

Supplemental material for Partial Fermionization: Spectral Universality in 1D Repulsive Bose Gases

Quirin Hummel, Juan Diego Urbina, and Klaus Richter
Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

Appendix A: Noninteracting case

The QCE for *noninteracting* bosonic or fermionic systems has been addressed in Ref. [1]. The results needed for the presented work are here briefly recapped for convenience and in order to adapt the notation. The general form

$$Z_{0,\pm}^{(N)}(\beta) = \frac{1}{N!} \sum_{\mathfrak{N} \vdash N} (\pm 1)^{N-|\mathfrak{N}|} c_{\mathfrak{N}}^{(N)} \mathcal{A}_{\mathfrak{N}}(-i\hbar\beta) \quad (\text{A1})$$

of the multi-particle partition function for noninteracting bosons (+) or fermions (-) is based on the cycle decomposition of permutations P involved in the symmetrization of the Hilbert space due to indistinguishability. A specific clustering, i.e., decomposition of P into cycles of particular lengths n_i , is characterized by the multiset $\mathfrak{N} = \{n_1, n_2, \dots, n_{|\mathfrak{N}|}\}$, summing up to a total of $\sum_{n \in \mathfrak{N}} n = \sum_{i=1}^{|\mathfrak{N}|} n_i = N$. The sum in Eq. (A1) thus runs over all partitions of N , denoted by $\mathfrak{N} \vdash N$, while $|\mathfrak{N}|$ denotes the number of parts and the combinatorial factor

$$c_{\mathfrak{N}}^{(N)} := \frac{N!}{\prod_{n \in \mathfrak{N}} n \prod_{n'} m_{\mathfrak{N}}(n')!} \quad (\text{A2})$$

is the number of distinct permutations of N with a cycle-decomposition corresponding to \mathfrak{N} , where $m_{\mathfrak{N}}(n)$ is the multiplicity of n in \mathfrak{N} .

The amplitude of each clustering \mathfrak{N} in Eq. (A1) is the product

$$\mathcal{A}_{\mathfrak{N}}(-i\hbar\beta) = \prod_{n \in \mathfrak{N}} \mathcal{A}_n(-i\hbar\beta) \quad (\text{A3})$$

of the amplitudes \mathcal{A}_n of the individual clusters, specified by their cluster sizes n , i.e., the number of particles involved in the cycles.

Using the semigroup property of the single-particle propagator $K_0^{(1)}$ and identifying $\mathbf{q}_{n+1} \equiv \mathbf{q}_1 = \mathbf{q}$ yields the n -body cluster amplitude

$$\mathcal{A}_n(t) = \int d^D q K_0^{(1)}(\mathbf{q}, \mathbf{q}; nt) = \mathcal{A}_1(nt). \quad (\text{A4})$$

Equivalently, the noninteracting N particle partition function (A1) can be written as

$$Z_{0,\pm}^{(N)}(\beta) = \frac{1}{N!} \sum_{\mathfrak{N} \vdash N} (\pm 1)^{N-|\mathfrak{N}|} c_{\mathfrak{N}}^{(N)} \prod_{n \in \mathfrak{N}} Z^{(1)}(n\beta) \quad (\text{A5})$$

in terms of the single-particle partition function $Z^{(1)}(\beta)$. For smooth and homogeneously scaling external potentials $U(\mathbf{q})$ the latter is evaluated in short-time approximation by replacing

$$K_0^{(1)}(\mathbf{q}, \mathbf{q}; t) \simeq \exp\left[-\frac{i}{\hbar} U(\mathbf{q})t\right] K_{\text{free}}^{(1)}(\mathbf{q}, \mathbf{q}; t), \quad (\text{A6})$$

where K_{free} stands for unconfined propagation; resulting in

$$Z^{(1)}(\beta) = \mathcal{A}_1(-i\hbar\beta) = \frac{V_{\text{eff}}}{\lambda_{\text{T}}^d} \propto \beta^{-d/2} \quad (\text{A7})$$

and consequently

$$Z^{(1)}(n\beta) = \mathcal{A}_n(-i\hbar\beta) = \frac{V_{\text{eff}}}{\lambda_{\text{T}}^d} n^{-d/2}. \quad (\text{A8})$$

The scaling with the effective dimension

$$d = D + \frac{2}{\mu} D \quad (\text{A9})$$

with μ the degree of homogeneity in the external potential $U(\mathbf{q}) = w^\mu U(\mathbf{q}/w)$ allows to absorb the dependence on cluster sizes $n \in \mathfrak{N}$ into combinatorial coefficients separated from the dependence on the relevant physical quantities, which are the temperature encoded in the thermal de Broglie wavelength

$$\lambda_{\text{T}} = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{-\frac{1}{2}} \quad (\text{A10})$$

and the (effective) volume

$$V_{\text{eff}} = \left(\frac{2\pi\hbar^2}{me_0}\right)^{D/\mu} \int d^D q \exp[-U(\mathbf{q})/e_0] \quad (\text{A11})$$

with an arbitrary unit of energy e_0 , which, for $\hbar^2/(2m) = 1$, coincides with the definition given in the main text.

The final explicit expression [see Eq. (1) of the main text]

$$Z_{0,\pm}^{(N)}(\beta) = \sum_{l=1}^N z_{\pm,l}^{(N,d)} \left(\frac{V_{\text{eff}}}{\lambda_{\text{T}}^d}\right)^l \quad (\text{A12})$$

involves the coefficients

$$z_{\pm,l}^{(N,d)} = (\pm 1)^{N-l} C_l^{(N,d)} / l!, \quad (\text{A13})$$

where the index l corresponds to the number of clusters $|\mathfrak{N}|$ in Eq. (A1)] the total number of particles N is

divided into, or equivalently the number of cycles in a permutation. The universal coefficients $C_l^{(N,d)}$ are given by

$$\begin{aligned} C_l^{(N,d)} &= \sum_{\substack{\mathfrak{M} \vdash N \\ |\mathfrak{M}|=l}} \frac{l!}{\prod_n m_{\mathfrak{M}}(n)!} \left(\prod_{n \in \mathfrak{M}} \frac{1}{n} \right)^{d/2+1} \\ &= \sum_{\substack{n_1, \dots, n_l=1 \\ \sum n_k=N}}^N \left(\prod_{k=1}^l \frac{1}{n_k} \right)^{d/2+1} \end{aligned} \quad (\text{A14})$$

and result from the scaling (A7) of single-particle partition functions with the effective dimension d together with summing up all contributions with the same number l of clusters, irrespective of their individual sizes, absorbing the combinatorial factors $c_{\mathfrak{M}}^{(N)}$, Eq. (A2). A full combinatorial derivation of Eq. (A14) as well as a recursive method for fast evaluation at larger values of N was given in [1].

Appendix B: QCE in thermal equilibrium

1. Arbitrary order

In full generality, i.e., arbitrary order, dimensionality D , and interaction with short-range character, the QCE partition function [see Eq. (4) of the main text] is entirely determined by interaction kernels $a_n^{\mathfrak{C}}(\beta\alpha)$, each associated with an irreducible cluster of size n , uniquely labeled by a symbol \mathfrak{C} and represented by an irreducible diagram [see, e.g., Figs. 2(b), 2(e), and 2(f) of the main text]. The kernels are defined via their unique relation to the amplitudes

$$\mathcal{A}_n^{\mathfrak{C}}(-i\hbar\beta) = \frac{V_{\text{eff}}}{\lambda_T^d} n^{-d/2} a_n^{\mathfrak{C}}(\beta\alpha) \quad (\text{B1})$$

that denote the value of the corresponding diagrams, where α denotes the energy associated with the coupling strength. The generic scaling property (B1) can be shown by consistent use of short-time dynamical information [2]. It expresses the fact that interactions only affect the local internal dynamics of a cluster, independent of the external potential $U(\mathbf{q})$, while confinement effects are separated, affecting the cluster as a whole. The information about $U(\mathbf{q})$ is carried by the effective volume (A11) and the effective dimension (A9). In the general expression for the QCE partition function [Eq. (4) of the main text] the generic scaling (B1) allows to subsume the effect of the interaction-kernels in the interaction-related terms $\Delta z_{\pm,l}^{(N,d)}(\beta\alpha)$. They add functional dependence on $\beta\alpha$ to the coefficients of the corresponding noninteracting partition function [Eq. (1) of the main text], while the polynomial structure in $V_{\text{eff}}\beta^{-d/2}$ is unchanged. Due to the significance of this scaling we introduce the thermal interaction strength

$$s = \beta\alpha. \quad (\text{B2})$$

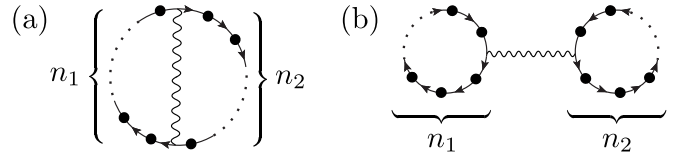


FIG. B1. The two classes of interacting cluster diagrams in first-order QCE: (a) The intra-cycle cluster where the interaction effect happens between two particles within the same cycle. (b) The inter-cycle structure where the interaction effect between two particles links two distinct cycles together to a single large cluster.

2. First order

In first-order QCE, the cluster structure \mathfrak{C} is fully determined by specifying intra- or inter-cycle configuration, the cluster size n , and its partition into n_1 and $n - n_1$, referring to the location of the interacting pair within the cyclic structure of the permutation (see Fig. B1). After symmetrization of the inter- and intra-cycle configuration Eq. (B1) reduces to Eq. (3) of the main text, involving only first-order kernels $a_{n_1, n-n_1}^{\pm}(s)$. A combinatorial refinement of Eq. (2) of the main text yields the relation

$$\Delta z_{\pm,l}^{(N,d)}(s) = \sum_{n=2}^{N-l+1} \frac{(\pm 1)^n}{n^{d/2}} z_{\pm,l-1}^{(N-n,d)} \sum_{n_1=1}^{n-1} a_{n_1, n-n_1}^{\pm}(s). \quad (\text{B3})$$

3. Delta-type contact interaction

We turn now to the case of contact interaction in 1D [see Eq. (6) of the main text]. For two distinguishable particles of equal mass m that live on an infinite line and are interacting via a repulsive Dirac delta pseudo-potential a separation into relative and center-of-mass coordinates allows to relate the interacting two-body propagator

$$K_0^{(2)}(\mathbf{q}^f, \mathbf{q}^i; t) + \Delta K_{\alpha}^{(2)}(\mathbf{q}^f, \mathbf{q}^i; t) \quad (\text{B4})$$

to the known 1D propagator for a single particle on a line with a Dirac delta barrier (see, e.g., [3]). In imaginary time $t = -i\hbar\beta$ and coordinates

$$\begin{aligned} X^{i,f} &:= \frac{1}{2} (x_1^{i,f} + x_2^{i,f}), \\ \Delta x^{i,f} &:= x_1^{i,f} - x_2^{i,f}, \\ x_j &:= \lambda_T^{-1} q_j \end{aligned} \quad (\text{B5})$$

that are scaled with the thermal de Broglie wavelength λ_T , the interacting part of the two-body propagator reads

$$\begin{aligned} \Delta K_{\alpha}^{(2)}(\mathbf{q}^f, \mathbf{q}^i; -i\hbar\beta) &= -\sqrt{s} \lambda_T^{-2} e^{-2\pi(X^f - X^i)^2} \\ &\times \int_0^{\infty} du \exp \left[-\sqrt{\pi s} u - \frac{\pi}{2} (|\Delta x^f| + |\Delta x^i| + u)^2 \right]. \end{aligned} \quad (\text{B6})$$

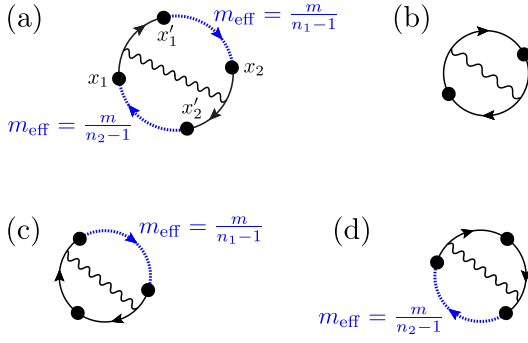


FIG. B2. The four cases of reduced effective intra-cluster diagrams (see Fig. B1a) after convolution of consecutive single-particle propagators. (a) $n_{1,2} \geq 2$ reduces to an effective cluster of four constituents with scaled coordinates x_i, x'_i . (b) $n_{1,2} = 1$ is not reduced and remains a two-body cluster. (c) $n_1 \geq 2, n_2 = 1$ reduces to an effective three-body cluster as well as the case (d) $n_1 = 1, n_2 \geq 2$. Single particle propagators of effective masses are marked with broken blue thick lines. All four cases are subsumed by the integral in Eq. (B7).

