathrm{Tr}[\hat{H}\hat{\Delta}_\lambda(\bar{\alpha},\alpha)], \quad \lambda\in[0,1], \tag{A.14}$$

where

$$\hat{\Delta}_\lambda(\bar{\alpha},\alpha) = \int \frac{d^2\xi}{\pi\hbar} e^{-(1-2\lambda)\bar{\xi}\xi/2\hbar} e^{\{\xi(\bar{\alpha}-\hat{A}^\dagger)-\bar{\xi}(\alpha-\hat{A})\}/\hbar}. \tag{A.15}$$

The choice of the λ-symbol is related to the λ-quantization scheme in sense of Berezin [8]. The particular cases of $\lambda = 0, \frac{1}{2}, 1$ correspond to the covariant, Wigner-Weyl and contravariant symbols, respectively. We remark that after the change of variables (A.13) the operator kernel $\hat{\Delta}_{1/2}(\bar{\alpha},\alpha)$ coincides with $\hat{\Delta}(q,p)$ given by (A.1), provided that $\xi = (-u+iv)/\sqrt{2}$.

Operator kernel (A.15) can be expressed

$$\hat{\Delta}_\lambda(\bar{\alpha},\alpha) = \int \frac{d^2\xi}{\pi\hbar} e^{-(1-2\lambda)\bar{\xi}\xi/2\hbar} e^{\{\xi\bar{\alpha}-\bar{\xi}\alpha\}/\hbar}\hat{T}_{-\xi} \tag{A.16}$$

in terms of the Heisenberg operator

$$\hat{T}(\bar{\xi},\xi) \equiv \hat{T}_\xi = e^{\{\xi\hat{A}^\dagger-\bar{\xi}\hat{A}\}/\hbar}, \tag{A.17}$$

which shifts the operators $\hat{A}$ and $\hat{A}^\dagger$:

$$\hat{T}_\xi\hat{A}\hat{T}_\xi^\dagger = \hat{A}-\xi, \quad \hat{T}_\xi\hat{A}^\dagger\hat{T}_\xi^\dagger = \hat{A}^\dagger-\bar{\xi}. \tag{A.18}$$

Due to the relation

$$\hat{T}_{-\xi} = \int \frac{d^2\alpha'}{\pi\hbar} e^{+(1-2\lambda')\bar{\xi}\xi/2\hbar} e^{-\{\xi\bar{\alpha}'-\bar{\xi}\alpha'\}/\hbar}\hat{\Delta}_{\lambda'}(\bar{\alpha}',\alpha'), \tag{A.19}$$

which is inverse to (A.16), we can derive the integral relation between different λ-symbols

$$H^{(\lambda)}(\bar{\alpha},\alpha) = \int \frac{d^2\xi}{\pi\hbar}\frac{d^2\alpha'}{\pi\hbar} H^{(\lambda')}(\bar{\alpha}',\alpha') e^{-(\lambda'-\lambda)\bar{\xi}\xi/\hbar} e^{\{\xi(\bar{\alpha}'-\bar{\alpha})-\bar{\xi}(\alpha'-\alpha)\}/\hbar}. \tag{A.20}$$

The integral over $d^2\xi$ converges if $\lambda<\lambda'$. For $\lambda=\lambda'$ we obtain an integral representation for δ-function, and therefore we recover the identity $H^{(\lambda)} = H^{(\lambda)}$.

For the particular values $\lambda = 0$ and $\lambda' = \frac{1}{2}$ we obtain the expression

$$H^{(0)}(\bar{\alpha},\alpha) = 2\int \frac{d^2\alpha'}{\pi\hbar} H^{(1/2)}(\bar{\alpha}',\alpha') e^{-2|\alpha'-\alpha|^2/\hbar}. \tag{A.21}$$

For a density operator $\hat{\rho}$, it relates Husimi $\rho^{(0)}$ and Wigner $\rho^{(1/2)}$ distributions.

The arbitrary λ-symbol is linked to the covariant symbol through the differential relation

$$H^{(0)}(\bar{\alpha},\alpha) = e^{\hbar\lambda\Delta} H^{(\lambda)}(\bar{\alpha},\alpha), \tag{A.22}$$

where Δ is the Laplace operator on the complex plane given by (2.45). In the semi-classical limit $\hbar \to 0$ *r.h.s.* of (A.22) can be expanded as

$$H^{(0)} = H^{(\lambda)} + \hbar\lambda\Delta H^{(\lambda)} + O(\hbar^2). \tag{A.23}$$

Therefore, for arbitrary $\lambda, \lambda' \in [0,1]$ we have

$$H^{(\lambda')} = H^{(\lambda)} - \hbar(\lambda' - \lambda)\Delta H^{(\lambda)} + O(\hbar^2). \tag{A.24}$$

A quantum operator can be inversely expressed through the λ-symbol by

$$\hat{H} = \int \frac{d^2\alpha}{\pi\hbar} H^{(\lambda)}(\bar{\alpha},\alpha)\hat{\Delta}_{1-\lambda}(\bar{\alpha},\alpha). \tag{A.25}$$

Below we quote the list of properties which constitute the necessary and sufficient input for the unique construction of the λ-symbol (A.14):

