General relations for quantum gases in two and three dimensions: Two-component fermions

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We derive exact general relations between various observables for N spin-1/2 fermions with zero-range or short-range interactions, in continuous space or on a lattice, in two or three dimensions, in an arbitrary external potential. Some of our results generalize known relations between the large-momentum behavior of the momentum distribution, the short-distance behaviors of the pair distribution function and of the one-body density matrix, the norm of the regular part of the wave function, the derivative of the energy with respect to the scattering length or to time, and the interaction energy (in the case of finite-range interactions). The expression relating the energy to a functional of the momentum distribution is also generalized. Moreover, we find expressions (in terms of the regular part of the wave function) for the derivative of the energy with respect to the effective range r_e in three dimensions (3D), and to the effective range squared in two dimensions (2D). They express the fact that the leading corrections to the eigenenergies due to a finite-interaction range are linear in the effective range in 3D (and in its square in 2D) with model-independent coefficients. There are subtleties in the validity condition of this conclusion, for the 2D continuous space (where it is saved by factors that are only logarithmically large in the zero-range limit) and for the 3D lattice models (where it applies only for some magic dispersion relations on the lattice that sufficiently weakly break Galilean invariance and that do not have cusps at the border of the first Brillouin zone; an example of such relations is constructed). Furthermore, the subleading short-distance behavior of the pair distribution function and the subleading $1/k^6$ tail of the momentum distribution are related to $\partial E/\partial r_e$ [or to $\partial E/\partial(r_e^2)$ in 2D]. The second-order derivative of energy with respect to the inverse (or the logarithm in the two-dimensional case) of the scattering length is found to be expressible for any eigenstate in terms of the eigen-wave-function's regular parts; this implies that, at thermal equilibrium, this second-order derivative, taken at fixed entropy, is negative. Applications of the general relations are presented: We compute corrections to exactly solvable two-body and three-body problems and find agreement with available numerics; for the unitary gas in an isotropic harmonic trap, we determine how the finite-$1/a$ and finite-range energy corrections vary within each energy ladder (associated with the SO(2,1) dynamical symmetry) and we deduce the frequency shift and the collapse time of the breathing mode; for the bulk unitary gas, we compare to fixed-node Monte Carlo data, and we estimate the deviation from the Bertsch parameter due to the finite interaction-range in typical experiments.

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I. GENERAL INTRODUCTION

The experimental breakthroughs of 1995 having led to the first realization of a Bose-Einstein condensate in an atomic vapor [1–3] have opened the era of experimental studies of ultracold gases with non-negligible or even strong interactions and in dimension lower than or equal to three [4–8]. In these systems, the thermal de Broglie wavelength and the typical distance between atoms are much larger than the range of the interaction potential. This so-called *zero-range* regime has interesting universal properties: Several quantities such as the thermodynamic functions of the gas depend on the interaction potential only through the scattering length a, a length that can be defined in any dimension and that characterizes the low-energy scattering amplitude of two atoms.

This universality property holds for the weakly repulsive Bose gas in three dimensions [9] up to the order of expansion in $(na^3)^{1/2}$ corresponding to Bogoliubov theory [10,11], with n being the gas density. It also holds for the weakly repulsive Bose gas in two dimensions [12–15], even at the next order beyond Bogoliubov theory [16]. For a much larger than the range of the interaction potential, the ground state of N bosons in two dimensions is a universal N-body bound state [17–21]. In one dimension, the universality holds for any scattering length, as exemplified by the fact that the Bose gas with zero-range interaction is exactly solvable by the Bethe ansatz both in the repulsive case [22] and in the attractive case [23–25].

For spin 1/2 fermions, the universality properties are expected to be even stronger. The weakly interacting regimes in three dimensions (3D) [26–31] and in two dimensions (2D) [32] are universal, as well as for any scattering length in the Bethe-ansatz-solvable one-dimensional (1D) case [33,34]. Universality is also expected to hold for an arbitrary scattering length even in 3D, as was recently tested by experimental studies on the BEC-BCS crossover using a Feshbach resonance (see Ref. [8], references therein, and, e.g., Refs. [35–52]) and in agreement with unbiased quantum Monte Carlo calculations [53–59]; and in 2D, a similar universal crossover from BEC to BCS is expected when the parameter $\ln(k_F a)$ [where k_F is the Fermi momentum] varies from $-\infty$ to $+\infty$ [60–67]. Mathematically, results on universality were obtained for the N-body problem in 2D [68]. In 3D, mathematical results were obtained for the three-body problem (see, e.g., Refs. [69–73]). The universality for the fermionic equal-mass N-body problem in 3D remains mathematically unproven.[1]

[1]The proof given in Ref. [68] that, for a sufficiently large number of equal-mass fermions, the energy is unbounded from below is actually

Universality is also expected for mixtures in 2D [64,77,78], and in 3D for Fermi-Fermi mixtures below a critical mass ratio [76,77,79,80]. Above a critical mass ratio, the Efimov effect takes place, as it also takes place for bosons [81,82]. In this case, the three-body problem depends on a single additional parameter: the three-body parameter. The Efimov physics is presently under active experimental investigation [83–89]. It is not the subject of this paper (see Ref. [90]).

In the zero-range regime, it is intuitive that the short-range or high-momentum properties of the gas are dominated by two-body physics. For example, the pair distribution function $g^{(2)}(\mathbf{r}_{12})$ of particles at distances r_{12} much smaller than the de Broglie wavelength is expected to be proportional to the modulus squared of the zero-energy two-body scattering-state wave function $\phi(\mathbf{r}_{12})$, with a proportionality factor Λ_g depending on the many-body state of the gas. Similarly, the tail of the momentum distribution $n(\mathbf{k})$, at wave vectors much larger than the inverse de Broglie wavelength is expected to be proportional to the modulus squared of the Fourier component $\tilde{\phi}(\mathbf{k})$ of the zero-energy scattering-state wave function, with a proportionality factor Λ_n depending on the many-body state of the gas: Whereas two colliding atoms in the gas have a center of mass wave vector of the order of the inverse de Broglie wavelength, their relative wave vector can access much larger values, up to the inverse of the interaction range, simply because the interaction potential has a width in the space of relative momenta of the order of the inverse of its range in real space.