Using this expression, the value of intra-cluster diagrams $A_{n_1, n_2}^{\text{intra}}$ [see Fig. B1(a), and Fig. 2(e) of the main text] is found to be

$$A_{n_1, n_2}^{\text{intra}} = -\frac{L}{\lambda_T n^{1/2}} \frac{\sqrt{2s}}{4\pi} \int_0^\infty dr \int_{-\infty}^\infty dz \int_0^\infty du \times \exp \left[-\frac{1}{8} z^2 - \sqrt{\frac{s}{2}} u - \frac{1}{8} (\nu z + r + |r| + u)^2 \right], \quad (\text{B7})$$

where $L = V_{\text{eff}}$ is the available length of the 1D system and $n = n_1 + n_2$ and $\nu = \sqrt{(2n_1 n_2)/n - 1}$.

Expression (B7) is found after using the semigroup convolution property on all consecutive single-particle propagators reducing the cluster diagram to a maximum number of four constituents (see Fig. B2), some of which have altered (effective) masses (or equivalently modified propagation times). The remaining integration variables refer to the relative coordinate of the two interacting particles scaled with λ_T , with the initial distance $r = x_2 - x_1$ and the average distance $z = ((x_2 - x_1) + (x'_2 - x'_1))/\nu$ during the process.

Analogue considerations can be made on the inter-cycle cluster diagrams [see Fig. B1(b) and Fig. 2(f) of the main text] and lead to the exact identity

$$\mathcal{A}_{n_1, n_2}^{\text{intra}} = \mathcal{A}_{n_1, n_2}^{\text{inter}} \equiv \mathcal{A}_{n_1, n_2}, \quad (\text{B8})$$

which is a special feature of the delta-type interaction and implies the redundancy of delta-interactions characteristic for *spinless fermions*. This special implication of the Pauli exclusion principle is thereby confirmed within QCE to first order, instead of being imposed explicitly. In the cluster expansion this happens by rendering the sum in Eq. (2) of the main text of all (first-order) interacting irreducible diagrams of a specific size n equal to null, since $\mathcal{A}_{n_1, n-n_1}^- = (\mathcal{A}_{n_1, n-n_1}^{\text{intra}} - \mathcal{A}_{n_1, n-n_1}^{\text{inter}})/2 = 0$. While,

as a physical fact, this circumstance is expected we find it here as a nontrivial cancellation effect confirming the whole approach.

The bosonic cluster contribution $\mathcal{A}^+ = \mathcal{A} = \mathcal{A}^{\text{intra}}$, Eq. (B7), fulfills the generic scaling (B1) [see also Eq. (3) of the main text], in this case reading

$$\mathcal{A}_{n_1, n_2}^+(\alpha, \beta) = \frac{L}{\lambda_T} n^{-1/2} a_{n_1, n_2}^+(\beta\alpha), \quad (\text{B9})$$

where further evaluation of Eq. (B7) results in the interaction kernel

$$a_{n_1, n_2}^+(s) = -\frac{2}{\pi} \tan^{-1} \frac{1}{\nu} + \frac{2}{\sqrt{\pi}} \left[\frac{\nu^2}{\sqrt{1+\nu^2}} \sqrt{s} - \nu \sqrt{s} e^s \operatorname{erfc}(\sqrt{s}) + (1-2\nu^2 s) F_\nu(s) \right] \quad (\text{B10})$$

with

$$F_\nu(s) = \int_0^\infty dz \exp \left[-z \left(z + 2\sqrt{(1+\nu^2)s} \right) \right] \operatorname{erfc}(\nu z). \quad (\text{B11})$$

Setting $\nu = 0$ one recovers the case involving only two particles $\mathcal{A}_{1,1} = \frac{L}{\lambda_T \sqrt{2}} (-1 + e^s \operatorname{erfc}(\sqrt{s}))$ on a line [4], also related to a corresponding expression in fully balanced spin-one-half Fermi gases which has been derived in the context of second-order virial expansion [5].

Appendix C: QCE in spectral representation

The general relation between the level counting function and the canonical partition function via inverse Laplace transform,

$$\mathcal{N}_\alpha(E) = \mathcal{L}_\beta^{-1} \left[\frac{1}{\beta} Z_{\alpha, \pm}^{(N)}(\beta) \right] (E), \quad (\text{C1})$$

applied to Eq. (4) of the main text gives the general QCE expression [Eq. (5) of the main text] for $\mathcal{N}_\alpha(E)$ with spectral ‘‘coefficient functions’’

$$g_{\pm, l}^{(N, d)}(\epsilon) = \epsilon^{-\frac{ld}{2}} \mathcal{L}_s^{-1} \left[\Delta z_{\pm, l}^{(N, d)}(s) s^{-\frac{ld}{2}-1} \right] (\epsilon), \quad (\text{C2})$$

defined in terms of the interaction kernels $a_n^{\mathcal{C}}(s)$ and the effective dimension d , where we used the identity $\mathcal{L}_\beta^{-1}[f(\beta)](E) = 1/a \mathcal{L}_a^{-1}[f(\beta)](E/a)$.

We focus on the explicit computation of the spectral coefficients $g_{+, l}^{(N, d)}(\epsilon)$ in first-order QCE for contact interactions (see previous section) by applying Eq. (C2) to Eq. (B3) using the explicit kernels (B10). For more clarity in calculus we split the internal factors of first-order cluster diagrams, according to

$$a_{n_1, n-n_1}^+(s) = a_1(s, \nu) + a_2(s, \nu) + a_3(s, \nu) + a_4(s, \nu), \quad (\text{C3})$$

into their four addends

$$\begin{aligned}
a_1(s, \nu) &= \frac{2}{\pi} \tan^{-1} \nu - 1 + \frac{2\nu^2}{\sqrt{\pi(1+\nu^2)}} \sqrt{s}, \\
a_2(s, \nu) &= -\frac{2}{\sqrt{\pi}} \nu \sqrt{s} e^s \operatorname{erfc}(\sqrt{s}), \\
a_3(s, \nu) &= \frac{2}{\sqrt{\pi}} F_\nu(s), \\
a_4(s, \nu) &= -\frac{4}{\sqrt{\pi}} \nu^2 s F_\nu(s) = -2\nu^2 s a_3(s, \nu),
\end{aligned} \tag{C4}$$

where we have absorbed the dependence on n_1 and the cluster size n into ν . Combining the explicit expressions (C4) for the contact-interacting 1D Bose gas with the general first-order QCE formula (B3) for the coefficients $\Delta z_{+,l}^{(N,d)}(s)$ of the partition function and subsequently plugging it into Eq. (C2) gives

$$g_{+,l}^{(N,d)}(\epsilon) = \sum_{n=2}^{N-l+1} n^{-\frac{d}{2}} z_{+,l-1}^{(N-n,d)} \sum_{n_1=1}^{n-1} \sum_{j=1}^4 b_j^{(ld)}(\epsilon, \nu) \tag{C5}$$

with

$$b_j^{(ld)}(\epsilon, \nu) = \epsilon^{-\frac{ld}{2}} \mathcal{L}_s^{-1} \left[s^{-\frac{ld}{2}-1} a_j(s, \nu) \right] (\epsilon). \tag{C6}$$

In the following explicit expressions for the four b_j are calculated for the case of integer upper index $ld \in \mathbb{N}$. This covers all possible contributions one can get for integer effective dimension $d \in \mathbb{N}$, Eq. (A9), including the important 1D cases of

- i) vanishing external potential $U = 0$ (Lieb-Liniger), where $\mu = \infty$, $d = D = 1$,
- ii) the harmonically trapped Bose gas $U(q) \propto q^2$, where $\mu = 2$, $d = 2D = 2$, and
- iii) linear potentials like a linear well $U(q) \propto |q|$, where $\mu = 1$, $d = 3D = 3$.

To ease notation for the computations, the effective dimension is assumed to be $d = 1$ without loss of generality, since all $d \in \mathbb{N}$ are also covered by renaming $l \mapsto ld \in \mathbb{N}$.

1. Calculation of $b_1^{(l)}(\epsilon, \nu)$

Applying standard rules of inverse Laplace transformation to powers of s gives

$$\begin{aligned}
b_1^{(l)}(\epsilon, \nu) &= \left(\frac{2}{\pi} \tan^{-1} \nu - 1 \right) \frac{\theta(\epsilon)}{\Gamma\left(\frac{l}{2} + 1\right)} \\
&\quad + \frac{2\nu^2}{\sqrt{\pi(1+\nu^2)}} \frac{\theta(\epsilon)}{\Gamma\left(\frac{l}{2} + \frac{1}{2}\right) \sqrt{\epsilon}}.
\end{aligned} \tag{C7}$$

2. Calculation of $b_2^{(l)}(\epsilon, \nu)$

Following the recursive approach in [4] gives

$$\begin{aligned}
b_2^{(l)}(\epsilon, \nu) &= -\frac{2\nu}{\sqrt{\pi}} \frac{\left(1 + \frac{1}{\epsilon}\right)^{\frac{l}{2}-\frac{1}{2}}}{\Gamma\left(\frac{l}{2} + \frac{1}{2}\right) \sqrt{\epsilon}} h_\lambda(\epsilon) \\
&\quad + \frac{2\nu}{\pi} \sum_{k=1}^{\lfloor \frac{l}{2} \rfloor} \frac{\Gamma\left(\frac{l}{2} - k + \frac{1}{2}\right)}{\Gamma\left(\frac{l}{2} - k + 1\right) \Gamma\left(\frac{l}{2} + \frac{1}{2}\right)} \left(1 + \frac{1}{\epsilon}\right)^{k-1} \frac{\theta(\epsilon)}{\epsilon},
\end{aligned} \tag{C8}$$

with the definitions

$$h_\lambda(\epsilon) = \begin{cases} \frac{2\nu}{\pi} \theta(\epsilon) \tan^{-1}(\sqrt{\epsilon}) & : \lambda = \frac{1}{2}, \\ \theta(\epsilon) & : \lambda = 0, \end{cases} \tag{C9}$$

and

$$\lambda = \frac{1}{2} (l \bmod 2) = \begin{cases} \frac{1}{2} & : l \text{ odd}, \\ 0 & : l \text{ even}. \end{cases} \tag{C10}$$

Here $[q]$ denotes the integer $n \leq q$ that is closest to q .

3. Calculation of $b_3^{(l)}(\epsilon, \nu)$

To simplify the following analysis we define

$$\tilde{F}_\nu(s) := e^{-(1+\nu^2)s} F_\nu(s). \tag{C11}$$

The integral in $\tilde{F}_\nu(s)$ can not be evaluated to elementary expressions directly. In contrast to that its inverse Laplace transform can be related to the solvable derivative given by

$$e^{(1+\nu^2)s} \tilde{F}'_\nu(s) = \frac{\nu}{2} s^{-\frac{1}{2}} e^s \operatorname{erfc}(\sqrt{s}) - \frac{1}{2} \sqrt{1+\nu^2} s^{-\frac{1}{2}}. \tag{C12}$$

Using this observation we calculate

$$\begin{aligned}
\mathcal{L}_s^{-1}[F_\nu(s)](\epsilon) &= \mathcal{L}_s^{-1}[\tilde{F}_\nu(s)](\epsilon + (1+\nu^2)) \\
&= -\frac{\mathcal{L}_s^{-1}[\tilde{F}'_\nu(s)](\epsilon + (1+\nu^2))}{\epsilon + (1+\nu^2)} \\
&= -\frac{\mathcal{L}_s^{-1}[e^{(1+\nu^2)s} \tilde{F}'_\nu(s)](\epsilon)}{\epsilon + (1+\nu^2)} \\
&= (\epsilon + (1+\nu^2))^{-1} \\
&\quad \times \left(\frac{\sqrt{1+\nu^2}}{2\sqrt{\pi}} \frac{\theta(\epsilon)}{\sqrt{\epsilon}} - \frac{\nu}{2\sqrt{\pi}} \frac{\theta(\epsilon)}{\sqrt{1+\epsilon}} \right).
\end{aligned} \tag{C13}$$

From there we get

$$\begin{aligned} \mathcal{L}_s^{-1}[s^{-1}F_\nu(s)](\epsilon) &= \int_{-\infty}^{\epsilon} dx \mathcal{L}_s^{-1}[F_\nu(s)](x) \\ &= \frac{\theta(\epsilon)}{\sqrt{\pi}} \left[\tan^{-1} \left(\sqrt{\frac{\epsilon}{1+\nu^2}} \right) \right. \\ &\quad \left. + \tan^{-1} \left(\sqrt{\frac{\nu^2}{1+\epsilon}} \right) - \tan^{-1} \nu \right], \end{aligned} \quad (\text{C14})$$

and

$$\begin{aligned} \mathcal{L}_s^{-1}[s^{-\frac{1}{2}}F_\nu(s)](\epsilon) &= \int_{-\infty}^{\infty} dx \mathcal{L}_s^{-1}[s^{-\frac{1}{2}}](\epsilon-x) \mathcal{L}_s^{-1}[F_\nu(s)](x) \\ &= \frac{\theta(\epsilon)}{2\pi} \int_0^{\epsilon} dx \frac{1}{\sqrt{\epsilon-x}} \left[\frac{\sqrt{1+\nu^2}}{\sqrt{x(x+(1+\nu^2))}} \right. \\ &\quad \left. - \frac{\nu}{\sqrt{1+x(x+(1+\nu^2))}} \right] \\ &= \frac{\theta(\epsilon)}{\pi} (\epsilon+(1+\nu^2))^{-\frac{1}{2}} \tan^{-1} \left(\frac{1}{\nu} \sqrt{1+\frac{1+\nu^2}{\epsilon}} \right). \end{aligned} \quad (\text{C15})$$