0) linearity, i.e. $\hat{H} \longrightarrow H^{(\lambda)}(\bar{\alpha},\alpha)$ is one-to-one linear map;

i) reality
$$(\hat{H}^\dagger)^{(\lambda)}(\bar{\alpha},\alpha) = [H^{(\lambda)}(\bar{\alpha},\alpha)]^*; \tag{A.26}$$

ii) standartization
$$\mathrm{Tr}[\hat{H}] = \int \frac{d^2\alpha}{\pi\hbar} H^{(\lambda)}(\bar{\alpha},\alpha); \tag{A.27}$$

iii) traciality
$$\mathrm{Tr}[\hat{F}\hat{G}] = \int \frac{d^2\alpha}{\pi\hbar} F^{(\lambda)}(\bar{\alpha},\alpha)G^{(1-\lambda)}(\bar{\alpha},\alpha) = \int \frac{d^2\alpha}{\pi\hbar} F^{(1-\lambda)}(\bar{\alpha},\alpha)G^{(\lambda)}(\bar{\alpha},\alpha) \tag{A.28}$$

(we note that it generalizes (A.6) and reproduces the latter at $\lambda = \frac{1}{2}$);

iv) covariance
$$(\hat{T}_\xi \hat{H} \hat{T}_\xi^\dagger)^{(\lambda)}(\bar{\alpha},\alpha) = H^{(\lambda)}(\bar{\alpha} - \bar{\xi}, \alpha - \xi). \tag{A.29}$$

We remark that the above construction of symbols relies on the commutation relation (2.21). However, one can define operators

$$\begin{pmatrix} \hat{A}_\nu \\ \hat{A}_\nu^\dagger \end{pmatrix} = \begin{pmatrix} \cos\frac{\nu}{2} & \sin\frac{\nu}{2} \\ -\sin\frac{\nu}{2} & \cos\frac{\nu}{2} \end{pmatrix} \begin{pmatrix} \hat{A} \\ \hat{A}^\dagger \end{pmatrix}, \tag{A.30}$$

where $\nu \in [0,\pi)$, with the same commutation relation $[\hat{A}_\nu, \hat{A}_\nu^\dagger] = \hbar$. One is then able to construct even a wider class of symbols (labelled by ν and λ) which are associated to a given quantum operator [23, 2]. In particular, a family of symbols constructed for $\nu = \frac{\pi}{2}$ ($\hat{A}_\nu = \hat{q}$, $\hat{A}_\nu^\dagger = -i\hat{p}$) is of the special interest in physical applications.

Appendix B

Quantum phase corrections

B.1 Calculation of Maslov indices

An important ingredient to the Trace Formula (2.3) is the Maslov index. It is an invariant property of a periodic orbit which can change only when the orbit undergoes a bifurcation or when a continuous symmetry is broken or restored under the variation of a system parameter (e.g., energy, deformation or an external field). The calculation of the Maslov index is not always straightforward, in particular for systems with many degrees of freedom or systems which are not of the "kinetic plus potential energy" type. In the standard methods used in the literature [69, 34, 36, 27], the determination of the Maslov index of a stable orbit necessitates the explicit use of an "intrinsic" coordinate system that follows the orbit (as introduced by Gutzwiller [45]), which can be numerically quite cumbersome. Easy-to-use calculational recipes using the method of [27] have been given in Appendix D of [18].

Recently, Sugita [88] has presented the formula (2.17) for the Maslov index which only contains canonically invariant ingredients. He has also discussed in [88] the relation of the winding number m to the homotopy theory. However, no practical recipes were given for the explicit calculation of the winding number m.

This subject has been partially explained in a recent review article on the Periodic Orbit Theory [74]. The winding number m has been identified as the Gel'fand-Lidski winding number [42], and it has been explained how to calculate it in principle. There has been also discussed a relation of σ_r given by (2.17) to an index which is known in the mathematical literature after the names of Conley and Zehnder [24], and extensive references on the latter subject have been provided. However, in [74] the way of extracting a unique value of the stability angle χ_i from the the eigenvalues $e^{\pm i\chi_i}$ of the stability matrix has only been hinted at, and a practical algorithm still remained to be specified. We also want to remark that a representation similar to (2.17) appears in a mathematical paper [70] where the admissible normal forms of the elements of Sp(2d) are classified.

Below the specification of the definitions of χ_i and m is given, which makes the presentation of σ_r in (2.17) complete and useful for practical applications [81].