For these intuitive reasons, and with the notable exception of one-dimensional systems, one expects that the mean interaction energy E_{int} of the gas, being sensitive to the shape of $g^{(2)}$ at distances on the order of the interaction range, is not universal but diverges in the zero-range limit; one also expects that, apart from the 1D case, the mean kinetic energy, being dominated by the tail of the momentum distribution, is not universal and diverges in the zero-range limit, a well-known fact in the context of Bogoliubov theory for Bose gases and of BCS theory for Fermi gases. Since the total energy of the gas is universal, and E_{int} is proportional to Λ_g while E_{kin} is proportional to Λ_n, one expects that there exists a simple relation between Λ_g and Λ_n.

The precise link between the pair distribution function, the tail of the momentum distribution, and the energy of the gas was first established for one-dimensional systems. In Ref. [22] the value of the pair distribution function for $r_{12} = 0$ was expressed in terms of the derivative of the gas energy with respect to the one-dimensional scattering length, thanks to the Hellmann-Feynman theorem. In Ref. [91] the tail of $n(k)$ was also related to this derivative of the energy, by using a simple and general property of the Fourier transform of a function having discontinuous derivatives in isolated points.

In three dimensions, results in these directions were first obtained for weakly interacting gases. For the weakly interacting Bose gas, Bogoliubov theory contains the expected properties, in particular on the short-distance behavior of the pair distribution function [92–94] and the fact that the momentum distribution has a slowly decreasing tail. For the weakly interacting spin-1/2 Fermi gas, it was shown that the BCS anomalous average (or pairing field) $\langle\hat{\psi}_\uparrow(\mathbf{r}_1)\hat{\psi}_\downarrow(\mathbf{r}_2)\rangle$ behaves at short distances as the zero-energy two-body scattering wave function $\phi(\mathbf{r}_{12})$ [95], resulting in a $g^{(2)}$ function indeed proportional to $|\phi(\mathbf{r}_{12})|^2$ at short distances. It was however understood later that the corresponding proportionality factor Λ_g predicted by BCS theory is incorrect [96]; for example, at zero temperature the BCS prediction drops exponentially with $1/a$ in the noninteracting limit $a \to 0^-$, whereas the correct result drops as a power law in a.

More recently, in a series of two articles [97,98], explicit expressions for the proportionality factors Λ_g and Λ_n were obtained in terms of the derivative of the gas energy with respect to the inverse scattering length for a spin-1/2 interacting Fermi gas in three dimensions and for an arbitrary value of the scattering length; that is, not restricted to the weakly interacting limit. Later on, these results were rederived in Ref. [99–101], and also in Ref. [102] with very elementary methods building on the aforementioned intuition that $g^{(2)}(\mathbf{r}_{12}) \propto |\phi(\mathbf{r}_{12})|^2$ at short distances and $n(\mathbf{k}) \propto |\tilde{\phi}(\mathbf{k})|^2$ at large momenta. These relations were tested by numerical four-body calculations [103]. An explicit relation between Λ_g and the interaction energy was derived in Ref. [101]. Another fundamental relation discovered in Ref. [97] and recently generalized in Refs. [104,105] to fermions in 2D expresses the total energy as a functional of the momentum distribution and the spatial density.

II. CONTENTS

Here we derive generalizations of the relations of Refs. [22, 91,97,98,101,104,105] to two-dimensional gases and to the case of a small but nonzero interaction range (both on a lattice and in continuous space). We also obtain results for the first-order derivative of the energy with respect to the effective range, as well as for the second-order derivative with respect to the scattering length. We shall also include rederivations of known relations using our elementary methods. We treat in detail the case of spin-1/2 fermions, with equal masses in the two spin states, both in three dimensions and in two dimensions. The discussion of spinless bosons and arbitrary mixtures is deferred to another article, because it may involve the Efimov effect in three dimensions [106].

This article is organized as follows: Models, notations and some basic properties are introduced in Sec. III. Relations for zero-range interactions are summarized in Table II and derived for pure states in Sec. IV. We then consider lattice models (Table III and Sec. V) and finite-range models in continuous space (Table IV and Sec. VI). In Sec. VII we derive a

incorrect, since the fermionic antisymmetry was not properly taken into account. A theorem was published without proof in Ref. [74] implying that the spectrum of the Hamiltonian of $N_\uparrow$ same-spin-state fermions of mass $m_\uparrow$ interacting with a distinguishable particle of mass $m_\downarrow$ is unbounded below, not only for $m_\uparrow = m_\downarrow$ and large enough $N_\uparrow$, but also for $N_\uparrow = 3$ and $m_\uparrow/m_\downarrow$ larger than the critical mass ratio $5.29\ldots$. No proof was found yet for this theorem; it was only proven that no Efimov effect occurs for $N_\uparrow = 3$, $N_\downarrow = 1$ provided $m_\uparrow/m_\downarrow$ is sufficiently small [75]. It was recently shown that a four-body Efimov effect occurs in this $(3+1)$-body problem (for an angular momentum $l = 1$ and not for any other $l \leqslant 10$) and makes the spectrum unbounded below; however, for a widely different critical mass ratio $m_\uparrow/m_\downarrow \simeq 13.384$ [76], which sheds some doubts on Ref. [74].