We calculate $\mathcal{L}_s^{-1}[s^{-n}\tilde{F}_\nu(s)]$ for larger negative powers of s using a recursive approach, where Eqs. (C14) and (C15) will serve as initial values. We define

$$G_n(s) := \Gamma(n)s^{-n}\tilde{F}_\nu(s), \quad (\text{C16})$$

where n may be either integer or half-integer. Taking the derivative of Eq. (C16) with respect to s leads to

$$G_{n+1}(s) = -\frac{\partial}{\partial s}G_n(s) + \Gamma(n)s^{-n}\tilde{F}'_\nu(s), \quad (\text{C17})$$

which implies the recursion relation

$$\begin{aligned} \mathcal{L}_s^{-1}[G_{n+1}(s)](\epsilon) &= \epsilon \mathcal{L}_s^{-1}[G_n(s)](\epsilon) \\ &\quad + \Gamma(n) \mathcal{L}_s^{-1}[s^{-n}\tilde{F}'_\nu(s)](\epsilon) \end{aligned} \quad (\text{C18})$$

for the inverse Laplace transformed objects, where the initial values $\mathcal{L}_s^{-1}[G_1(s)]$ or $\mathcal{L}_s^{-1}[G_{\frac{1}{2}}(s)]$ are given explicitly by Eqs. (C14) and (C15). The solution to Eq. (C18)

is either given by

$$\begin{aligned} \mathcal{L}_s^{-1}[G_{n+1}(s)](\epsilon) &= \epsilon^n \mathcal{L}_s^{-1}[G_1(s)](\epsilon) \\ &\quad + \sum_{k=1}^n \epsilon^{n-k} \Gamma(k) \mathcal{L}_s^{-1}[s^{-k}\tilde{F}'_\nu(s)](\epsilon) \end{aligned} \quad (\text{C19})$$

for integer indexes or by

$$\begin{aligned} \mathcal{L}_s^{-1}[G_{n+\frac{1}{2}}(s)](\epsilon) &= \epsilon^n \mathcal{L}_s^{-1}[G_{\frac{1}{2}}(s)](\epsilon) \\ &\quad + \sum_{k=0}^{n-1} \epsilon^{n-1-k} \Gamma\left(k+\frac{1}{2}\right) \mathcal{L}_s^{-1}[s^{-k-\frac{1}{2}}\tilde{F}'_\nu(s)](\epsilon) \end{aligned} \quad (\text{C20})$$

for half-integer indexes. In the given form, both solutions (C19) and (C20) are valid for $n \in \mathbb{N}_0$. After reintroducing the exponential prefactor Eqs. (C19) and (C20) become

$$\begin{aligned} \Gamma(n+1) \mathcal{L}_s^{-1}[s^{-n-1}F_\nu(s)](\epsilon) &= (\epsilon+(1+\nu^2))^n \mathcal{L}_s^{-1}[s^{-1}F_\nu(s)](\epsilon) \\ &\quad + \sum_{k=1}^n (\epsilon+(1+\nu^2))^{n-k} \Gamma(k) \\ &\quad \times \mathcal{L}_s^{-1}[s^{-k}e^{(1+\nu^2)s}\tilde{F}'_\nu(s)](\epsilon), \end{aligned} \quad (\text{C21})$$

and

$$\begin{aligned} \Gamma\left(n+\frac{1}{2}\right) \mathcal{L}_s^{-1}[s^{-n-\frac{1}{2}}F_\nu(s)](\epsilon) &= \sqrt{\pi}(\epsilon+(1+\nu^2))^n \mathcal{L}_s^{-1}[s^{-\frac{1}{2}}F_\nu(s)](\epsilon) \\ &\quad + \sum_{k=1}^n (\epsilon+(1+\nu^2))^{n-k} \Gamma\left(k-\frac{1}{2}\right) \\ &\quad \times \mathcal{L}_s^{-1}[s^{-k+\frac{1}{2}}e^{(1+\nu^2)s}\tilde{F}'_\nu(s)](\epsilon), \end{aligned} \quad (\text{C22})$$

where $n \in \mathbb{N}_0$. The remaining step is to calculate $\mathcal{L}_s^{-1}[s^{-n}e^{(1+\nu^2)s}\tilde{F}'_\nu(s)](\epsilon)$ for n being either integer or half-integer. Using Eq. (C12) leads to

$$\begin{aligned} \mathcal{L}_s^{-1}[s^{-n}e^{(1+\nu^2)s}\tilde{F}'_\nu(s)](\epsilon) &= \frac{\nu}{2} \mathcal{L}_s^{-1}[s^{-n-1}\sqrt{s} \operatorname{erfc}(\sqrt{s})](\epsilon) \\ &\quad - \frac{1}{2} \sqrt{1+\nu^2} \mathcal{L}_s^{-1}[s^{-n-\frac{1}{2}}](\epsilon) \\ &= -\frac{\sqrt{\pi}}{4} \epsilon^n b_2^{(2n)}(\epsilon, \nu) - \frac{\sqrt{1+\nu^2}}{2\Gamma(n+\frac{1}{2})} \epsilon^{n-\frac{1}{2}} \theta(\epsilon). \end{aligned} \quad (\text{C23})$$

For $l \geq -1$ we get

$$b_3^{(l)}(\epsilon, \nu) = \frac{\left(1 + \frac{1+\nu^2}{\epsilon}\right)^{\frac{l}{2}}}{\Gamma\left(\frac{l}{2} + 1\right)} \left[t_\lambda(\epsilon, \nu) - \frac{1}{\sqrt{\pi}} \sum_{k=1}^{\lceil \frac{l}{2} \rceil} \Gamma(k - \lambda) \left(1 + \frac{1+\nu^2}{\epsilon}\right)^{\lambda - k} \left(\frac{\sqrt{\pi}}{2} b_2^{(2(k-\lambda))}(\epsilon, \nu) + \frac{\sqrt{1+\nu^2}}{\Gamma\left(k - \lambda + \frac{1}{2}\right)} \frac{\theta(\epsilon)}{\sqrt{\epsilon}} \right) \right], \quad (\text{C24})$$

where $\lceil q \rceil$ denotes the integer $n \geq q$ that is closest to q and the function t_λ is defined as

$$t_\lambda(\epsilon, \nu) = \begin{cases} \frac{2}{\pi} \theta(\epsilon) \tan^{-1} \left(\frac{1}{\nu} \sqrt{1 + \frac{1+\nu^2}{\epsilon}} \right) & : \lambda = \frac{1}{2}, \\ \frac{2}{\pi} \theta(\epsilon) \left[\tan^{-1} \left(\sqrt{\frac{\epsilon}{1+\nu^2}} \right) + \tan^{-1} \left(\sqrt{\frac{\nu^2}{1+\epsilon}} \right) - \tan^{-1} \nu \right] & : \lambda = 0. \end{cases} \quad (\text{C25})$$

4. Calculation of $b_4^{(l)}(\epsilon, \nu)$

Since Eq. (C24) is not only valid for $l \in \mathbb{N}$ but also for the values $l = -1, 0$ we can use the simple relation between a_3 and a_4 [see Eq. (C4)] to get

$$b_4^{(l)}(\epsilon, \nu) = -\frac{2\nu^2}{\epsilon} b_3^{(l-2)}(\epsilon, \nu) \quad (\text{C26})$$

for all $l \in \mathbb{N}$.

Appendix D: QCE in fermionization regime—Strong-coupling expansion

We employ an exact mapping [6] of 1D bosonic systems with delta interaction to spinless fermionic systems with an effective attractive zero-range interaction potential, here referred to as *anti delta*. Application of first-order QCE to the effective fermionic theory relies on the two-body propagator for the anti delta interaction. To relate it to the propagator in the original system we define, for any two-body propagator K , the swapping operation, denoted by \bar{K} , as

$$\begin{aligned} \bar{K}((q'_1, q'_2), (q_1, q_2)) \\ = \begin{cases} K((q'_1, q'_2), (q_1, q_2)), & \text{for } (q_1 - q_2)(q'_1 - q'_2) > 0, \\ -K((q'_1, q'_2), (q_1, q_2)), & \text{for } (q_1 - q_2)(q'_1 - q'_2) < 0, \end{cases} \end{aligned} \quad (\text{D1})$$

which gives a relative sign inversion when the two particles have to cross each other along any classical path from (q_1, q_2) to (q'_1, q'_2) . The interacting propagator K of two distinguishable particles subject to delta interaction is built from its symmetric part K_+ and its antisymmetric part K_- w.r.t. particle exchange,

$$K = K_+ + K_-, \quad (\text{D2})$$

where $K_+(K_-)$ is defined by all symmetric(antisymmetric) eigenfunctions $\psi_\pm(R, r)$ of the

two-body system, where R, r denote center-of-mass and relative coordinates, respectively. The delta interaction only has an effect on the symmetric wavefunctions $\psi_+(R, r)$, whereas the antisymmetric ones are unaffected $\psi_-(R, r) = \psi_{0,-}(R, r)$, thus we write

$$K_+ = K_{0,+} + K_\alpha, \quad (\text{D3})$$

$$K_- = K_{0,-}, \quad (\text{D4})$$

where $K_{0,\pm}$ denotes the (anti)symmetric part of the non-interacting propagator and K_α the modification to the symmetric part due to finite interaction.

For the anti delta interaction (which will be denoted by a tilde) the opposite is the case and one has unaffected symmetric wavefunction $\tilde{\psi}_+(R, r) = \psi_{0,+}(R, r)$ whereas the antisymmetric wavefunctions $\tilde{\psi}_-(R, r)$ feel the interaction in form of a jump discontinuity at vanishing relative distance r of the particles. Because of the exact mapping, those antisymmetric wavefunctions are equivalent with the symmetric ones for the delta interaction with a conditional sign inversion

$$\tilde{\psi}_-(R, r) = \text{sign}(r) \psi_+(R, r), \quad (\text{D5})$$

reflected in the propagator \tilde{K} of two distinguishable particles with anti delta interaction as

$$\begin{aligned} \tilde{K} &= K_{0,+} + \bar{K}_+ \\ &= K_{0,+} + \bar{K}_{0,+} + \bar{K}_\alpha. \end{aligned} \quad (\text{D6})$$

For first-order QCE calculations one needs then only the modification \tilde{K}_α of the propagator due to anti delta interaction, thus we write

$$\begin{aligned} \tilde{K} &= K_0 + \tilde{K}_\alpha \\ &= K_{0,+} + K_{0,-} + \tilde{K}_\alpha, \end{aligned} \quad (\text{D7})$$

and obtain the final result

$$\tilde{K}_\alpha = \bar{K}_{0,+} + \bar{K}_\alpha - K_{0,-}. \quad (\text{D8})$$

A simple test of this result can be done in the limit $\alpha \rightarrow \infty$ where the symmetric propagator for delta interaction becomes just the swapped version of the free antisymmetric propagator

$$K_{0,+} + K_\alpha \xrightarrow{\alpha \rightarrow \infty} \bar{K}_{0,-}, \quad (\text{D9})$$

so that

$$\tilde{K}_\alpha \xrightarrow{\alpha \rightarrow \infty} 0, \quad (\text{D10})$$

which means the fermionic theory is noninteracting in this limit, confirming the fermionization effect [7, 8].