All information about the Maslov index of an isolated orbit is contained in its matrizant $M(t)$ describing the time propagation of a small perturbation $\delta\mathbf{q}, \delta\mathbf{p}$ around the orbit in phase space:

$$\begin{pmatrix} \delta\mathbf{q}(t) \\ \delta\mathbf{p}(t) \end{pmatrix} = M(t) \begin{pmatrix} \delta\mathbf{q}(0) \\ \delta\mathbf{p}(0) \end{pmatrix}, \tag{B.1}$$

where $\mathbf{q}(t)$ and $\mathbf{p}(t)$ are d-dimensional coordinate and momentum variables. $M(t)$ is obtained by solving the linearized equations of motion of a classical system characterized by its Hamiltonian $H(\mathbf{q},\mathbf{p})$, which leads to the differential equations

$$\frac{d}{dt}M(t) = \mathcal{J}H''(t)M(t), \qquad M(0) = I_{2d}\,, \tag{B.2}$$

where

$$\mathcal{J} = \begin{pmatrix} 0 & I_d \\ -I_d & 0 \end{pmatrix}, \qquad H''(t) = \begin{pmatrix} \frac{\partial^2 H}{\partial\mathbf{q}\partial\mathbf{q}} & \frac{\partial^2 H}{\partial\mathbf{q}\partial\mathbf{p}} \\ \frac{\partial^2 H}{\partial\mathbf{p}\partial\mathbf{q}} & \frac{\partial^2 H}{\partial\mathbf{p}\partial\mathbf{p}} \end{pmatrix}. \tag{B.3}$$

$\mathcal{J}$ is the unit symplectic matrix in the $2d$-dimensional phase space, and I_{2d}, I_d are the $2d$- and d-dimensional unit matrices, respectively. At the time of the orbit's period T, the matrix $M(T)$ is called the monodromy matrix. One can always transform $M(T)$ into block form. One parabolic (2×2) block contains the trivial unit eigenvalues related to energy conservation; the remaining $(2d-2)$-dimensional part of $M(T)$ is called the reduced monodromy matrix M_{red} or stability matrix. M_{red} falls into (inverse) parabolic, elliptic, or (inverse) hyperbolic (2×2) blocks or, for $d>2$ dimensions, loxodromic (4×4) blocks, depending on the stability of the respective orbits.

Following [74], we split $M(t)$ into a product of a periodic and an average part (Floquet decomposition):

$$M(t) = M_{\text{per}}(t)M_{\text{av}}(t) \tag{B.4}$$

with

$$M_{\text{av}}(t) = \exp(tK), \tag{B.5}$$

where K is a constant matrix. By definition, the periodic part of the matrizant in (B.4) satisfies the condition $M_{\text{per}}(t) = M_{\text{per}}(t+T)$. In particular, $M_{\text{per}}(0) = M_{\text{per}}(T) = I_{2d}$. We then can specify the constant matrix K by equating

$$M_{\text{av}}(T) \equiv \exp(TK) = M(T)\,. \tag{B.6}$$

Then,

$$K = \frac{1}{T}\ln[M(T)]\,. \tag{B.7}$$

To take the logarithm on *r.h.s.* of (B.7), we diagonalize $M(T)$, calculate the logarithms of the eigenvalues of $M(T)$, and then return to the initial basis. However, the relation (B.7) remains symbolic until we adopt a certain phase convention for the eigenvalues of K.

In the standard definition of the function $\ln(z)$ with $z = |z|e^{i\phi}$ the phase range $\phi \in (-\pi,\pi]$ is chosen, corresponding to the branch-cut line being taken along the negative real axis. Let us consider the eigenvalue problem

$$M(T)\xi_i^{\pm} = e^{\pm i\tilde{\chi}_i}\xi_i^{\pm}, \tag{B.8}$$

where $\xi_i^- = [\xi_i^+]^*$ and

$$\widetilde{\chi}_i = -i \ln[e^{+i\widetilde{\chi}_i}] \in (0, \pi). \tag{B.9}$$

The case $\widetilde{\chi}_i = \pi$ will be discussed separately below.

Let us introduce the symplectic product

$$s_i = +[\mathrm{Re}(\xi_i^+)]^{\mathrm{T}} \mathcal{J} \,\mathrm{Im}(\xi_i^+) \equiv -[\mathrm{Re}(\xi_i^-)]^{\mathrm{T}} \mathcal{J} \,\mathrm{Im}(\xi_i^-)\,, \tag{B.10}$$

which is known as Krein invariant [59, 4]. With this, we can adopt the following convention for the eigenvalues $\pm i \frac{\chi_i}{T}$ of K

$$K\xi_i^\pm = \pm i \frac{\chi_i}{T} \xi_i^\pm, \tag{B.11}$$

so that

$$\chi_i = \widetilde{\chi}_i, \quad \text{if} \quad s_i > 0, \tag{B.12}$$
$$\chi_i = 2\pi - \widetilde{\chi}_i, \quad \text{if} \quad s_i < 0. \tag{B.13}$$

These relations fully determine the constant matrix K and specify uniquely the stability angle to be used in the formula (2.17). In our phase convention χ_i takes values in the range $(0, 2\pi)$.

The case of inverse parabolic block with $e^{\pm i\widetilde{\chi}_i} = -1$ is degenerate and requires special consideration. It corresponds to the stability changing between elliptic and inverse hyperbolic. In this case we choose the value $\chi_i = \pi$ by the continuity reasons.