TABLE I. Notation for the regular part A of the N-body wave function appearing in the contact conditions [first line, with $\mathbf{R}_{ij} = (\mathbf{r}_i + \mathbf{r}_j)/2$ fixed], for the scalar product between such regular parts (second line) and for corresponding matrix elements of operators $\mathcal{H}_{ij}$ acting on $\mathbf{R}_{ij}$ and on the $\mathbf{r}_k$, $k \neq i, j$ (third line).

Three dimensions		Two dimensions	
$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) \underset{r_{ij}\to 0}{=} \left(\frac{1}{r_{ij}} - \frac{1}{a}\right) A_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}) + O(r_{ij})$	(1a)	$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) \underset{r_{ij}\to 0}{=} \ln(r_{ij}/a) A_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}) + O(r_{ij})$	(1b)
$(A^{(1)},A^{(2)}) \equiv \sum_{i<j} \int \left(\prod_{k\neq i,j} d^d r_k\right) d^d R_{ij}\, A_{ij}^{(1)*}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}) A_{ij}^{(2)}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j})$			(2)
$(A^{(1)},\mathcal{H}A^{(2)}) \equiv \sum_{i<j} \int \left(\prod_{k\neq i,j} d^d r_k\right) d^d R_{ij}\, A_{ij}^{(1)*}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}) \mathcal{H}_{ij} A_{ij}^{(2)}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j})$			(3)

model-independent expression for the correction to the energy due to a finite range or a finite effective range of the interaction, and we relate this energy correction to the subleading short-distance behavior of the pair distribution function and to the coefficient of the $1/k^6$ subleading tail of the momentum distribution (see Table V). The case of general statistical mixtures of pure states or of stationary states is discussed in Sec. VIII, and the case of thermodynamic equilibrium states in Sec. IX. Finally, we present applications of the general relations: For two particles and three particles in harmonic traps we compute corrections to exactly solvable cases (Secs. X A and X B). For the unitary gas trapped in an isotropic harmonic potential, we determine how the equidistance between levels within a given energy ladder [resulting from the SO(2,1) dynamical symmetry] is affected by finite $1/a$ and finite-range corrections, which leads to a frequency shift and a collapse of the breathing mode of the zero-temperature gas (Sec. X C). For the bulk unitary gas, we check that general relations are satisfied by existing fixed-node Monte Carlo data [107–109] for correlation functions of the unitary gas (Sec. X D). We quantify the finite-range corrections to the unitary gas energy in typical experiments, which is required for precise measurements of its equation of state (Sec. X E). We conclude in Sec. XI.

III. MODELS, NOTATIONS, AND BASIC PROPERTIES

We now introduce the three models used in this work to account for interparticle interactions and associated notations, together with some basic properties to be used in some of the derivations.

For a fixed number N_σ of fermions in each spin state $\sigma = \uparrow,\downarrow$, one can consider that particles $1,\ldots,N_\uparrow$ have a spin $\uparrow$ and particles $N_\uparrow + 1,\ldots,N_\uparrow + N_\downarrow = N$ have a spin $\downarrow$, so that the wave function $\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ (normalized to unity) changes sign when one exchanges the positions of two particles having the same spin.[2]

A. Zero-range model

In this well-known model (see, e.g., [81,82,110–115] and references therein) the interaction potential is replaced by boundary conditions on the N-body wave function: For any pair of particles $i \neq j$, there exists a function A_{ij}, hereafter called the regular part of ψ, such that Table I, Eq. (1a) holds in the 3D case and Table I, Eq. (1b) holds in the 2D case, where the limit of vanishing distance r_{ij} between particles i and j is taken for a fixed position of their center of mass $\mathbf{R}_{ij} = (\mathbf{r}_i + \mathbf{r}_j)/2$ and fixed positions of the remaining particles $(\mathbf{r}_k)_{k\neq i,j}$ different from $\mathbf{R}_{ij}$. Fermionic symmetry of course imposes $A_{ij} = 0$ if particles i and j have the same spin. When none of the $\mathbf{r}_i$'s coincide, there is no interaction potential and Schrödinger's equation reads $H\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) = E\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ with $H = -\frac{\hbar^2}{2m}\sum_{i=1}^N \Delta_{\mathbf{r}_i} + H_{\text{trap}}$, where m is the atomic mass and the trapping potential energy is

$$H_{\text{trap}} \equiv \sum_{i=1}^N U(\mathbf{r}_i), \tag{1}$$

U being an external trapping potential. The crucial difference between the Hamiltonian H and the noninteracting Hamiltonian is the boundary condition Table I, Eqs. (1a) and (1b).

B. Lattice models

These models are used for quantum Monte Carlo calculations [53–56,58,116]. They can also be convenient for analytics, as used in Refs. [15,16,102,117] and in this work. Particles live on a lattice; that is, the coordinates are integer multiples of the lattice spacing b. The Hamiltonian is

$$H = H_{\text{kin}} + H_{\text{int}} + H_{\text{trap}}, \tag{2}$$

with, in first quantization, the kinetic energy

$$H_{\text{kin}} = -\frac{\hbar^2}{2m}\sum_{i=1}^N \Delta_{\mathbf{r}_i}, \tag{3}$$

the interaction energy

$$H_{\text{int}} = g_0 \sum_{i<j} \delta_{\mathbf{r}_i,\mathbf{r}_j} b^{-d}, \tag{4}$$

and the trapping potential energy defined by (1); namely, in second quantization,

$$H_{\text{kin}} = \sum_\sigma \int_D \frac{d^d k}{(2\pi)^d} \epsilon_{\mathbf{k}} c_\sigma^\dagger(\mathbf{k}) c_\sigma(\mathbf{k}), \tag{5}$$

$$H_{\text{int}} = g_0 \sum_{\mathbf{r}} b^d (\psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\downarrow \psi_\uparrow)(\mathbf{r}), \tag{6}$$

$$H_{\text{trap}} = \sum_{\mathbf{r},\sigma} b^d U(\mathbf{r}) (\psi_\sigma^\dagger \psi_\sigma)(\mathbf{r}). \tag{7}$$