Using the relation (D8) in the calculation of the corresponding QCE diagrams involved in the cluster contribution $\tilde{A}_{n_1, n-n_1}(s)$ for the fermionic theory one gets then a replacement of the functions $a_{n_1, n-n_1} \mapsto \tilde{a}_{n_1, n-n_1}$ given by [see Eq. (C4) for comparison]

$$\begin{aligned}\tilde{a}_1(s, \nu) &= -\frac{2}{\pi} \frac{\nu}{1+\nu^2} - \frac{2\nu^2}{\sqrt{\pi(1+\nu^2)}} \sqrt{s}, \\ \tilde{a}_2(s, \nu) &= \frac{2}{\sqrt{\pi}} \nu \sqrt{s} e^s \operatorname{erfc}(\sqrt{s}) = -a_2(s, \nu), \\ \tilde{a}_3(s, \nu) &= \frac{2}{\sqrt{\pi}} F_\nu(s) = a_3(s, \nu), \\ \tilde{a}_4(s, \nu) &= \frac{4}{\sqrt{\pi}} \nu^2 s F_\nu(s) = -a_4(s, \nu),\end{aligned}\quad (\text{D11})$$

and consequently

$$\begin{aligned}\tilde{b}_1^{(l)}(\epsilon, \nu) &= -\frac{2}{\pi} \frac{\nu}{1+\nu^2} \frac{\theta(\epsilon)}{\Gamma(\frac{l}{2}+1)} \\ &\quad - \frac{2\nu^2}{\sqrt{\pi(1+\nu^2)}} \frac{\theta(\epsilon)}{\Gamma(\frac{l}{2}+\frac{1}{2})\sqrt{\epsilon}}, \\ \tilde{b}_2^{(l)}(\epsilon, \nu) &= -b_2^{(l)}(\epsilon, \nu), \\ \tilde{b}_3^{(l)}(\epsilon, \nu) &= b_3^{(l)}(\epsilon, \nu), \\ \tilde{b}_4^{(l)}(\epsilon, \nu) &= -b_4^{(l)}(\epsilon, \nu),\end{aligned}\quad (\text{D12})$$

which can then be used in the fermionic version

$$\tilde{g}_{-,l}^{(N,d)}(\epsilon) = \sum_{n=2}^{N-l+1} n^{-\frac{d}{2}} z_{-,l-1}^{(N-n,d)} \sum_{n_1=1}^{n-1} \sum_{j=1}^4 \tilde{b}_j^{(ld)}(\epsilon, \nu) \quad (\text{D13})$$

of the coefficients (C5) modified to anti delta interaction, plugged into the fermionic counting function [Eq. (5) of the main text] together with the noninteracting fermionic coefficients (A13)

$$z_{-,l}^{(n,d)} = (-1)^{n-l} z_{+,l}^{(n,d)} \quad (\text{D14})$$

to get the corresponding counting functions for the fermionization regime.

Appendix E: Energy shifting method

We write the ansatz of the shifting method, i.e., expressing the effect of interactions as a shift in all energies (see Fig. E1), as

$$\mathcal{N}_\alpha(E) = \mathcal{N}_0(E - \Delta_\alpha). \quad (\text{E1})$$

The energy shifts Δ_α are in general allowed to vary with their location in the spectrum. Besides E , also d , V_{eff} , N , and α are free variables in the formal definition (E1) of Δ_α , which can be thought of as a reformulation of the

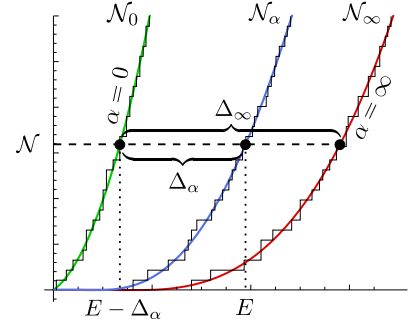


FIG. E1. Schematic method of energy shifting.

problem to find $\mathcal{N}_\alpha(E)$: Provided that the noninteracting smooth spectrum (represented by $\mathcal{N}_0(E)$) is known, Δ_α contains all information to construct the interacting one (represented by $\mathcal{N}_\alpha(E)$). As is pointed out in the following, the shifts Δ_α have a systematic form induced by the QCE for \mathcal{N}_0 and \mathcal{N}_α which allows then for an iterative approximation in a controlled way. This way one obtains, via Eq. (E1), a method to determine \mathcal{N}_α in an approximative order-by-order manner that is far more efficient than the direct approximation of \mathcal{N}_α using QCE up to a specific order.

1. The full shifts—Infinite coupling

For the purpose of this section we write the noninteracting counting function as

$$\mathcal{N}_0(\tilde{E}) = c_N \tilde{E}^{Nd/2} + c_{N-1} \tilde{E}^{(N-1)d/2} + \dots, \quad (\text{E2})$$

with the dimensionless total energy

$$\tilde{E} = \rho_0 E, \quad (\text{E3})$$

measured in units of the characteristic energy

$$\rho_0^{-1} = \frac{2\pi\hbar^2}{m} V_{\text{eff}}^{-2/d} \quad (\text{E4})$$

related to the (effective) system size V_{eff} (A11) and using the short-hand notation

$$c_l = \frac{z_{+,l}^{(N,d)}}{\Gamma(\frac{ld}{2}+1)} \quad (\text{E5})$$

for the constant coefficients. We note that, while we explicitly focus on bosonic systems here, the approach can be easily applied to fermionic systems, replacing $z_+ \mapsto z_-$ in Eq. (E5), as well.

To start with, we consider 1D bosonic systems with contact interactions and in particular focus on the fermionization limit $\alpha \rightarrow \infty$, which can be mapped to noninteracting spinless fermions [7, 8]. We thus demand equivalence with the noninteracting fermionic counting function

$$\mathcal{N}_\infty(E) \stackrel{!}{=} c_N \tilde{E}^{Nd/2} - c_{N-1} \tilde{E}^{(N-1)d/2} + \dots, \quad (\text{E6})$$

invoking a requirement on the full shift $\Delta_\infty = \lim_{\alpha \rightarrow \infty} \Delta_\alpha$ by comparison (E1) with the shifted non-interacting counting function. Up to next-to-leading order in the regime of high energy—or equivalently high temperature and weak quantum degeneracy—the latter reads

$$\begin{aligned} \mathcal{N}_0(E - \Delta_\infty) &= c_N \tilde{E}^{Nd/2} \left(1 - \tilde{E}^{-1} \tilde{\Delta}_\infty\right)^{Nd/2} + c_{N-1} \tilde{E}^{(N-1)d/2} + \dots \\ &= c_N \tilde{E}^{Nd/2} - \frac{Nd}{2} c_N \left(\tilde{\Delta}_\infty \tilde{E}^{Nd/2-1}\right) \\ &\quad + c_{N-1} \tilde{E}^{(N-1)d/2} + \dots \end{aligned} \quad (\text{E7})$$

with the dimensionless full energy shift defined as

$$\tilde{\Delta}_\infty = \rho_0 \Delta_\infty. \quad (\text{E8})$$

Equating Eq. (E7) with Eq. (E6) the second term in the expansion (E7) has to contribute to the term of order $\mathcal{O}(\tilde{E}^{(N-1)d/2})$ to correct its sign. Here we find the case $d = 2$ to be of special simplicity, because it corresponds to a full shift Δ_∞ that is a constant. From comparison one easily finds in this case

$$\tilde{\Delta}_\infty = \frac{2c_{N-1}}{Nc_N} = \frac{1}{2}N(N-1) \quad \text{for } d = 2, \quad (\text{E9})$$

which is remarkably accurate when applied to the 1D harmonic trapping (for which $d = 2$), where the exact spectra of noninteracting bosons and fermions are related level-by-level by an exact constant shift coinciding with the prediction (E9) from the universal consideration of smooth spectra.

For arbitrary effective dimensionality d the matching (E6) demands that the full shifts asymptotically behave like

$$\tilde{\Delta}_\infty \sim \text{const.} \times \tilde{E}^{1-d/2} \quad \text{as } \tilde{E} \rightarrow \infty. \quad (\text{E10})$$

By comparing ideal bosonic and fermionic smooth counting functions for several different values of the effective dimension d and numbers of particles N one finds that the prescription

$$\tilde{\Delta}_\infty = \text{const.} \times [\mathcal{N}]^{(2/d-1)/N} \quad (\text{E11})$$

is way more favorable than an energy-dependent prescription as in Eq. (E10). It effectively (in a smooth way) expresses the full fermionization shift of each level as a function of its quantum number \mathcal{N} rather than its (fermionized) energy E , related here by $\mathcal{N} = \mathcal{N}_\infty(E)$. While exhibiting the same correct asymptotics for large \tilde{E} the \mathcal{N} -dependent prescription (E11) quite accurately produces the fully fermionized limit on all energy scales. So far the explicit \mathcal{N} -prescription, Eq. (E11), is heuristic (if $d \neq 2$) and only motivated by observation. For finite coupling α on the other hand, the *partial* shift Δ_α also involves the infinite shift Δ_∞ (see subsequent subsection).

There, expressing Δ_∞ as a function of $\mathcal{N} = \mathcal{N}_\alpha(E)$ is crucial and can be justified by consistency w.r.t. “interaction flow” (see the subsection after the next).

A direct comparison of the next-to-leading order terms in Eqs. (E7) and (E6), using $\mathcal{N} = \mathcal{N}_\infty(E)$, yields the explicit full shift

$$\rho_0 \Delta_\infty = \underbrace{\frac{4}{Nd} c_{N-1} c_N^{-1-(2/d-1)/N}}_{\text{const.}} [\mathcal{N}]^{(2/d-1)/N}. \quad (\text{E12})$$

2. The partial shifts—Arbitrary coupling strengths

The next step in extending the shifts to arbitrary interaction strength crucially relies on the generic structure [Eq. (5) of the main text] of the QCE: The effect of arbitrary α is a correction of the coefficients c_l by functions (C2) of the energy in units of the coupling parameter, E/α , while keeping the polynomial structure in $V_{\text{eff}} E^{d/2}$, or equivalently $\tilde{E}^{d/2}$. Therefore we apply the same separation in the two distinct energy scales given by α and V_{eff} to the shifts. The corresponding ansatz reads, in the first-order implementation of the shifting,

$$\Delta_\alpha = \chi^{(N,d)} \left(\frac{E}{\alpha}\right) \Delta_\infty, \quad (\text{E13})$$

where the partial shift as fraction $\chi \in [0, 1]$ of the full shift is a function of the energy in units of the coupling strength, E/α , not involving the energy scale given by V_{eff} . The system size on the other hand enters the full shift Δ_∞ (see also Fig. E1), which should in contrast be independent of α in the following sense. For finite α , Δ_∞ refers to the “horizontal” line which should not change while the interacting energy E moves along the horizontal line when changing α . To illuminate this meaning of the separation of energy scales and the prescription (E11) a bit more, consider the shift of a single exact MB level. Say, we talk about the n -th excited state $E^{(n)}(\alpha)$, start from its noninteracting energy $E^{(n)}(0)$ and adiabatically switch on interactions. The full shift (E11) is expressed in terms of the counting function $\mathcal{N} = \mathcal{N}_\alpha(E^{(n)}(\alpha))$ which simply becomes the quantum number n . It does not change during the process of turning on interactions. The ansatz (E13) then suggests that the ratio $E^{(n)}(\alpha)/\alpha$ of the actual interacting energy of this level and the energy-like coupling parameter is in unique relation to how far this level has moved from the noninteracting $E^{(n)}(0)$ to the fully fermionized counter-part $E^{(n)}(\infty)$. This notion of invariance of Δ_∞ during a change of α can be expressed by writing it as a function of the *noninteracting* energy $E_0 \equiv E - \Delta_\alpha$ to eliminate an explicit α -dependence. By using $\mathcal{N} = \mathcal{N}_\alpha(E) = \mathcal{N}_0(E_0)$ in Eq. (E11) one may write

$$\Delta_\infty^{(N,d)}(E, \alpha, V_{\text{eff}}) = \Delta_\infty^{(N,d)}(E_0, V_{\text{eff}}). \quad (\text{E14})$$

From the analytical point of view the ansatz (E13) allows a matching in the next-to-leading order term of the

expansion in \tilde{E} . The separation into two different energy scales is here crucial. Matching coefficients in a power expansion in \tilde{E} can be thought of as matching power expansions in the (effective) volume V_{eff} , while E/α is considered as an independent variable. This way of separating combines the high amount of analytical control one has over power series expansions with the high value of a nonperturbative description in the interaction. This separation can also be exploited to extend the shifting method to higher-order (see below).

We briefly comment on the generality of the approach. The interpretation of Δ_∞ , Eq. (E12), as full shifts $\lim_{\alpha \rightarrow \infty} \Delta_\alpha$ between noninteracting levels and infinite strong coupling or *fermionized* energies only applies to the 1D bosonic case with contact interactions. Nevertheless, for arbitrary particle exchange symmetry, effective dimension d and short-range interaction potential, the general approach (E13) together with the \mathcal{N} prescription (E11), (E12) is still a fully valid and meaningful ansatz. Matching within the first-order ansatz (E13) the next-to-leading order contribution in an expansion similar to (E7) of the RHS of Eq. (E1) with the QCE expansion [Eq. (5) of the main text] on the LHS determines the ratio

$$\chi^{(N,d)}\left(\frac{E}{\alpha}\right) = -\frac{1}{2c_{N-1}}g_{\pm,N-1}^{(N,d)}\left(\frac{E}{\alpha}\right) \quad (\text{E15})$$

in terms of the coefficient functions (C2). In the case of contact-interacting bosons in one dimension the latter are given by the explicit expressions (C5) and one has the exact fermionization property, implemented as

$$g_{+,N-1}^{(N,d)}\left(\frac{E}{\alpha}\right) \xrightarrow{\alpha \rightarrow \infty} -2c_{N-1}, \quad (\text{E16})$$

for which one reobtains the correct full shifts as $\lim_{\alpha \rightarrow \infty} \chi^{(N,d)}(E/\alpha) = \chi(0) = 1$, meaning *in this case* the subscript ∞ can be taken literally in the sense $\Delta_\infty = \lim_{\alpha \rightarrow \infty} \Delta_\alpha$. In the general case, where actual fermionization may be absent, the label Δ_∞ just refers to the explicit expression (E12).