The winding number m is an invariant characteristic of $M_{\mathrm{per}}(t) = M(t) M_{\mathrm{av}}^{-1}(t)$. To determine it, it is convenient to employ the so-called polar decomposition of the symplectic matrix M_{per} into a product of an orthogonal matrix R_{per} and a positive definite symmetric matrix W_{per}:

$$M_{\mathrm{per}} = R_{\mathrm{per}} W_{\mathrm{per}}\,. \tag{B.14}$$

In turn, the orthogonal matrix R_{per} admits the representation

$$R_{\mathrm{per}} = \begin{pmatrix} X_{\mathrm{per}} & Y_{\mathrm{per}} \\ -Y_{\mathrm{per}} & X_{\mathrm{per}} \end{pmatrix}. \tag{B.15}$$

Therefore, the winding number m can be defined as

$$m = \varphi(T) - \varphi(0), \tag{B.16}$$

where

$$\varphi(t) = \frac{1}{2\pi} \mathrm{Arg}\det\left[X_{\mathrm{per}}(t) + iY_{\mathrm{per}}(t)\right]. \tag{B.17}$$

Since $X_{\mathrm{per}}(t)$ and $Y_{\mathrm{per}}(t)$ are periodic, m is a (positive or negative) integer number.

The winding number (B.16) has been vastly discussed in the literature, both mathematical and physical (see [74] for extensive references). In particular, we would like to quote here that it has been introduced in [42] for a topological characterization of the structural stability of linear Hamiltonian flow.

The extraction of $R_{\text{per}}(t)$ from $M_{\text{per}}(t)$ provides a nice representation of the evolution of $\varphi(t)$, because $\det[X_{\text{per}}(t) + iY_{\text{per}}(t)]$ runs around the unit circle. However, the polar decomposition (B.14) is not essential for the calculation of the winding number m, even though the latter is encoded in $R_{\text{per}}(t)$. The same result as in (B.17) can be also obtained from $\psi(T) - \psi(0)$, where

$$\psi(t) = \frac{1}{2\pi} \text{Arg} \det \left[A_{\text{per}}(t) + iB_{\text{per}}(t)\right], \tag{B.18}$$

and the matrices $A_{\text{per}}(t)$ and $B_{\text{per}}(t)$ are the blocks of

$$M_{\text{per}}(t) = \begin{pmatrix} A_{\text{per}}(t) & B_{\text{per}}(t) \\ C_{\text{per}}(t) & D_{\text{per}}(t) \end{pmatrix}. \tag{B.19}$$

For a proof and further discussion of this point see Appendix A of [65].

Let us now consider the following canonical transformation

$$M(t) = S(t) M_{\text{av}}(t) S(0)^{-1}. \tag{B.20}$$

with $S(t) \equiv M_{\text{per}}(t)$. Since $S(0) = I_{2d}$, this expression is equivalent to (B.4). The relation between the Maslov indices σ of $M(t)$ and σ_{av} of $M_{\text{av}}(t)$ for $r = 1$ is given by [88]

$$\sigma = \sigma_{\text{av}} + 2m. \tag{B.21}$$

But the winding number in σ_{av} equals zero, since $M_{\text{av}}(t)$ belongs to the same homotopy class as the identity matrix, i.e., it can be continuously shrunk to the latter. Therefore, in order to determine σ_{av} we just need to find out the number of elliptic and inverse hyperbolic blocks of $M_{\text{av}}(T) = M(T)$. We emphasize that neither σ_{av} nor m depend on the choice of the starting point on the periodic orbit [88], as it should be for the canonically invariant quantities.

We can also introduce another prescription for calculating χ_i and m appearing in [88]. It is based on the alternative Floquet decomposition

$$M(t) = \widetilde{M}_{\text{per}}(t) \widetilde{M}_{\text{av}}(t) \equiv \widetilde{M}_{\text{per}}(t) \exp(t\widetilde{K}), \tag{B.22}$$

specified by a constant matrix $\widetilde{K}$ such that

$$\widetilde{K} \xi_i^{\pm} = \pm i \frac{\widetilde{\chi}_i}{T} \xi_i^{\pm}. \tag{B.23}$$

This actually represents another convention for the choice of the stability angle. The formula for the Maslov index (2.17) is then modified to

$$\sigma_r = \sum_{i=1}^{n_{\text{ell}}} \left(1 + 2\left[\text{sign}(s_i) \frac{r\widetilde{\chi}_i}{2\pi}\right]\right) + rn_{\text{ih}} + 2\widetilde{m}r. \tag{B.24}$$

If $s_i > 0$ for all i, we have $\widetilde{K} = K$ and $\widetilde{\chi}_i = \chi_i$, as well as $\widetilde{m} = m$. Therefore, there is no difference between (B.24) and (2.17). If $s_i < 0$ for some i, we can make the transformation

$$2\left[-\frac{r\tilde{\chi}_i}{2\pi}\right] = -2r + 2\left[\frac{r(2\pi - \tilde{\chi}_i)}{2\pi}\right] = -2r + 2\left[\frac{r\chi_i}{2\pi}\right]. \tag{B.25}$$

Correspondingly, the winding number m of $M_{\mathrm{per}}(t)$ changes to $\widetilde{m}$, which is the winding number of $\widetilde{M}_{\mathrm{per}}(t)$, such that

$$2\widetilde{m}r = 2mr + 2r. \tag{B.26}$$

Summing up (B.25) and (B.26), we see that the σ_r in both (B.24) and (2.17) coincide. Thus, the equivalence of both representations is established. We also note that, in general, the difference $(\widetilde{m} - m)$ equals to the winding number of $e^{t(K-\widetilde{K})}$, which is the number of elliptic blocks of K (or $\widetilde{K}$) with negative values of s_i.