[2]The corresponding state vector is $|\Psi\rangle = [N!/(N_\uparrow! N_\downarrow!)]^{1/2} \hat{A}(|\uparrow,\ldots,\uparrow,\downarrow,\ldots,\downarrow\rangle \otimes |\psi\rangle)$ where there are $N_\uparrow$ spins $\uparrow$ and $N_\downarrow$ spins $\downarrow$, and the operator $\hat{A}$ antisymmetrizes with respect to all particles. The wave function $\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is then proportional to $(\langle\uparrow,\ldots,\uparrow,\downarrow,\ldots,\downarrow| \otimes \langle \mathbf{r}_1,\ldots,\mathbf{r}_N|)|\Psi\rangle$, with the proportionality factor $[N!/(N_\uparrow! N_\downarrow!)]^{1/2}$.

Here d is the spatial dimension, $\epsilon_{\mathbf{k}}$ is the dispersion relation, and $\hat{\psi}$ obeys discrete anticommutation relations $\{\hat{\psi}_\sigma(\mathbf{r}),\hat{\psi}^\dagger_{\sigma'}(\mathbf{r}')\} = b^{-d}\delta_{\mathbf{r}\mathbf{r}'}\delta_{\sigma\sigma'}$. The operator $c^\dagger_\sigma(\mathbf{k})$ creates a particle in the plane wave state $|\mathbf{k}\rangle$ defined by $\langle\mathbf{r}|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}$ for any $\mathbf{k}$ belonging to the first Brillouin zone $D = (-\frac{\pi}{b},\frac{\pi}{b}]^d$. The corresponding anticommutation relations are $\{c_\sigma(\mathbf{k}),c^\dagger_{\sigma'}(\mathbf{k}')\} = (2\pi)^d\delta_{\sigma\sigma'}\delta(\mathbf{k}-\mathbf{k}')$ if $\mathbf{k}$ and $\mathbf{k}'$ are both in the first Brillouin zone.[3] The operator Δ in Eq. (3) is the lattice version of the Laplacian defined by $-\frac{\hbar^2}{2m}\langle\mathbf{r}|\Delta_{\mathbf{r}}|\mathbf{k}\rangle \equiv \epsilon_{\mathbf{k}}\langle\mathbf{r}|\mathbf{k}\rangle$. The simplest choice for the dispersion relation is $\epsilon_{\mathbf{k}} = \hbar^2k^2/(2m)$ [15,16,55,58,117]. Another choice, used in Refs. [54,116], is the dispersion relation of the Hubbard model: $\epsilon_{\mathbf{k}} = \frac{\hbar^2}{mb^2}\sum_{i=1}^d[1-\cos(k_ib)]$. More generally, what follows applies to any $\epsilon_{\mathbf{k}}$ such that $\epsilon_{\mathbf{k}} \underset{b\to0}{\to} \hbar^2k^2/(2m)$ sufficiently rapidly and $\epsilon_{-\mathbf{k}} = \epsilon_{\mathbf{k}}$.

A key quantity is the zero-energy scattering state $\phi(\mathbf{r})$, defined by the two-body Schrödinger equation (with the center of mass at rest):

$$\left(-\frac{\hbar^2}{m}\Delta_{\mathbf{r}} + g_0\frac{\delta_{\mathbf{r},\mathbf{0}}}{b^d}\right)\phi(\mathbf{r}) = 0 \tag{8}$$

and by the normalization conditions

$$\phi(\mathbf{r}) \underset{r\gg b}{\simeq} \frac{1}{r} - \frac{1}{a} \text{ in 3D}, \tag{9}$$

$$\phi(\mathbf{r}) \underset{r\gg b}{\simeq} \ln(r/a) \text{ in 2D}. \tag{10}$$

A two-body analysis, detailed in Appendix A, yields the relation between the scattering length and the bare coupling constant g_0, in three and two dimensions:

$$\frac{1}{g_0} \overset{\text{3D}}{=} \frac{m}{4\pi\hbar^2a} - \int_D\frac{d^3k}{(2\pi)^3}\frac{1}{2\epsilon_{\mathbf{k}}}, \tag{11}$$

$$\frac{1}{g_0} \overset{\text{2D}}{=} \lim_{q\to0}\left[-\frac{m}{2\pi\hbar^2}\ln\left(\frac{aqe^\gamma}{2}\right) + \int_D\frac{d^2k}{(2\pi)^2}\mathrm{P}\frac{1}{2(\epsilon_{\mathbf{q}}-\epsilon_{\mathbf{k}})}\right], \tag{12}$$

where $\gamma = 0.577\,216\ldots$ is Euler's constant and P is the principal value. This implies that (for constant b):

$$\frac{d\,(1/g_0)}{d\,(1/a)} = \frac{m}{4\pi\hbar^2} \text{ in 3D}, \tag{13}$$

$$\frac{d\,(1/g_0)}{d\,(\ln a)} = -\frac{m}{2\pi\hbar^2} \text{ in 2D}. \tag{14}$$

Another useful property derived in Appendix A is

$$\phi\,(\mathbf{0}) = -\frac{4\pi\hbar^2}{mg_0} \text{ in 3D}, \tag{15}$$

$$\phi\,(\mathbf{0}) = \frac{2\pi\hbar^2}{mg_0} \text{ in 2D}, \tag{16}$$

which, together with Eqs. (13) and (14), gives

$$|\phi\,(\mathbf{0})\,|^2 = \frac{4\pi\hbar^2}{m}\frac{d\,(-1/a)}{dg_0} \text{ in 3D}, \tag{17}$$

$$|\phi\,(\mathbf{0})\,|^2 = \frac{2\pi\hbar^2}{m}\frac{d\,(\ln a)}{dg_0} \text{ in 2D}. \tag{18}$$

[3]Otherwise $\delta(\mathbf{k}-\mathbf{k}')$ has to be replaced by the periodic version $\sum_{\mathbf{K}\in(2\pi/b)\mathbb{Z}^d}\delta(\mathbf{k}-\mathbf{k}'-\mathbf{K})$.