The analytic matching (E15) together with the full shifts (E12) determines the partial shifts (E13) as a function of E/α and \mathcal{N} . When expressing \mathcal{N} as a function of E it is crucial to use the unknown (already shifted) $\mathcal{N} = \mathcal{N}_\alpha(E)$ in the expression for the full shifts (E12), as demanded by the ‘‘interaction flow consistency’’ argument (see next subsection). In order to determine the final counting function (or equivalently the shifts Δ_α) from known objects involves therefore a self-consistent solution: Using the deduced analytical knowledge, Eqs. (E13), (E12), (E15), about Δ_α in the ansatz (E1) results in a highly nontrivial algebraic equation for $\mathcal{N}_\alpha(E)$. The most practical way to formulate the corresponding equation is by solving for E with a given quantum number \mathcal{N} instead of the other way around. The process of solving can be thought of as starting with a noninteracting level of energy E_0 and pushing its energy

until the requirement given by the matching is fulfilled. When fixing a starting value E_0 the corresponding shift Δ_α is determined by the equation

$$\rho_0 \Delta_\alpha = \text{const.} \times [\mathcal{N}_0(E_0)]^{(2/d-1)/N} \times \chi^{(N,d)}\left(\frac{E_0 + \Delta_\alpha}{\alpha}\right), \quad (\text{E17})$$

where the constant prefactor and the partial fermionization function χ are analytically given by Eq. (E12) and Eq. (E15), respectively. As the root of Eq. (E17), the shifts are determined as functions

$$\Delta_\alpha = \Delta_\alpha(d, N, V_{\text{eff}}, E_0, \alpha) \quad (\text{E18})$$

of E_0 and α as well as the fixed system parameters d, N, V_{eff} . Equivalently one can solve for the partial fermionization χ [see also Eq. (11) of the main text] as a function of E_0 and α by finding the root x of

$$x = \chi^{(N,d)}\left(\frac{E_0 + x \Delta_\infty^{(N,d)}(E_0, V_{\text{eff}})}{\alpha}\right), \quad (\text{E19})$$

giving $\chi = x$ as

$$\chi = \chi(d, N, V_{\text{eff}}, E_0, \alpha). \quad (\text{E20})$$

To extend the first-order implementation of the shifting method to higher-order one can again exploit the separation into the energy scales \tilde{E} and E/α inherent to the QCE counting function to arbitrary order [Eq. (5) of the main text] in full generality. To achieve this the ansatz (E13) has to be modified to admit corrections to χ in terms of powers of the small parameter

$$y = N^{1+d/2} \left[\frac{\mathcal{N}}{c_N} \right]^{-1/N} \quad (\text{E21})$$

that increases when one approaches the deeply quantum degenerate regime. This characterization becomes more obvious when expressed in terms of the scaled noninteracting energy [see Eq. (13) of the main text and [appendix F, subsection 2](#)],

$$y = (E_0^{\text{sc}})^{-d/2} + \mathcal{O}\left((E_0^{\text{sc}})^{-2d/2}\right). \quad (\text{E22})$$

The extended ansatz (to order J) reads

$$\Delta_\alpha = \Delta_\infty \left[\chi_1^{(N,d)}\left(\frac{E}{\alpha}\right) + \sum_{j=1}^J y^j \chi_{j+1}^{(N,d)}\left(\frac{E}{\alpha}\right) \right], \quad (\text{E23})$$

where the higher-order contributions $\chi_{j \geq 2}^{(N,d)}(E/\alpha)$, similarly to the first-order implementation, get fixed by successive analytical matching of next-to-next-to-leading (and higher) order terms in the large- \tilde{E} expansion of the shifted noninteracting counting function similar to (E7) with the QCE counting function [Eq. (5) of the main text], which then involves three-body (and larger) clusters, encoded in $g_{+,\leq N-2}^{(N,d)}(E/\alpha)$.

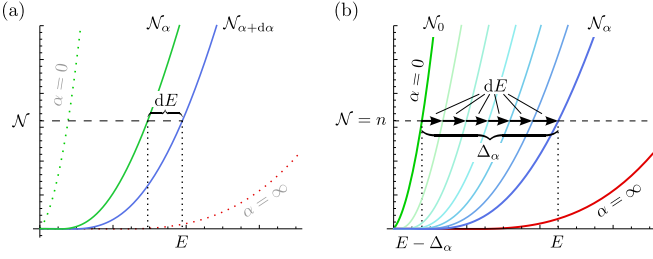


FIG. E2. (a) Scheme of an infinitesimal energy shifting, where \mathcal{N}_α is the initial point (green). (b) Sketch of integrated infinitesimal shifts dE (along $\mathcal{N} = \text{const.}$), reproducing the finite shift Δ_α .

3. Interaction flow consistency—A justification of the \mathcal{N} -prescription

In this subsection an analytical argument is presented clarifying why the \mathcal{N} -dependent prescription (E11) is favorable to an energy dependent one (E10). The argument is based on an infinitesimal version of the shifting method. Instead of applying the shifting to noninteracting counting functions \mathcal{N}_0 , Eq. (E2), or equivalently individual MB levels, in order to approximately reproduce the interacting case, the starting point is here the case of finite arbitrary coupling strength α . One could think of the situation with the coupling set to α as an unperturbed system, while an infinitesimal increase $d\alpha$ in the interaction can be regarded as a small perturbation. The attempt is then to implement this perturbation as an infinitesimal version of the energy shifting method applied to \mathcal{N}_α , expressed by

$$\mathcal{N}_{\alpha+d\alpha}(E) = \mathcal{N}_\alpha(E - dE). \quad (\text{E24})$$

Similar to the direct finite shift (E13) the ansatz for the infinitesimal shift is

$$dE = \underbrace{\text{const.} \times \mathcal{N}^{(2/d-1)/N}}_{=\Delta_\infty} d\chi \sim \tilde{E}^{1-d/2} d\chi, \quad (\text{E25})$$

where $\mathcal{N} = \mathcal{N}_{\alpha+d\alpha}(E)$ can be regarded as the quantum number of a level to be shifted. The situation is sketched in Fig. E2(a). The function $d\chi$ is here assumed to depend on the ratio $E/d\alpha$ of energy and the (here infinitesimal *additional*) coupling $d\alpha$. Again a separation into different energy scales given by $d\alpha$ and V_{eff} is crucial. As in the previous subsection, the shift dE gets then determined by matching (E24) term by term in an expansion in \tilde{E} associated with the energy scale given by the system size. This is here demonstrated as a first-order shift involving only the matching of terms of next-to-leading order $\mathcal{O}(\tilde{E}^{(N-1)d/2})$. Up to this order, and expanded linearly in infinitesimal quantities, the shifted counting function,

according to QCE, reads

$$\begin{aligned} \mathcal{N}_\alpha(E - dE) &= c_N \tilde{E}^{Nd/2} \\ &+ \left[c_{N-1} + g\left(\frac{E}{\alpha}\right) - 2c_{N-1} d\chi \right. \\ &\quad \left. - \underbrace{\frac{4}{Nd} c_{N-1} c_N^{-1} \frac{E}{\alpha} g'\left(\frac{E}{\alpha}\right) \tilde{E}^{-d/2} d\chi}_{\text{subdominant as } \tilde{E} \rightarrow \infty} \right] \tilde{E}^{(N-1)d/2} \\ &+ \dots, \end{aligned} \quad (\text{E26})$$

which has to be matched with the QCE prediction

$$\begin{aligned} \mathcal{N}_{\alpha+d\alpha}(E) &= c_N \tilde{E}^{Nd/2} \\ &+ \left[c_{N-1} + g\left(\frac{E}{\alpha}\right) - g'\left(\frac{E}{\alpha}\right) \frac{E}{\alpha^2} d\alpha \right] \tilde{E}^{(N-1)d/2} + \dots, \end{aligned} \quad (\text{E27})$$

where $g(E/\alpha)$ is short hand for $g_{\pm, N-1}^{(N,d)}(E/\alpha)$. There is a subtle issue in identifying the order of terms in \tilde{E} . Since in the infinitesimal shift the energy scale regarded distinctly from \tilde{E} should be $E/d\alpha$ instead of E/α , the latter could be associated with the volume scale by $E/\alpha = \tilde{E}/\tilde{\alpha}$ with a scaled dimensionless parameter $\tilde{\alpha} = \rho_0 \alpha$. However, α could be considered as a third energy scale, fixed as system parameter of the starting point system, independent of both, the (additional) interaction $d\alpha$ and the system size V_{eff} . The corresponding behaviour $\tilde{\alpha} \rightarrow \infty$ as $V_{\text{eff}} \rightarrow \infty$ keeps the ratio $E/\alpha = \tilde{E}/\tilde{\alpha}$ finite when considering the regime of large volume that underlies the expansion in dominant powers of \tilde{E} . Moreover, even if α is not considered as fixed parameter but rather scaling with V_{eff} , including the otherwise subdominant terms in Eqs. (E26) and (E27) does not affect the discussion and leads to the same result, as will be shown in the following. The only restriction is then that those terms do not become predominant, which would require that $g(\epsilon) \sim \epsilon^{d/2}$ when $\epsilon \rightarrow \infty$, in clear contradiction to the assumption that the effect of interaction vanishes as $\alpha \rightarrow 0$, expressed as $g(E/\alpha) \rightarrow 0$. Recognizing that

$$\frac{d}{d\alpha} g\left(\frac{E}{\alpha}\right) = g'\left(\frac{E}{\alpha}\right) \left(-\frac{E}{\alpha^2} + \frac{1}{\alpha} \frac{dE}{d\alpha} \right), \quad (\text{E28})$$

and using Eq. (E25) allows to refine

$$\begin{aligned} \frac{E}{\alpha^2} g'\left(\frac{E}{\alpha}\right) d\alpha &= -dg\left(\frac{E}{\alpha}\right) \\ &+ \underbrace{\frac{4}{Nd} c_{N-1} c_N^{-1} \frac{E}{\alpha} g'\left(\frac{E}{\alpha}\right) \tilde{E}^{-d/2} d\chi}_{\text{subdominant as } \tilde{E} \rightarrow \infty} + \dots \end{aligned} \quad (\text{E29})$$

The matching then directly leads to the infinitesimal shift

$$\frac{d\chi}{d\alpha} = -\frac{1}{2c_{N-1}} \frac{d}{d\alpha} g\left(\frac{E}{\alpha}\right), \quad (\text{E30})$$

implying a flow equation for $E(\alpha)$ that depends on the particular choice of Δ_∞ in Eq. (E25).

Finally, the \mathcal{N} -prescription (E12) for Δ_∞ becomes crucial when integrating the infinitesimal shifts (see sketch in Fig. E2b) to obtain the finite shift

$$\Delta_\alpha = \int_0^\alpha d\alpha' \frac{dE(\alpha')}{d\alpha'}. \quad (\text{E31})$$

While the energy $E(\alpha)$ of a point on the counting function, or equivalently of an individual MB level $E^{(n)}(\alpha)$, naturally changes during the integration, its quantum number $\mathcal{N} = n$ remains constant. Thus, combining Eq. (E25) with Eq. (E30), the integrated shift becomes

$$\Delta_\alpha = - \underbrace{\frac{1}{2c_{N-1}} \Delta_\infty}_{\text{const.}} \times \left(g\left(\frac{E}{\alpha}\right) - \underbrace{\lim_{\epsilon \rightarrow \infty} g(\epsilon)}_{=0} \right), \quad (\text{E32})$$

which exactly coincides with the direct finite shift (E13) with Eq. (E15). This feature is here referred to as interaction flow consistency: The direct, finite version of the shifting with \mathcal{N} -prescription is consistent with the integrated flow when applied as infinitesimal version at all steps in between, a very special feature that is, e.g., not inherent in an energy-dependent prescription.

4. Generality of the method

First, although the method was deduced based on fermionization, the matching of the ansatz (E13) together with the prescription (E11) that results in Eq. (E15) does not rely on this peculiarity of delta-interactions in 1D. Instead, it applies to other types of interaction, dimensionality and also statistics. The term ‘‘full shifts’’ should then not be taken literally, whereas the final implementation of the method in form of Eqs. (E17) and (E19) should still hold, even if $\alpha \rightarrow \infty$ produces infinite shifts, then reflected by $\lim_{\epsilon \rightarrow 0} \chi(\epsilon) = \infty$.