The sign of s_i may change from positive to negative (or vice versa) away from bifurcation or symmetry breaking points. As a consequence, $\widetilde{m}$ changes its value by $+1$ or -1, but such as to conserve the total Maslov index. The prescription for $\widetilde{K}$ based on (B.23) is not relevant from the point of view of a canonically invariant formulation, but such a representation often appears to be more convenient in numerical computations.

The following remark is in place here. In the presence of *inverse hyperbolic* blocks in an orbit's monodromy matrix $M(T)$, the Floquet decomposition (B.4) is, strictly speaking, ill-defined because both parts $M_{\mathrm{per}}(t)$ and $M_{\mathrm{av}}(t)$ in (B.4) are in general not symplectic. For such an orbit it would be more rigorous to calculate the winding number of its second repetition whose monodromy matrix contains no inverse hyperbolic blocks, and then to reconstruct the winding number of the first repetition.

B.2 Phase corrections to the flat phase-space propagator

Below we discuss the prescription (2.19) for including phase correction to the classical action in the semiclassical expression for a propagator and its trace. Taking into account a definite correspondence between the choice of a phase-space symbol and an ordering of an operator, one can also intepret the emergence of the extra phase $\delta H/\hbar$ as an artefact of the operator ordering.

For a more detailed explanation, we would like to discuss the results of [58]. In particular, the relation between semiclassical results for a propagator obtained within different quantization schemes has been established there. We refer to Appendix A.2 for the specification of notations.

The semiclassical propagator in the λ-quantization scheme reads [58]

$$K_{sc}^{flat} = \left(i\frac{\partial^2 \mathcal{R}_{cl}^{(\lambda)}}{\partial\bar{\alpha}_f \partial\alpha_i} \right)^{1/2} \exp\left\{ i\frac{\mathcal{R}_{cl}^{(\lambda)}}{\hbar} + i\left(\frac{1}{2}-\lambda\right) \int_0^T B^{(\lambda)} dt \right\}, \tag{B.27}$$

where

$$\begin{aligned} \mathcal{R}^{(\lambda)}(\bar{\alpha}_f, \alpha_i, T) &= -\frac{i}{2}\left(\bar{\alpha}_f \alpha_{cl}(T) + \bar{\alpha}_{cl}(0)\alpha_i - |\alpha_f|^2 - |\alpha_i|^2\right) \\ &+ \int_0^T dt \left(-\frac{i}{2}(\dot{\bar{\alpha}}_{cl}\alpha_{cl} - \bar{\alpha}_{cl}\dot{\alpha}_{cl}) - H^{(\lambda)}(\bar{\alpha}_{cl}, \alpha_{cl}) \right) \end{aligned} \tag{B.28}$$

and

$$B^{(\lambda)} = \Delta H^{(\lambda)} = \Delta H^{(1/2)} + O(\hbar) = \Delta H^{(0)} + O(\hbar). \tag{B.29}$$

The terms of the order $O(\hbar)$ in $B^{(\lambda)}$ as well as the dependence of the prefactor on λ are inessential due to the very structure of the asymptotic expression (B.27). $O(\hbar)$-terms are also negligible in the classical equations of motion:

$$\dot{\alpha} = -i\frac{\partial H^{(\lambda)}}{\partial\bar{\alpha}} + O(\hbar), \quad \alpha(0) = \alpha_i, \tag{B.30}$$

$$\dot{\bar{\alpha}} = i\frac{\partial H^{(\lambda)}}{\partial\alpha} + O(\hbar), \quad \bar{\alpha}(T) = \bar{\alpha}_f. \tag{B.31}$$

For $\lambda = 1$ we have the semiclassical expression obtained within the contravariant quantization scheme.

Note that for $\lambda = \frac{1}{2}$ (Weyl quantization) the B-term drops out from (B.27). Since the semiclassical propagator should not depend on λ, i.e. on the choice of the quantization scheme, the extra-phase correction just compensates for the difference between λ and Wigner-Weyl symbols in the next-to-leading order in $\hbar$ [see (A.24) for $\lambda' = \frac{1}{2}$].

Suppose that the quantum Hamiltonian $\hat{H}$ belongs to a family of specifically ordered Hamiltonians [22], also parametrized by $\lambda \in [0, 1]$,

$$\hat{H}_\lambda(\hat{A}^\dagger, \hat{A}) = \frac{1}{(\pi\hbar)^2} \int d^2\alpha d^2\beta H(\bar{\alpha}, \alpha) e^{(1-2\lambda)\bar{\beta}\beta/2\hbar} e^{\{\beta(\bar{\alpha}-\hat{A}^\dagger) - \bar{\beta}(\alpha-\hat{A})\}/\hbar}, \tag{B.32}$$

where the particular cases of $\lambda = 0, \frac{1}{2}, 1$ correspond to the normal, Weyl and antinormal orderings, respectively. One can establish the one-to-one correspondence between the operators (B.32) and the symbols (A.14). It follows from the observation that the λ-symbol of the λ-ordered operator yields the principal symbol $H(\bar{\alpha}, \alpha)$, higher order $\hbar$-terms vanishing. Thus, the result (B.27) of [58] actually proves the proposition (2.19) for the Hamiltonians (B.32).