In the zero-range limit ($b\to0$ with g_0 adjusted in such a way that a remains constant), it is expected that the spectrum of the lattice model converges to the one of the zero-range model, as explicitly checked for three particles in Ref. [117], and that any eigenfunction $\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ of the lattice model tends to the corresponding eigenfunction of the zero-range model provided all interparticle distances remain much larger than b. For any stationary state, let us denote by $1/k_{\text{typ}}$ the typical length-scale on which the zero-range model's wave function varies; for example, for the lowest eigenstates, this is on the order of the mean interparticle distance, or on the order of a in the regime where a is small and positive and dimers are formed. The zero-range limit is then reached if $k_{\text{typ}}b \ll 1$. This notion of typical wave vector k_{typ} can also be applied to the case of a thermal equilibrium state, since most significantly populated eigenstates then have a k_{typ} on the same order; it is then expected that the thermodynamic potentials converge to the ones of the zero-range model when $b\to0$, and that this limit is reached provided $k_{\text{typ}}b \ll 1$. For the homogeneous gas, defining a thermal wave vector k_T by $\hbar^2k_T^2/(2m) = k_BT$, we have $k_{\text{typ}} \sim \max(k_F,k_T)$ for $a<0$ and $k_{\text{typ}} \sim \max(k_F,k_T,1/a)$ for $a>0$.

For lattice models, it will prove convenient to define the regular part A by

$$\begin{aligned}\psi(\mathbf{r}_1,\ldots,\mathbf{r}_i=\mathbf{R}_{ij},\ldots,\mathbf{r}_j=\mathbf{R}_{ij},\ldots,\mathbf{r}_N)\\ = \phi(\mathbf{0})A_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}).\end{aligned} \tag{19}$$

In the zero-range regime $k_{\text{typ}}b \ll 1$, when the distance r_{ij} between two particles of opposite spin is $\ll 1/k_{\text{typ}}$ while all the other interparticle distances are much larger than b and than r_{ij}, the many-body wave function is proportional to $\phi(\mathbf{r}_j-\mathbf{r}_i)$, with a proportionality constant given by (19):

$$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) \simeq \phi(\mathbf{r}_j-\mathbf{r}_i)A_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}), \tag{20}$$

where $\mathbf{R}_{ij} = (\mathbf{r}_i+\mathbf{r}_j)/2$. If, moreover, $r_{ij} \gg b$, ϕ can be replaced by its asymptotic form [Eqs. (9) and (10)]. Since the contact conditions [Table I, Eqs. (1a) and (1b)] of the zero-range model must be recovered, we see that the lattice model's regular part tends to the zero-range model's regular part in the zero-range limit.

C. Finite-range continuous-space models

Such models are used in numerical few-body correlated Gaussian and many-body fixed-node Monte Carlo calculations (see, e.g., Refs. [5,65,103,107,118–120] and references therein). They are also relevant to neutron matter [121]. The Hamiltonian reads

$$H = H_0 + \sum_{i=1}^{N_\uparrow}\sum_{j=N_\uparrow+1}^{N} V(r_{ij}), \tag{21}$$

with H_0 being defined by Eq. (3) where $\Delta_{\mathbf{r}_i}$ now stands for the usual Laplacian, and $V(r)$ is an interaction potential between particles of opposite spin, which vanishes for $r>b$ or at least decays quickly enough for $r\gg b$. The two-body zero-energy scattering state $\phi(r)$ is again defined by the Schrödinger equation $-(\hbar^2/m)\Delta_{\mathbf{r}}\phi + V(r)\phi = 0$ and the boundary condition (9) or (10). The zero-range regime is again reached for $k_{\text{typ}}b \ll 1$ with k_{typ} the typical relative wave

TABLE II. Relations for spin-1/2 fermions with zero-range interactions. The definition (1) of C, as well as the relations in lines 3, 5, 6, and 7, concern any (nonpathological) statistical mixture of states which satisfy the contact conditions [Table I, line 1] (with real wave functions for line 7). Line 2 holds for any pure state; here A is the regular part of the wave function appearing in the contact condition, and (A,A) is its squared norm (defined in Table I). Lines 4 and 8 hold for any stationary state. Lines 9–11 hold at thermal equilibrium in the canonical ensemble. Line 12 holds for any time dependence of scattering length and trapping potential and any corresponding time-dependent statistical mixture. Many of the 3D relations were originally obtained in Refs. [97,98] (see text), while the 2D relation (5b) was obtained in Ref. [105] for the homogeneous system and in Ref. [104] (in a different form) for the general case.