Second, since the first-order energy shift (E15) only depends on the two-body clusters, it does not suffer from the truncation of QCE to first order, making it exact at the smooth level. This reduction of the universal properties of a few-body system to the solution of the isolated two-body problem in particular opens the application to generic (short-range) interaction potentials. It also suggests an interpretation as a quantum few-body analogue of leading-order virial expansions of classical macroscopic systems, that, e.g., lead to the Van-der-Waals equation. Both incorporate interaction effects at the two-body level and both are restricted to describing smooth features. While the latter applies to classical grand canonical ensembles of typically macroscopic numbers of particles, our approach describes canonical ensembles of indistinguishable particles down to the regime of quantum degeneracy.

Appendix F: Large N asymptotics of partial fermionization

1. The asymptotic fermionization function $\chi^{(N,d)}(\epsilon)$

We analyse the asymptotics of the partial fermionization function $\chi^{(N,d)}(\epsilon)$ [see Eq. (8) of the main text] in the regime of $N \gg 1$. First we work on a general level that applies to arbitrary dimensionality and arbitrary short range interaction. To first order of the shifting method this involves, due to Eq. (E15), the asymptotics of the function $g_{\pm, N-1}^{(N,d)}(\epsilon)$. Expressing the latter in terms of the interaction kernels $a^\pm(s)$ via Eq. (C2) and (B3) reduces the problem to find the large- N behavior of

$$\epsilon^{-(N-1)d/2} \mathcal{L}_s^{-1} \left[s^{-(N-1)d/2-1} a_{1,1}^\pm(s) \right] (\epsilon). \quad (\text{F1})$$

In general, we consider here an arbitrary clustering $\mathfrak{N} = \{n_1, n_2, \dots, n_{|\mathfrak{N}|}\}$, including also three-body and higher order clusters, possibly involving both interacting ones and noninteracting, purely symmetry-related ones. The corresponding contribution to the spectral coefficient functions $g_{\pm, l}^{(N,d)}(\epsilon)$ involves terms of the form

$$\langle f(s) \rangle_\epsilon \equiv \Gamma(\mu + 1) \epsilon^{-\mu} \mathcal{L}_s^{-1} \left[s^{-\mu-1} f(s) \right] (\epsilon), \quad (\text{F2})$$

where $\mu = ld/2$ with $l = |\mathfrak{N}|$ the total number of clusters in the specific contribution and $f(s) = \prod_{n \in \mathfrak{N}} a_n(s)$ the product of interaction kernels of all nontrivial, interacting clusters. We set $a(s) \equiv 1$ for the trivial one-body clusters as well as noninteracting cyclic clusters of more than one particle. This definition, in view of the noninteracting amplitudes (A8), is compatible with the definition (B1)

While for first-order shifting only the term (F1) with $l = N - 1$ clusters is needed, the general expressions (F2) are required for shifting of order $N - l$ and higher. A large number of particles N thus implies a large number of clusters $l \simeq N$ contributing to the shifting method unless the level of approximation becomes comparable to N . The results presented in the main text [see Fig. 3 of the main text], based on only first- and second-order shifting, show that this criterion can be met easily while providing sufficient accuracy to describe average spectra down to the quantum degenerate regime.

Eqs. (F1) and (F2) can be interpreted as (inverse) thermal ‘‘average’’ in the following sense. It transfers functions of temperature, i.e., $a_{1,1}^\pm(s)$ or in general $f(s)$, from the canonical equilibrium picture of definite temperature (represented by $s = \beta\alpha$) to the corresponding microcanonical picture of definite energy (represented by $\epsilon = E/\alpha$). The identity

$$\langle f(s) \rangle_\epsilon = \frac{\mathcal{L}_\beta^{-1} [Z_l(\beta) \beta^{-1} f(\beta\alpha)] (E)}{\mathcal{L}_\beta^{-1} [Z_l(\beta) \beta^{-1}] (E)} \quad (\text{F3})$$

with $Z_l(\beta) \propto \beta^{-\mu} = \beta^{-ld/2}$ reveals the nature of the ensemble over which this ‘‘average’’ is taken: $Z_l(\beta)$ can

be seen as the partition function of l independent, distinguishable particles. Therefore each cluster, as far as concerns the ensemble average, acts as a single effective particle independent of the other clusters. On the other hand, the interaction effects that add more detail to such a composite particle picture by accounting for the internal dynamics are represented by the interaction kernels in $f(s)$ and “averaged” over in this ensemble rather than defining it. For instance, replacing $f(\beta\alpha) \mapsto \beta$ in Eq. (F3) results in an “average” of β that coincides with the microcanonical definition of inverse temperature

$$\bar{\beta}_E = \frac{d}{dE} \log \mathcal{N}_l(E) = \frac{d}{2} l E^{-1} \quad (\text{F4})$$

for a system of l distinguishable particles at given total energy E , in accordance with the equipartition theorem

$$\bar{E}_\beta = -\frac{d}{d\beta} \log Z_l(\beta) = \frac{d}{2} l \beta^{-1} \quad (\text{F5})$$

for the average energy in the corresponding canonical ensemble at given inverse temperature β .

Considering the limit $N \rightarrow \infty$ and hence $l, \mu \rightarrow \infty$ leads then to an equivalence of the microcanonical and canonical ensembles of clusters in the sense that

$$\langle f(s) \rangle_\epsilon \rightarrow f(\bar{\beta}_E \alpha) = f(\mu/\epsilon), \quad (\text{F6})$$

showing that, during the limiting process, the energy per particle E/N is the quantity that should be kept fixed rather than the total energy E in order to get a non-trivial result. Thermal fluctuations for a finite number of particles or, more precisely, clusters, lead to subdominant corrections that can be obtained as an expansion in the “central moments”:

$$\langle f(s) \rangle_\epsilon = f(\bar{s}) + \frac{1}{2!} f''(\bar{s}) \langle (s - \bar{s})^2 \rangle_\epsilon + \dots, \quad (\text{F7})$$

where we introduced the notation

$$\bar{s} \equiv \langle s \rangle_\epsilon = \bar{\beta}_E \alpha = \mu/\epsilon, \quad (\text{F8})$$

which should be considered as a quantity of $\mathcal{O}(1)$. From the definition (F2) the “central moments” can be evaluated to be

$$\langle (s - \bar{s})^n \rangle_\epsilon = \bar{s}^n \sum_{k=0}^n (-1)^{n-k} \binom{n}{k} \prod_{j=0}^{k-1} \left(1 - \frac{j}{\mu}\right). \quad (\text{F9})$$

To analyse the dominance of higher moment corrections for large μ we write

$$\prod_{j=0}^{k-1} \left(1 - \frac{j}{\mu}\right) = \begin{cases} \sum_{l=0}^{k-1} (-\mu)^{-l} P_l(k) & k \geq 1 \\ 1 & k = 0 \end{cases} \quad (\text{F10})$$

where $P_l(k)$ are polynomials in the natural numbers k of degree $2l$, recursively defined by

$$P_l(k) = \sum_{j=l}^{k-1} j P_{l-1}(j), \quad P_0(k) \equiv 1 \quad (\text{F11})$$

in the case $l < k$. One can easily show that these polynomials fulfill $P_l(k) = 0$ for $l \geq k \in \mathbb{N}_0$, except for $P_0(0) = 1$. Therefore one can lift the upper limit in the l -summation in Eq. (F10) from $k-1$ to $n-1$ and reorder the sum in Eq. (F9) to get the expansion in inverse powers of μ

$$\langle (s - \bar{s})^n \rangle_\epsilon = \bar{s}^n \sum_{l=0}^{n-1} (-\mu)^{-l} \sum_{k=0}^n (-1)^{n-k} \binom{n}{k} P_l(k). \quad (\text{F12})$$

Since the $P_l(k)$ are of degree $2l$, all terms from $\mathcal{O}(1)$ up to $\mathcal{O}(\mu^{-n/2})$ vanish, due to the identity

$$\sum_{k=0}^n (-1)^{n-k} \binom{n}{k} k^\nu = 0 \quad \text{for } \nu < n, \nu \in \mathbb{N}_0. \quad (\text{F13})$$

The higher central moments therefore are of order

$$\langle (s - \bar{s})^n \rangle_\epsilon = \mathcal{O}(\mu^{-\lceil n/2 \rceil}), \quad (\text{F14})$$

where $\lceil \cdot \rceil$ denotes the ceiling function. In particular, the first-order correction $\mathcal{O}(\mu^{-1})$ only involves the “variance” ($n = 2$) in the (inverse) thermal “average”. One gets

$$\langle f(s) \rangle_\epsilon = f(\bar{s}) - \frac{1}{2} f''(\bar{s}) \bar{s}^2 \mu^{-1} + \mathcal{O}(\mu^{-2}). \quad (\text{F15})$$

We return now to the asymptotics for partial fermionization functions. At the level of first-order energy shifting (E15) the exact relation to the two-body interaction kernels is

$$\chi^{(N,d)}(\epsilon) = -\langle a_{1,1}^\pm(s) \rangle_\epsilon \quad (\text{F16})$$

with $\mu = (N-1)d/2$, i.e., $l = N-1$ clusters in the ensemble. For large systems $N \gg 1$, in view of Eq. (F15), one has

$$\chi^{(N,d)}(N\tilde{\epsilon}) = -a_{1,1}^\pm\left(\frac{d}{2\tilde{\epsilon}}\right) + \mathcal{O}(N^{-1}) \quad (\text{F17})$$

in the fully general case and, by using Eq. (B10),

$$\chi^{(N,d)}(N\tilde{\epsilon}) = 1 - e^{d/(2\tilde{\epsilon})} \operatorname{erfc}\left(\sqrt{d/(2\tilde{\epsilon})}\right) + \mathcal{O}(N^{-1}) \quad (\text{F18})$$

for the repulsive Dirac delta contact interaction in 1D Bose gases [see Eq. (12) of the main text]. Crucial for the nontrivial limit when $N \rightarrow \infty$ is the scaling of the total energy with N , which we expressed by introducing $\tilde{\epsilon} = \epsilon/N = E/(N\alpha)$, i.e., the energy *per particle* in units of the coupling strength α .

We note that while the asymptotic first-order partial fermionization function (F18) is determined by only the dominant term in Eq. (F15), this turns out to be not the case for energy shifting to higher order, where thermal fluctuations become non-negligible. This is due to the fact that to higher order, a sum of more than one “average” of the form (F15) is involved and the corresponding dominant terms $f(\bar{s})$ are divergent as positive powers of

N . In the overall sum, however, all divergent terms cancel each other, leaving again a nontrivial limit $N \rightarrow \infty$ when $\bar{\epsilon}$ is fixed. In the case of asymptotic second-order shifting, for instance, the variance term $\sim f''(\bar{s})$ survives, while higher moments are of vanishing order in N .

2. Asymptotic scaling of the full fermionization shifts $\Delta_\infty^{(N,d)}(E_0, V_{\text{eff}})$

In the following we consider the thermodynamic limit $N, V_{\text{eff}} \rightarrow \infty$ while keeping N/V_{eff} fixed. Henceforth,

$$X \stackrel{\text{TL}}{=} Y \quad \text{or} \quad X \stackrel{\text{TL}}{\simeq} Y \quad (\text{F19})$$

denotes identity or approximate identity of two quantities X and Y in this limit, respectively. We will show that the full energy shift $\Delta_\infty^{(N,d)}(E_0, V_{\text{eff}})$ is an (asymptotically) *extensive* quantity in the sense of

$$\Delta_\infty^{(\lambda N, d)}(\lambda E_0, \lambda V_{\text{eff}}) \stackrel{\text{TL}}{=} \lambda \Delta_\infty^{(N, d)}(E_0, V_{\text{eff}}). \quad (\text{F20})$$

From matching fully shifted and fermionized spectra in the high temperature regime we inferred the full shift Δ_∞ , Eq. (E12), in an \mathcal{N} -dependent prescription (E11) that was motivated by interaction flow consistency (see appendix E, subsection 3). Considering $N \gg 1$ in the coefficients (E5), (A13) the full shift asymptotically becomes

$$\rho_0 \Delta_\infty^{(N, d)}(E_0, V_{\text{eff}}) \stackrel{\text{TL}}{=} 2^{-\frac{d}{2}} e^{\frac{d}{2} - \frac{2}{d}} N^{1 + \frac{2}{d}} [\mathcal{N}_0(E_0)]^{(\frac{2}{d} - 1)/N}. \quad (\text{F21})$$

In order to express all relevant quantities in a dimensionless way that additionally reflects finite (effective) particle density $n_{\text{eff}} = N/V_{\text{eff}}$ in the thermodynamic limit, we introduce the (intensive) unit of energy

$$\mathcal{E} = \rho_0^{-1} N^{2/d} = \frac{2\pi\hbar^2}{m} n_{\text{eff}}^{2/d} \quad (\text{F22})$$

with ρ_0 given by Eq. (E4) and define the scaled energy E_0^{sc} and scaled full shift $\Delta_\infty^{\text{sc}}$ as the energy and full shift *per particle* in units of \mathcal{E} , Eq. (F22):

$$E_0^{\text{sc}} \equiv \frac{E_0}{N\mathcal{E}}, \quad \Delta_\infty^{\text{sc}} \equiv \frac{\Delta_\infty}{N\mathcal{E}}. \quad (\text{F23})$$

For simplicity, we set $k_B = 1$ and identify the microcanonical entropy S of the noninteracting Bose gas in the usual way

$$S(N, E_0, V_{\text{eff}}) = \log \mathcal{N}_0(E_0). \quad (\text{F24})$$

The difference in using the counting function instead of the DOS becomes insignificant in the thermodynamic limit. The only assumption needed to go on is extensivity of the entropy (F24) in the sense $S(\lambda N, \lambda E_0, \lambda V_{\text{eff}}) \stackrel{\text{TL}}{=} \lambda S(N, E_0, V_{\text{eff}})$, which can be inferred from extensivity of the grand potential of the non-interacting Bose gas

together with equivalence of ensembles in the thermodynamic limit. A simple dimensional analysis shows that extensivity of S , itself a dimensionless quantity, implies the scaling law

$$S(N, E_0, V_{\text{eff}}) \stackrel{\text{TL}}{=} N s(E_0^{\text{sc}}). \quad (\text{F25})$$

It follows that the scaled full shift per particle (F23), expressed in terms of the microcanonical entropy per particle s , is

$$\Delta_\infty^{\text{sc}}(N, E_0, V_{\text{eff}}, d) \stackrel{\text{TL}}{=} 2^{-\frac{d}{2}} e^{\frac{d}{2} - \frac{2}{d}} \exp \left[s(E_0^{\text{sc}}) \left(\frac{2}{d} - 1 \right) \right], \quad (\text{F26})$$

which, in view of Eqs. (F22) and (F23), implies the extensivity (F20) of Δ_∞ .