B.3 Solari-Kochetov phase correction

We can obtain [80] the Solari-Kochetov phase correction to the semiclassical spin coherent-state propagator (4.1) in a way similar to that prescribed for the flat phase-space propagator in (2.19). For this purpose we employ the special Holstein-Primakoff representation [48] for the spin operators

$$\begin{aligned}
\hat{s}_+ &= \hat{s}_1 + i\hat{s}_2 = \hat{a}^\dagger\sqrt{2s - \hat{a}^\dagger\hat{a}}, \\
\hat{s}_- &= \hat{s}_1 - i\hat{s}_2 = \sqrt{2s - \hat{a}^\dagger\hat{a}}\,\hat{a}, \\
\hat{s}_3 &= \hat{a}^\dagger\hat{a} - s,
\end{aligned} \tag{B.33}$$

in terms of the standard annihilation and creation operators $\hat{a}$ and $\hat{a}^\dagger$ with the commutation relation $[\hat{a}, \hat{a}^\dagger] = 1$. It is easy to check that the operators (B.33) satisfy the su(2) algebra (3.2) as well as

$$\frac{1}{2}\left(\hat{s}_+\hat{s}_- + \hat{s}_-\hat{s}_+\right) + \hat{s}_3^2 = s(s+1). \tag{B.34}$$

Let us introduce the semiclassical parameter $h = 1/(2s)$ and define $\hat{A} = \hat{a}\sqrt{h}$ and $\hat{A}^\dagger = \hat{a}^\dagger\sqrt{h}$, such that

$$[\hat{A}, \hat{A}^\dagger] = h. \tag{B.35}$$

We also define the operators

$$\begin{aligned}
\hat{S}_+ &= \hat{A}^\dagger\sqrt{1 - \hat{A}^\dagger\hat{A}}, \\
\hat{S}_- &= \sqrt{1 - \hat{A}^\dagger\hat{A}}\,\hat{A}, \\
\hat{S}_3 &= h\hat{s}_3 = \hat{A}^\dagger\hat{A} - \frac{1}{2},
\end{aligned} \tag{B.36}$$

which satisfy the commutation relations

$$[\hat{S}_+, \hat{S}_-] = 2h\hat{S}_3, \quad [\hat{S}_3, \hat{S}_\pm] = \pm h\hat{S}_\pm. \tag{B.37}$$

The square root in (B.36) should be understood as an expasion in a Taylor series

$$\sqrt{1-x} = 1 + \sum_{l=1}^{\infty} c_l x^l \tag{B.38}$$

with x replaced by $\hat{A}^\dagger\hat{A}$.

One can immediately notice that the operators (B.36), when expressed through $\hat{A}$ and $\hat{A}^\dagger$, do not depend explicitly on h, and that (B.35) is similar to (2.21). This enables us to apply formally the Moyal formula (A.10) with the Poisson bracket (A.12) to the operators (B.36), replacing everywhere $\hbar$ by h. Considering α and $\bar{\alpha}$ to be the "Weyl symbols" of $\hat{A}$ and $\hat{A}^\dagger$, respectively, we can thus define the "Weyl symbols" of the operators (B.36).

First, we find

$$
\begin{aligned}
(\hat{A}^\dagger \hat{A})_W &= \bar{\alpha}\alpha - \frac{h}{2} + O(h^2), && \text{(B.39)}\\
(\hat{A}\hat{A}^\dagger)_W &= \bar{\alpha}\alpha + \frac{h}{2} + O(h^2), && \text{(B.40)}\\
((\hat{A}^\dagger \hat{A})^l)_W &= (\bar{\alpha}\alpha)^l - \frac{hl}{2}(\bar{\alpha}\alpha)^{l-1} + O(h^2). && \text{(B.41)}
\end{aligned}
$$

Exploiting the latter relation and the trivial equality

$$
\frac{d}{dx}\sqrt{1-x} = -\frac{1}{2\sqrt{1-x}} = \sum_{l=1}^{\infty} l c_l x^{l-1} \tag{B.42}
$$

we establish

$$
(\sqrt{1-\hat{A}^\dagger \hat{A}})_W = \sqrt{1-\bar{\alpha}\alpha} + \frac{h}{4}\frac{1}{\sqrt{1-\bar{\alpha}\alpha}} + O(h^2). \tag{B.43}
$$