Three dimensions		Two dimensions	
$C \equiv \lim_{k\to+\infty} k^4 n_\sigma(\mathbf{k})$	(1)		
$C = (4\pi)^2\,(A,A)$	(2a)	$C = (2\pi)^2 (A,A)$	(2b)
$\int d^3R\, g^{(2)}_{\uparrow\downarrow}\left(\mathbf{R}+\frac{\mathbf{r}}{2},\mathbf{R}-\frac{\mathbf{r}}{2}\right) \underset{r\to 0}{\sim} \frac{C}{(4\pi)^2}\frac{1}{r^2}$	(3a)	$\int d^2R\, g^{(2)}_{\uparrow\downarrow}\left(\mathbf{R}+\frac{\mathbf{r}}{2},\mathbf{R}-\frac{\mathbf{r}}{2}\right) \underset{r\to 0}{\sim} \frac{C}{(2\pi)^2}\ln^2 r$	(3b)
$\frac{dE}{d(-1/a)} = \frac{\hbar^2 C}{4\pi m}$	(4a)	$\frac{dE}{d(\ln a)} = \frac{\hbar^2 C}{2\pi m}$	(4b)
$E - E_{\rm trap} = \frac{\hbar^2 C}{4\pi m a} + \sum_\sigma \int \frac{d^3k}{(2\pi)^3}\frac{\hbar^2 k^2}{2m}\left[n_\sigma(\mathbf{k}) - \frac{C}{k^4}\right]$	(5a)	$E - E_{\rm trap} = \lim_{\Lambda\to\infty}\left[-\frac{\hbar^2 C}{2\pi m}\ln\left(\frac{a\Lambda e^\gamma}{2}\right) + \sum_\sigma \int_{k<\Lambda}\frac{d^2k}{(2\pi)^2}\frac{\hbar^2k^2}{2m} n_\sigma(\mathbf{k})\right]$	(5b)
$\int d^3R\, g^{(1)}_{\sigma\sigma}\left(\mathbf{R}+\frac{\mathbf{r}}{2},\mathbf{R}-\frac{\mathbf{r}}{2}\right) \underset{r\to 0}{=} N_\sigma - \frac{C}{8\pi}r + O(r^2)$	(6a)	$\int d^2R\, g^{(1)}_{\sigma\sigma}\left(\mathbf{R}+\frac{\mathbf{r}}{2},\mathbf{R}-\frac{\mathbf{r}}{2}\right) \underset{r\to 0}{=} N_\sigma + \frac{C}{4\pi}r^2\ln r + O(r^2)$	(6b)
$\frac{1}{3}\sum_{i=1}^3\sum_\sigma \int d^3R\, g^{(1)}_{\sigma\sigma}\left(\mathbf{R}+\frac{r\mathbf{u_i}}{2},\mathbf{R}-\frac{r\mathbf{u_i}}{2}\right)$ $\underset{r\to 0}{=} N - \frac{C}{4\pi}r - \frac{m}{3\hbar^2}\left(E - E_{\rm trap} - \frac{\hbar^2 C}{4\pi m a}\right)r^2 + o(r^2)$	(7a)	$\frac{1}{2}\sum_{i=1}^2\sum_\sigma \int d^2R\, g^{(1)}_{\sigma\sigma}\left(\mathbf{R}+\frac{r\mathbf{u_i}}{2},\mathbf{R}-\frac{r\mathbf{u_i}}{2}\right)$ $\underset{r\to 0}{=} N + \frac{C}{4\pi}r^2\left[\ln\left(\frac{r}{a}\right) - 1\right] - \frac{m}{2\hbar^2}\left(E - E_{\rm trap}\right)r^2 + o(r^2)$	(7b)
$\frac{1}{2}\frac{d^2E_n}{d(-1/a)^2} = \left(\frac{4\pi\hbar^2}{m}\right)^2 \sum_{n',E_{n'}\neq E_n}\frac{\lvert\langle A^{(n')},A^{(n)}\rangle\rvert^2}{E_n - E_{n'}}$	(8a)	$\frac{1}{2}\frac{d^2E_n}{d(\ln a)^2} = \left(\frac{2\pi\hbar^2}{m}\right)^2 \sum_{n',E_{n'}\neq E_n}\frac{\lvert\langle A^{(n')},A^{(n)}\rangle\rvert^2}{E_n - E_{n'}}$	(8b)
$\left(\frac{d\bar{E}}{d(-1/a)}\right)_S = \left(\frac{dF}{d(-1/a)}\right)_T = \frac{\hbar^2 C}{4\pi m}$	(9a)	$\left(\frac{d\bar{E}}{d(\ln a)}\right)_S = \left(\frac{dF}{d(\ln a)}\right)_T = \frac{\hbar^2 C}{2\pi m}$	(9b)
$\left(\frac{d^2F}{d(-1/a)^2}\right)_T < 0$	(10a)	$\left(\frac{d^2F}{d(\ln a)^2}\right)_T < 0$	(10b)
$\left(\frac{d^2\bar{E}}{d(-1/a)^2}\right)_S < 0$	(11a)	$\left(\frac{d^2\bar{E}}{d(\ln a)^2}\right)_S < 0$	(11b)
$\frac{dE}{dt} = \frac{\hbar^2 C}{4\pi m}\frac{d(-1/a)}{dt} + \left\langle\frac{dH_{\rm trap}}{dt}\right\rangle$	(12a)	$\frac{dE}{dt} = \frac{\hbar^2 C}{2\pi m}\frac{d(\ln a)}{dt} + \left\langle\frac{dH_{\rm trap}}{dt}\right\rangle$	(12b)

vector.[4] Equation (20) again holds in the zero-range regime, where A now simply stands for the zero-range model's regular part.

IV. RELATIONS IN THE ZERO-RANGE LIMIT

We now derive relations for the zero-range model. For some of the derivations we will use a lattice model and then take the zero-range limit. We recall that we derive all relations for pure states in this section, the generalization to statistical mixtures and the discussion of thermal equilibrium being deferred to Secs. VIII and IX.