From equivalence of grand canonical and microcanonical ensembles in the thermodynamic limit, formally justified by saddle point approximation, one finds

$$s(E_0^{\text{sc}}) = \left(1 + \frac{2}{d} \right) (\text{Li}_{d/2}[z_0(E_0^{\text{sc}})])^{2/d} E_0^{\text{sc}} - \log[z_0(E_0^{\text{sc}})] \quad (\text{F27})$$

with the fugacity $z_0(E_0^{\text{sc}})$ implicitly defined by

$$E_0^{\text{sc}} = \frac{d \text{Li}_{1+d/2}(z_0)}{2 [\text{Li}_{d/2}(z_0)]^{1+2/d}}, \quad (\text{F28})$$

as long as condensation effects do not play a role. The latter can only occur for $d > 2$, when this poses the restriction

$$E_0^{\text{sc}} > \frac{d \zeta(1 + \frac{d}{2})}{2 [\zeta(\frac{d}{2})]^{1+2/d}} \equiv E_{0, \text{crit}}^{\text{sc}} \quad (\text{F29})$$

to the validity of Eqs. (F27) and (F28). The polylogarithm in Eqs. (F27) and (F28) is defined as $\text{Li}_\nu(z) = \sum_{k=1}^{\infty} z^k / k^\nu$, $|z| < 1$. The implicit definition (F28) can be analytically resolved in two complementary regimes. In the low-temperature quantum regime $E_0^{\text{sc}} \ll 1$ (or $E_0^{\text{sc}} - E_{0, \text{crit}}^{\text{sc}} \ll 1$) the full shift reduces to (see also [9])

$$\Delta_\infty^{\text{sc}}(E_0^{\text{sc}}, d) \stackrel{\text{TL}}{\simeq} 2^{-\frac{d}{2}} e^{\frac{d}{2} - \frac{2}{d}} \exp \left[C(d) (E_0^{\text{sc}})^{\frac{d}{2+d}} \right] \quad (\text{F30})$$

with $C(d) = (\frac{4}{d^2} - 1) [\frac{d}{2} \zeta(1 + \frac{d}{2})]^{2/(2+d)}$. Remarkably, Eq. (F30) is also valid in the BEC regime $E_0^{\text{sc}} < E_{0, \text{crit}}^{\text{sc}}$, while Eqs. (F27) and (F28) are not applicable. This one finds by splitting off the contributions $N^{\text{cond}}, E_0^{\text{cond}}$, and S^{cond} to N , E_0 , and S that originate from the single-particle ground state while setting $z_0 = 1$ in the thermal contributions. While the occupation of the ground state N^{cond} becomes macroscopic in the BEC regime, the total energy E_0 and total entropy S are dominated by the thermal contributions in the thermodynamic limit. Formally, the low-temperature entropy per particle in the exponent of Eq. (F30) could also be viewed as continuation of the function implicitly defined by Eqs. (F27) and (F28) into the BEC regime.

In the classical regime $E_0^{\text{sc}} \gg 1$, on the other hand, the entropy per particle becomes logarithmic, resulting in a simple power-law for the full shift

$$\Delta_\infty^{\text{sc}}(E_0^{\text{sc}}, d) \stackrel{\text{TL}}{\simeq} 2^{1-d} d^{d/2-1} (E_0^{\text{sc}})^{1-d/2}. \quad (\text{F31})$$

In the case $d = 2$ (e.g., given by a harmonic trap in 1D), the scaled full shift asymptotically becomes a unique constant for all energies:

$$\Delta_\infty^{\text{sc}} \stackrel{\text{TL}}{=} \frac{1}{2} \quad \text{for } d = 2, \quad (\text{F32})$$

in accordance with the exact unscaled full shift (E9).

3. Asymptotic universality of partial fermionization $\chi(d, E_0^{\text{sc}}, \alpha^{\text{sc}})$

We address the final question of the asymptotic scaling of partial fermionization as a function of the noninteracting energy E_0 as contrasted to the interacting energy $E = E_0 + \Delta_\alpha$ of the already shifted levels. We express the generic asymptotic scaling (F17) of the fermionization function for arbitrary short-range interaction as

$$\chi^{(N,d)}\left(\frac{E}{\alpha}\right) \stackrel{\text{TL}}{=} f\left(\frac{2E}{dN\alpha}\right) \quad (\text{F33})$$

where, in the case of δ -type contact interaction,

$$f(y) = 1 - e^{1/y} \operatorname{erfc}\left(\sqrt{1/y}\right). \quad (\text{F34})$$

To get χ as a function of the noninteracting energy E_0 ,

$$\chi = \chi(d, N, E_0, \alpha, V_{\text{eff}}), \quad (\text{F35})$$

one has to solve [see Eq. (12) of the main text]

$$\chi = f\left(\frac{2}{dN\alpha} \left(E_0 + \chi \Delta_\infty^{(N,d)}(E_0, V_{\text{eff}})\right)\right), \quad (\text{F36})$$

which, by implementing Eq. (F26), reduces to

$$\chi \stackrel{\text{TL}}{=} f\left(\frac{2}{d\alpha^{\text{sc}}} \left(E_0^{\text{sc}} + \chi \Delta_\infty^{\text{sc}}(E_0^{\text{sc}}, d)\right)\right), \quad (\text{F37})$$

where $\alpha^{\text{sc}} = \alpha/\mathcal{E}$ is the coupling strength in units of the intensive unit of energy \mathcal{E} , Eq. (F22). We arrive at the universal scaling law [Eq. (14) of the main text]

$$\chi(d, N, E_0, \alpha, V_{\text{eff}}) \stackrel{\text{TL}}{=} \chi(d, E_0^{\text{sc}}, \alpha^{\text{sc}}). \quad (\text{F38})$$

The significance of Eq. (F38) is that it establishes universality in the sense that it relates smoothed spectra of interacting systems that differ in the number of particles with each other, involving a rescaling of the coupling α and the unshifted (noninteracting) energy E_0 . Remarkably, the implicit definition (F37) of the asymptotic χ

even admits to write it as a function of only two parameters $2E_0^{\text{sc}}/(d\alpha^{\text{sc}})$ and $2\Delta_\infty^{\text{sc}}/(d\alpha^{\text{sc}})$, which augments the universality to even unify systems that differ in effective dimension d , i.e., systems with all kinds of external potentials that are homogeneous functions. This statement can be put as a relation between χ for arbitrary d and the simplest case of $d = 2$ via

$$\chi(d, E_0^{\text{sc}}, \alpha^{\text{sc}}) = \chi\left(2, \frac{E_0^{\text{sc}}}{2\Delta_\infty^{\text{sc}}}, \frac{d\alpha^{\text{sc}}}{4\Delta_\infty^{\text{sc}}}\right). \quad (\text{F39})$$

Since it is based on the generic asymptotic scaling property of f , Eq. (F17), it applies to arbitrary short-range interaction potentials and physical dimension, as long as compatible with the QCE framework.

Appendix G: Regimes of χ and explicit approximants

We specify contact interaction in 1D and identify three basic regimes of the asymptotic $\chi = \chi(d, E_0^{\text{sc}}, \alpha^{\text{sc}})$, considering the thermodynamic limit, where the implicit definition (F37) can be resolved and shows characteristic behavior. First, we identify the perturbative regime (I), characterized by

$$\begin{aligned} \alpha^{\text{sc}} &\ll E_0^{\text{sc}}, \\ E_0^{\text{sc}} &\gg (\Delta_\infty^{\text{sc}})^{2/3} (\alpha^{\text{sc}})^{1/3}, \end{aligned} \quad (\text{G1})$$

where the first term of the argument on the RHS of Eq. (F37) becomes large while the second term can be neglected, i.e., $\chi \Delta_\infty^{\text{sc}}/E_0^{\text{sc}} \ll 1$, and

$$\chi \simeq f\left(\underbrace{2E_0^{\text{sc}}/(d\alpha^{\text{sc}})}_{\gg 1}\right) \simeq \sqrt{2d\alpha^{\text{sc}}/(\pi E_0^{\text{sc}})}. \quad (\text{G2})$$

This covers a ‘‘classical perturbative regime’’ (Ia) as well as a ‘‘quantum perturbative regime’’ (Ib), distinguished by either $E_0^{\text{sc}} > \Delta_\infty^{\text{sc}}$ or $E_0^{\text{sc}} < \Delta_\infty^{\text{sc}}$, respectively.

Second, we identify a nonperturbative quantum regime (II) by

$$\begin{aligned} \alpha^{\text{sc}} &\ll \Delta_\infty^{\text{sc}}, \\ E_0^{\text{sc}} &\ll (\Delta_\infty^{\text{sc}})^{2/3} (\alpha^{\text{sc}})^{1/3}, \end{aligned} \quad (\text{G3})$$

where the second term of the argument on the RHS of Eq. (F37) becomes large while the first term can be neglected, i.e., $\chi \Delta_\infty^{\text{sc}}/E_0^{\text{sc}} \gg 1$, and

$$\chi \simeq f\left(\underbrace{2\chi \Delta_\infty^{\text{sc}}/(d\alpha^{\text{sc}})}_{\gg 1}\right) \simeq \sqrt{2d\alpha^{\text{sc}}/(\pi \Delta_\infty^{\text{sc}} \chi)}, \quad (\text{G4})$$

which simplifies to

$$\chi \simeq \left(\frac{2d\alpha^{\text{sc}}}{\pi \Delta_\infty^{\text{sc}}}\right)^{1/3}. \quad (\text{G5})$$