Further use of the Moyal formula (A.10) leads to the desired definitions

$$
\begin{aligned}
(\hat{S}_+)_W &= (\hat{A}^\dagger\sqrt{1-\hat{A}^\dagger \hat{A}})_W = \bar{\alpha}\sqrt{1-\bar{\alpha}\alpha} + \frac{h}{2}\frac{\bar{\alpha}}{\sqrt{1-\bar{\alpha}\alpha}} + O(h^2),\\
(\hat{S}_-)_W &= (\sqrt{1-\hat{A}^\dagger \hat{A}}\hat{A})_W = \alpha\sqrt{1-\bar{\alpha}\alpha} + \frac{h}{2}\frac{\alpha}{\sqrt{1-\bar{\alpha}\alpha}} + O(h^2), && \text{(B.44)}\\
(\hat{S}_3)_W &= (\hat{A}^\dagger \hat{A} - \frac{1}{2})_W = \bar{\alpha}\alpha - \frac{1}{2} - \frac{h}{2} + O(h^2).
\end{aligned}
$$

There exists, however, a subtlety that should be spelled out here. The spin operators (B.36) act in the finite Hilbert space in contrast to the operators $\hat{q}, \hat{p}$ and $\hat{H}(\hat{q}, \hat{p})$ which act in a different – infinite – Hilbert space. Nevertheless, the “Weyl symbols” (B.44) of the operators (B.36) do make sense locally in the semiclassical limit $h \to 0$, and, as we shall see, reproduce the Solari-Kochetov phase.

For the Hamiltonian (3.13), rewritten as

$$
\hat{H} = \frac{1}{h}\mathbf{C}\cdot\hat{\mathbf{S}} = \frac{1}{h}\left[\frac{1}{2}C_+\hat{S}_- + \frac{1}{2}C_-\hat{S}_+ + C_3\hat{S}_3\right], \tag{B.45}
$$

we are going to relate the phase in question to the difference between the principal and “Weyl” symbols of (B.45)

$$
H(\bar{\alpha}, \alpha) - H_W(\bar{\alpha}, \alpha) = \delta H(\bar{\alpha}, \alpha) + O(h), \tag{B.46}
$$

similarly to the respective prescription (2.19) in the flat case. (There is a small distinction in notations in comparison with the flat case since the classical action and the naive classical Hamiltonian for spin are already divided by the semiclassical parameter h and therefore $H(\bar{\alpha}, \alpha)$ and $\delta H(\bar{\alpha}, \alpha)$ are of order $O(h^{-1})$ and $O(1)$, respectively.)

According to (B.44) the principal symbol and the next-order correction of (B.45) are given, respectively, by

$$
\begin{aligned}
H(\bar{\alpha}, \alpha) &= \frac{1}{h}\left[A(2\bar{\alpha}\alpha - 1) + (\bar{f}\alpha + f\bar{\alpha})\sqrt{1-\bar{\alpha}\alpha}\right], && \text{(B.47)}\\
\delta H(\bar{\alpha}, \alpha) &= A - \frac{\bar{f}\alpha + f\bar{\alpha}}{2\sqrt{1-\bar{\alpha}\alpha}}. && \text{(B.48)}
\end{aligned}
$$

To compare these expressions with (3.14) and (4.7), respectively, we use the Darboux transformation

$$z = \frac{\alpha}{\sqrt{1-\bar{\alpha}\alpha}}, \quad \bar{z} = \frac{\bar{\alpha}}{\sqrt{1-\bar{\alpha}\alpha}}. \tag{B.49}$$

It makes the Kähler symplectic structure locally flat and converts the classical equations of motion (4.3) into

$$\dot{\alpha} = -ih\frac{\partial H(\bar{\alpha},\alpha)}{\partial\bar{\alpha}} + O(h), \quad \dot{\bar{\alpha}} = ih\frac{\partial H(\bar{\alpha},\alpha)}{\partial\alpha} + O(h). \tag{B.50}$$

The terms $O(h)$ appear due to the finiteness of the $(\alpha,\bar{\alpha})$ phase space which is a disc on the complex plane. However, they become negligible as $h\to 0$. All the other terms in (B.50) have the order $O(1)$.

Thus, after the transformation (B.49) we observe the coincidence of the principal symbols (3.14) and (B.47) and obtain the relation

$$\frac{1}{2}B = \delta H, \tag{B.51}$$

where the B-term (4.6) for the Hamiltonian linear in spin equals

$$B = 2A - (\bar{f}z + f\bar{z}). \tag{B.52}$$

In conclusion we construct the approximate realization of the su(2) algebra with respect to the Poisson bracket (A.12). Taking into account (A.11) and the commutation relations (B.37) we deduce that

$$i\{(\hat{S}_+)_W,(\hat{S}_-)_W\}_{\bar{\alpha},\alpha} = 2(\hat{S}_3)_W + O(h^2), \tag{B.53}$$

$$i\{(\hat{S}_3)_W,(\hat{S}_\pm)_W\}_{\bar{\alpha},\alpha} = \pm(\hat{S}_\pm)_W + O(h^2). \tag{B.54}$$

These formulae can be checked by straitforward calculation using (B.44).