A. Tail of momentum distribution

In this subsection as well as in the following subsections IV B, IV D, IV E, and IV G, we consider a many-body pure state whose wave function ψ satisfies the contact condition [Table I, Eqs. (1a) and (1b)]. We now show that the momentum distribution $n_\sigma(\mathbf{k})$ has a σ-independent tail proportional to $1/k^4$, with a coefficient denoted by C [Table II, Eq. (1)]. C is usually referred to as the "contact". We shall also show that C is related by Table II, Eqs. (2a) and (2b) to the norm of the regular part A of the wave function (defined in Table I). In 3D these results were obtained in [98].[5] Here, the momentum distribution is defined in second quantization by $n_\sigma(\mathbf{k}) = \langle\hat{n}_\sigma(\mathbf{k})\rangle = \langle c^\dagger_\sigma(\mathbf{k})c_\sigma(\mathbf{k})\rangle$ where $c_\sigma(\mathbf{k})$ annihilates a particle of spin σ in the plane-wave state $|\mathbf{k}\rangle$ defined by $\langle\mathbf{r}|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}$; this corresponds to the normalization

$$\int \frac{d^dk}{(2\pi)^d} n_\sigma(\mathbf{k}) = N_\sigma. \tag{22}$$

In first quantization,

$$n_\sigma(\mathbf{k}) = \sum_{i:\sigma}\int\left(\prod_{l\neq i} d^dr_l\right)\left|\int d^dr_i e^{-i\mathbf{k}\cdot\mathbf{r}_i}\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)\right|^2, \tag{23}$$

where the sum is taken over all particles of spin σ: i runs from 1 to $N_\uparrow$ for $\sigma = \uparrow$, and from $N_\uparrow + 1$ to N for $\sigma = \downarrow$.

Three dimensions. The key point is that, in the large-k limit, the Fourier transform with respect to $\mathbf{r}_i$ is dominated by the contribution of the short-distance divergence coming from the contact condition [Table I, Eq. (1a)]:

$$\int d^3r_i e^{-i\mathbf{k}\cdot\mathbf{r}_i}\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) \underset{k\to\infty}{\simeq} \int d^3r_i e^{-i\mathbf{k}\cdot\mathbf{r}_i}\sum_{j,j\neq i}\frac{1}{r_{ij}}A_{ij}(\mathbf{r}_j,(\mathbf{r}_l)_{l\neq i,j}). \tag{24}$$

[4] For purely attractive interaction potentials such as the square-well potential, above a critical particle number, the ground state is a collapsed state and the zero-range regime can only be reached for certain excited states (see, e.g., [122] and references therein).

[5] The existence of the $1/k^4$ tail had already been observed within a self-consistent approximate theory [123].

A similar link between the short-distance singularity of the wave function and the tail of its Fourier transform was used to derive exact relations in 1D in Ref. [91]. From $\Delta(1/r) = -4\pi\delta(\mathbf{r})$, we have $\int d^3r e^{-i\mathbf{k}\cdot\mathbf{r}}\frac{1}{r} = \frac{4\pi}{k^2}$, so that

$$\int d^3r_i e^{-i\mathbf{k}\cdot\mathbf{r}_i}\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) \underset{k\to\infty}{\simeq} \frac{4\pi}{k^2}\sum_{j,j\neq i} e^{-i\mathbf{k}\cdot\mathbf{r}_j} A_{ij}(\mathbf{r}_j,(\mathbf{r}_l)_{l\neq i,j}). \quad (25)$$

One inserts this into (23) and expands the modulus squared. After spatial integration over all the $\mathbf{r}_l, l\neq i$, the crossed terms rapidly vanish in the large-k limit, as they are the product of $e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_{j'})}$ and of regular functions of $\mathbf{r}_j$ and $\mathbf{r}_{j'}$.[6] This yields $n_\sigma(\mathbf{k}) \underset{k\to\infty}{\sim} C/k^4$, with the expression Table II, Eq. (2a) of C in terms of the norm (A,A) defined in Table I, Eq. (2).

Two dimensions. The 2D contact condition [Table I, Eq. (1b)] now gives

$$\int d^2r_i e^{-i\mathbf{k}\cdot\mathbf{r}_i}\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) \underset{k\to\infty}{\simeq} \int d^2r_i e^{-i\mathbf{k}\cdot\mathbf{r}_i}\sum_{j,j\neq i}\ln(r_{ij})A_{ij}(\mathbf{r}_j,(\mathbf{r}_l)_{l\neq i,j}). \quad (26)$$

From $\Delta(\ln r) = 2\pi\delta(\mathbf{r})$, one has $\int d^2r e^{-i\mathbf{k}\cdot\mathbf{r}}\ln r = -2\pi/k^2$ and

$$\int d^2r_i e^{-i\mathbf{k}\cdot\mathbf{r}_i}\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) \underset{k\to\infty}{\simeq} -\frac{2\pi}{k^2}\sum_{j,j\neq i} e^{-i\mathbf{k}\cdot\mathbf{r}_j} A_{ij}(\mathbf{r}_j,(\mathbf{r}_l)_{l\neq i,j}). \quad (27)$$

As in 3D this leads to Table II, Eq. (2b).