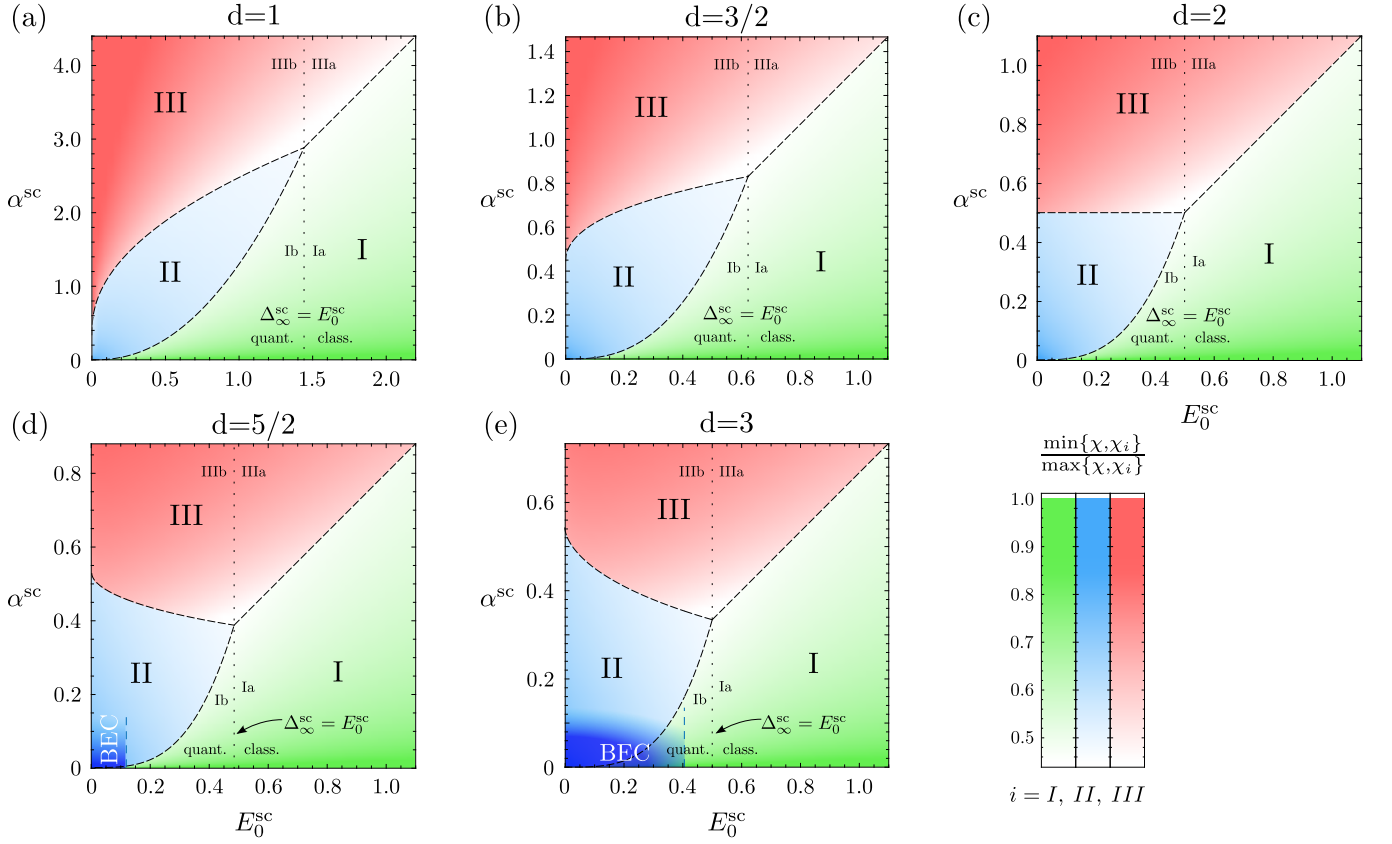


FIG. G1. The three regimes of partial fermionization in 1D Bose gases with contact interaction. I: perturbative regime, see Eq. (G1) [classical (Ia) and quantum (Ib)] (green); II: nonperturbative quantum regime, see Eq. (G3) (blue); III: fermionization regime, see Eq. (G6) [classical (IIIa) and quantum (IIIb)] (red). Validity of particular regimes is encoded by lightness. The separation of regimes is indicated by three boundaries (dashed) $\alpha^{\text{sc}}/2 = (E_0^{\text{sc}})^3(\Delta_\infty^{\text{sc}})^{-2}$ (I-II), $\alpha^{\text{sc}}/2 = \Delta_\infty^{\text{sc}}$ (II-III), and $\alpha^{\text{sc}}d/2 = E_0^{\text{sc}}$ (I-III), corresponding to Eqs. (G1), (G3), and (G6). The panels (a)–(e) show several cases of varying effective dimension: (a) $d = 1$, i.e., periodic boundary condition and $U(q) = 0$; (b) $d = 3/2$; (c) $d = 2$, i.e., harmonic trapping $U(q) \propto q^2$; (d) $d = 5/2$; (e) $d = 3$, i.e., linear well, e.g., $U(q) \propto |q|$. For $d > 2$ the noninteracting Bose gas enters the BEC regime (indicated in dark blue) when $E_0^{\text{sc}} \leq E_{0,\text{crit}}^{\text{sc}}$ (marked dashed blue), see Eq. (F29).

Regimes I and II are both characterized by a large argument to the function f in Eq. (F37), i.e., a low level of fermionization $\chi \ll 1$. They are complemented by the fermionization regime (III), i.e.,

$$\begin{aligned} E_0^{\text{sc}} &\ll \alpha^{\text{sc}}, \\ \Delta_\infty^{\text{sc}} &\ll \alpha^{\text{sc}}, \end{aligned} \quad (\text{G6})$$

where a small argument to the function f in Eq. (F37) implies $1 - \chi \ll 1$ and one gets

$$\chi \simeq 1 - \sqrt{2(E_0^{\text{sc}} + \Delta_\infty^{\text{sc}})/(\pi d \alpha^{\text{sc}})}, \quad (\text{G7})$$

covering both, a “classical fermionization regime” (IIIa) as well as a “quantum fermionization regime” (IIIb).

The identification of these regimes becomes especially simple in the case $d = 2$, where $\Delta_\infty^{\text{sc}} \stackrel{\text{TL}}{=} 1/2$ is constant. For this case, χ becomes a particularly rigid shift w.r.t. E_0^{sc} in the nonperturbative quantum regime.

Figure G1 shows the partition of the parameter space

into the regimes identified above and the validity of the respective approximations, Eqs. (G2),(G5), and (G7).

Finally, an overall good approximation is already obtained by a single iteration. Using the expression for regime II, Eq. (G5), on the RHS of Eq. (F37) gives

$$\chi \simeq f\left(\frac{2E_0^{\text{sc}}}{d\alpha^{\text{sc}}} + \left(\frac{4}{\pi}\right)^{1/3} \left(\frac{2\Delta_\infty^{\text{sc}}}{d\alpha^{\text{sc}}}\right)^{2/3}\right) \quad (\text{G8})$$

with f and $\Delta_\infty^{\text{sc}}(E_0^{\text{sc}})$ defined in Eqs. (F34) and (F26), respectively. In the full parameter range the interpolation function (G8) has a maximum relative error $\delta = |\chi_{\text{approx}} - \chi|/\chi$ of $\delta < 11.7\%$ w.r.t. the exact numerical solution of the implicit Eq. (F37). If one applies the iteration once more, i.e., plugging Eq. (G8) into the RHS of Eq. (F37) results in an explicit approximation with maximum relative error $\delta < 3.0\%$. The third and fourth iteration give $\delta < 0.99\%$ and $\delta < 0.38\%$. It is worth to note that for the second and higher iterations also the relative error in $1 - \chi$, i.e., $\bar{\delta} = |\chi_{\text{approx}} - \chi|/(1 - \chi)$, referring to the deviation from fermionization, is bound

by $\bar{\delta} < 5.3\%$, 0.88% , 0.23% , referring to the second, third and fourth iteration, respectively. Note that it is crucial to take the approximation in regime II as initial value. It is special in so far that it correctly produces the dominant behavior in all three regimes after just one iteration. In contrast, taking for instance $\chi \equiv 0, 1$, or Eq. (G2) as starting point results in unbounded relative errors δ , even after multiple iterations.

Appendix H: Relation between χ and local pair correlations for contact interaction

A relation between the local pair correlation function and the functions Δ_α and χ can be obtained by following standard steps relating the pair correlation with the dependence of thermodynamic potentials on the interaction strength, as in [10]. We first present a version of this analysis suitable to the microcanonical case of main interest, and then discuss its connection with the canonical scenario.

In second-quantized form, adequately describing the subspace of bosonic symmetry, the many-body Hamiltonian [Eq. (6) of the main text], that parametrically depends on the interaction strength α , takes the form ($\hbar^2/2m = 1$)

$$\begin{aligned} \hat{H}_\alpha = & \int \hat{\psi}^\dagger(q) \left(-\frac{\partial^2}{\partial q^2} \right) \hat{\psi}(q) dq \\ & - \sqrt{8\alpha} \int \hat{\psi}^\dagger(q) \hat{\psi}^\dagger(q) \hat{\psi}(q) \hat{\psi}(q) dq \end{aligned} \quad (\text{H1})$$

in terms of bosonic field operators $\hat{\psi}, \hat{\psi}^\dagger$. Denoting by $|E_\alpha^{(n)}\rangle$ the eigenstate indexed by n with energy $E_\alpha^{(n)}$, by applying the Hellmann-Feynman theorem we obtain

$$\begin{aligned} \frac{\partial E_\alpha^{(n)}}{\partial \alpha} &= \left\langle E_\alpha^{(n)} \left| \frac{\partial \hat{H}_\alpha}{\partial \alpha} \right| E_\alpha^{(n)} \right\rangle \\ &= \left\langle E_\alpha^{(n)} \left| \sqrt{\frac{2}{\alpha}} \int \hat{\psi}^\dagger(q) \hat{\psi}^\dagger(q) \hat{\psi}(q) \hat{\psi}(q) dq \right| E_\alpha^{(n)} \right\rangle. \end{aligned} \quad (\text{H2})$$

The (unnormalized) local pair correlation function $g^{(2)}(0; q)$ is defined as the expectation value of the density-density correlator at zero distance at position q . In a microcanonical setup, for an energy eigenstate $|E_\alpha^{(n)}\rangle$ the local pair correlation function depends, besides position q and coupling strength α , also on the level index n , and it is given by

$$g_{n,\alpha}^{(2)}(0; q) = \left\langle E_\alpha^{(n)} \left| \hat{\psi}^\dagger(q) \hat{\psi}^\dagger(q) \hat{\psi}(q) \hat{\psi}(q) \right| E_\alpha^{(n)} \right\rangle. \quad (\text{H3})$$

Comparing this definition with [Eq. (7) of the main text] we get

$$\left(\frac{\partial \chi(E/\alpha)}{\partial \alpha} \right)_n = \frac{1}{\Delta_\infty} \sqrt{\frac{2}{\alpha}} \int \langle g_{n,\alpha}^{(2)}(0; q) \rangle_n dq \quad (\text{H4})$$

that expresses the partial fermionization function χ in terms of the pair correlation averaged over a window of eigenstates and integrated over all positions. Realizing that E_0 , as opposed to $E = E_0 + \Delta_\alpha$, is invariant under changing α when the level index n is fixed, i.e.,

$$\left(\frac{\partial E_0}{\partial \alpha} \right)_n = 0 \quad (\text{H5})$$

and hence $(\partial \cdot / \partial \alpha)_n = (\partial \cdot / \partial \alpha)_{E_0}$, this gives direct access to χ as a function of α, E_0, d , and N , i.e., the function with universal characteristics [Eq. (14) of the main text] when $N \gg 1$. The relation reads

$$\frac{\partial \chi(N, d, \alpha^{\text{sc}}, E_0^{\text{sc}})}{\partial \alpha^{\text{sc}}} = \frac{1}{\Delta_\infty^{\text{sc}} \sqrt{2\pi\alpha^{\text{sc}}}} \frac{\langle g_{n,\alpha}^{(2)}(0; q) \rangle_{n,q}}{n_{\text{eff}}^{1+1/d}} \quad (\text{H6})$$

in rescaled variables [see Eq. (13) of the main text and (F23)] with effective particle density $n_{\text{eff}} = N/V_{\text{eff}}$ and the spatially and energy averaged local pair correlation defined as

$$\langle g_{n,\alpha}^{(2)}(0; q) \rangle_{n,q} = \frac{1}{V_{\text{eff}}} \int \langle g_{n,\alpha}^{(2)}(0) \rangle_n dq. \quad (\text{H7})$$

In the translationally invariant case of bosons on a ring of length L the spatial average becomes obsolete since $g^{(2)}(0; q) \equiv g^{(2)}(0)$ becomes independent of the position q , leading to the simple relation

$$\frac{\partial \chi(N, d, \alpha^{\text{sc}}, E_0^{\text{sc}})}{\partial \alpha^{\text{sc}}} = \frac{1}{\Delta_\infty^{\text{sc}} \sqrt{2\pi\alpha^{\text{sc}}}} \frac{\langle g_{n,\alpha}^{(2)}(0) \rangle_n}{(N/L)^2} \quad (\text{H8})$$

between the (universal) partial fermionization and (energy averaged) local pair correlations.

In case that the available experimental measurement of the pair correlation is performed in a canonical setup at temperature $k_B T$ to obtain $g_{T,\alpha}^{(2)}(0)$, one invokes the ensemble equivalence justified for $N \gg 1$ in order to relate the temperature with the mean energy, $T = T(E)$, through the microcanonical counting function to get the canonical form of the relation between pair correlations and partial fermionization,

$$\frac{\partial \chi(N, d, \alpha^{\text{sc}}, E_0^{\text{sc}})}{\partial \alpha^{\text{sc}}} = \frac{1}{\Delta_\infty^{\text{sc}} \sqrt{2\pi\alpha^{\text{sc}}}} \frac{g_{T(E_0),\alpha}^{(2)}(0)}{(N/L)^2}, \quad (\text{H9})$$

where

$$T(E_0) = T_0(E_0) \left[1 + \frac{\partial}{\partial E_0} (\chi \Delta_\infty) \right] \quad (\text{H10})$$

and $T_0(E_0) = (k_B \partial \log \mathcal{N}_0(E_0) / \partial E_0)^{-1}$ is the temperature of the *non-interacting* Bose gas at average energy E_0 .

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