Appendix C

Elements of the SU(2) representation theory

$(2s+1)$-dimensional matrices of the SU(2) irreducible representation labelled by the (half-)integer weight s can be expressed in terms of the Euler angles (α, β, γ) [91]

$$\mathcal{D}^s(\alpha, \beta, \gamma) = e^{-iJ_3^s \alpha} e^{-iJ_2^s \beta} e^{-iJ_3^s \gamma}, \tag{C.1}$$

where J_a^s $(a = 1, 2, 3)$ are the SU(2) matrix generators. Matrix elements of (C.1)

$$\mathcal{D}^s_{m'm''}(\alpha, \beta, \gamma) = \langle s, m' | \mathcal{D}^s(\alpha, \beta, \gamma) | s, m'' \rangle = e^{-im'\alpha} e^{-im''\gamma} d^s_{m'm''}(\beta) \tag{C.2}$$

are called the Wigner $\mathcal{D}$-functions. They are expressed through the reduced Wigner functions

$$\begin{aligned} d^s_{m'm''}(\beta) &= \sqrt{(s+m')!(s-m')!(s+m'')!(s-m'')!} \\ &\times \sum_k (-1)^k \frac{\left[\cos\frac{\beta}{2}\right]^{2s-2k+m'-m''} \left[\sin\frac{\beta}{2}\right]^{2k-m'+m''}}{k!(s+m'-k)!(s-m''-k)!(m''-m'+k)!}. \end{aligned} \tag{C.3}$$

Hereby k runs over all integer values for which the factorial arguments are non-negative.

For the particular value of the second lower index $m'' = s$, the expressions (C.2) and (C.3) yield

$$\mathcal{D}^s_{m's}(\alpha, \beta, \gamma) = \sum_{m'=-s}^{s} \sqrt{\frac{(2s)!}{(s-m')!(s+m')!}} \left[\cos\frac{\beta}{2}\right]^{s+m'} \left[\sin\frac{\beta}{2}\right]^{s-m'} e^{-im'\alpha - is\gamma}. \tag{C.4}$$

This can be equivalently rewritten in the form

$$\mathcal{D}^s_{m's}(\alpha, \beta, \gamma) = \mathcal{D}^s_{m',-s}(\alpha - \pi, \pi - \beta, \pi - \gamma), \tag{C.5}$$

which follows from the symmetry property

$$\mathcal{D}^s_{m'm''}(\alpha - \pi, \pi - \beta, \pi - \gamma) = (-1)^{s+m''} \mathcal{D}^s_{m',-m''}(\alpha, \beta, \gamma). \tag{C.6}$$

Below we consider the particular representations for values $s = \frac{1}{2}$ and $s = 1$.

For $s = \frac{1}{2}$ (fundamental representation) we have $J_a^s = \frac{1}{2}\sigma_a$, where σ_a are the Pauli matrices, and

$$\mathcal{D}^{1/2}(\alpha,\beta,\gamma) = \begin{pmatrix} \cos\frac{\beta}{2}e^{-\frac{i}{2}(\gamma+\alpha)} & -\sin\frac{\beta}{2}e^{\frac{i}{2}(\gamma-\alpha)} \\ \sin\frac{\beta}{2}e^{-\frac{i}{2}(\gamma-\alpha)} & \cos\frac{\beta}{2}e^{\frac{i}{2}(\gamma+\alpha)} \end{pmatrix}. \tag{C.7}$$

For $s = 1$

$$J_1^1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad J_2^1 = \frac{i}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad J_3^1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tag{C.8}$$

and

$$\mathcal{D}^1(\alpha,\beta,\gamma) = \begin{pmatrix} \frac{1}{2}(1+\cos\beta)e^{-i(\gamma+\alpha)} & -\frac{1}{\sqrt{2}}\sin\beta e^{-i\alpha} & \frac{1}{2}(1-\cos\beta)e^{i(\gamma-\alpha)} \\ \frac{1}{\sqrt{2}}\sin\beta e^{-i\gamma} & \cos\beta & -\frac{1}{\sqrt{2}}\sin\beta e^{i\gamma} \\ \frac{1}{2}(1-\cos\beta)e^{-i(\gamma-\alpha)} & \frac{1}{\sqrt{2}}\sin\beta e^{i\alpha} & \frac{1}{2}(1+\cos\beta)e^{i(\gamma+\alpha)} \end{pmatrix}. \tag{C.9}$$

This representation is called adjoint, since its dimensionality coincides with the number of the SU(2) generators, and with the number of variables (α,β,γ) parametrizing the group SU(2). One can perform the equivalence transformation

$$O = U_0\mathcal{D}^1U_0^\dagger \tag{C.10}$$

with

$$U_0 = \begin{pmatrix} -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & 1 & 0 \end{pmatrix}, \tag{C.11}$$

in order to obtain the orthogonal matrix O of rotations in three-dimensional Euclidean space. In explicit form it is given by

$$O = \begin{pmatrix} \cos\beta\cos\alpha\cos\gamma - \sin\alpha\sin\gamma & -\cos\beta\cos\alpha\sin\gamma - \sin\alpha\cos\gamma & \sin\beta\cos\alpha \\ \cos\beta\sin\alpha\cos\gamma + \cos\alpha\sin\gamma & -\cos\beta\sin\alpha\sin\gamma + \cos\alpha\cos\gamma & \sin\beta\sin\alpha \\ -\sin\beta\cos\gamma & \sin\beta\sin\gamma & \cos\beta \end{pmatrix}. \tag{C.12}$$

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