B. Pair distribution function at short distances

The pair distribution function gives the probability density of finding a spin-↑ particle at $\mathbf{r}_\uparrow$ and a spin-↓ particle at $\mathbf{r}_\downarrow$:

$$g^{(2)}_{\uparrow\downarrow}(\mathbf{r}_\uparrow,\mathbf{r}_\downarrow) = \langle(\hat\psi^\dagger_\uparrow\hat\psi_\uparrow)(\mathbf{r}_\uparrow)(\hat\psi^\dagger_\downarrow\hat\psi_\downarrow)(\mathbf{r}_\downarrow)\rangle = \int\left(\prod_{k=1}^N d^dr_k\right)|\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)|^2 \times\sum_{i=1}^{N_\uparrow}\sum_{j=N_\uparrow+1}^{N}\delta(\mathbf{r}_\uparrow-\mathbf{r}_i)\delta(\mathbf{r}_\downarrow-\mathbf{r}_j).$$

We set $\mathbf{r}_{\uparrow,\downarrow} = \mathbf{R}\pm\mathbf{r}/2$ and we integrate over $\mathbf{r}_i$ and $\mathbf{r}_j$:

$$g^{(2)}_{\uparrow\downarrow}\left(\mathbf{R}+\frac{\mathbf{r}}{2},\mathbf{R}-\frac{\mathbf{r}}{2}\right) = \sum_{i=1}^{N_\uparrow}\sum_{j=N_\uparrow+1}^{N}\int\left(\prod_{k\neq i,j}d^dr_k\right)\left|\psi\left(\mathbf{r}_1,\ldots,\mathbf{r}_i=\mathbf{R}+\frac{\mathbf{r}}{2},\ldots,\mathbf{r}_j=\mathbf{R}-\frac{\mathbf{r}}{2},\ldots,\mathbf{r}_N\right)\right|^2 \quad (28)$$

Let us define the spatially integrated pair distribution function[7]

$$G^{(2)}_{\uparrow\downarrow}(\mathbf{r}) \equiv \int d^dR\, g^{(2)}_{\uparrow\downarrow}\left(\mathbf{R}+\frac{\mathbf{r}}{2},\mathbf{R}-\frac{\mathbf{r}}{2}\right), \quad (29)$$

whose small-r singular behavior we will show to be related to C via Table II, Eqs. (3a) and (3b).

Three dimensions. Replacing the wave function in Eq. (28) by its asymptotic behavior given by the contact condition [Table I, Eq. (1a)] immediately yields

$$G^{(2)}_{\uparrow\downarrow}(\mathbf{r}) \underset{r\to0}{\sim} \frac{(A,A)}{r^2}. \quad (30)$$

Expressing (A,A) in terms of C through Table II, Eq. (2a) finally gives Table II, Eq. (3a).

In a measurement of all particle positions, the mean total number of pairs of particles of opposite spin which are separated by a distance smaller than s is $N_{\rm pair}(s) = \int_{r<s} d^dr G^{(2)}_{\uparrow\downarrow}(\mathbf{r})$, so that from Table II, Eq. (3a),

$$N_{\rm pair}(s) \underset{s\to0}{\sim} \frac{C}{4\pi}s, \quad (31)$$

as obtained in Refs. [97,98].

Two dimensions. The contact condition [Table I, Eq. (1b)] similarly leads to Table II, Eq. (3b). After integration over the region $r < s$ this gives

$$N_{\rm pair}(s) \underset{s\to0}{\sim} \frac{C}{4\pi}s^2\ln^2 s. \quad (32)$$

C. First order derivative of energy with respect to scattering length

The relations Table II, Eqs. (4a) and (4b) can be derived straightforwardly using the lattice model (see Sec. V E). Here, we derive them by directly using the zero-range model, which is more involved but also instructive.

Three dimensions. Let us consider a wave function ψ_1 satisfying the contact condition [Table I, Eq. (1a)] for a scattering length a_1. We denote by $A^{(1)}_{ij}$ the regular part of ψ_1 appearing in the contact condition [Table I, Eq. (1a)]. Similarly, ψ_2 satisfies the contact condition for a scattering length a_2 and

[6] For example, for $n_\downarrow(\mathbf{k})$ in the trapped three-body case, with particles 1 and 2 in state ↑ and particle 3 in state ↓, one has $i=3$ and $j,j'=1$ or 2. Then the crossed term $A_{31}(\mathbf{r}_1,\mathbf{r}_2)A_{32}(\mathbf{r}_2,\mathbf{r}_1)$ has to all orders finite derivatives with respect to $\mathbf{r}_1$ and $\mathbf{r}_2$, except if $\mathbf{r}_1=\mathbf{r}_2$ where it vanishes as $|\mathbf{r}_1-\mathbf{r}_2|^{2s-2}$, $s>0$ not integer [see, e.g., Eq. (H3) and below that equation]. By a power-counting argument, its Fourier transform with respect to $\mathbf{r}_1-\mathbf{r}_2$ contributes to the momentum distribution tail as $1/k^{2s+5} = o(1/k^4)$; one recovers the "three-close-particle" contribution mentioned in a note of Ref. [98].

[7] For simplicity, we refrain here from expressing C as the integral of a "contact density" $\mathcal{C}(\mathbf{R})$ related to the small-r behavior of the local pair distribution function $g^{(2)}_{\uparrow\downarrow}(\mathbf{R}+\mathbf{r}/2,\mathbf{R}-\mathbf{r}/2)$ as was done for the 3D case in Refs. [97–99]; this $\mathcal{C}(\mathbf{R})$ is then also related to the large-k tail of the Wigner distribution [i.e., the Fourier transform with respect to $\mathbf{r}$ of the one-body density matrix $\langle\psi^\dagger_\sigma(\mathbf{R}-\mathbf{r}/2)\psi_\sigma(\mathbf{R}+\mathbf{r}/2)\rangle$]; see Eq. (30) of Ref. [97].

TABLE III. Relations for spin-1/2 fermions for lattice models. $\hat{C}$ is defined in line 1 and $C = \langle \hat{C} \rangle$. Lines 2, 3, and 8 are relations between operators. Line 4 holds for any pure state [the regular part A being defined in Eq. (19) in the text]. Lines 5 and 6 hold for any stationary state. Line 7 holds at thermal equilibrium in the canonical ensemble. Lines 9 and 10 are expected to hold in the zero-range regime $k_{\rm typ} b \ll 1$, where $k_{\rm typ}$ is the typical wave vector, for any stationary state or at thermal equilibrium.

Three dimensions		Two dimensions	
$\hat{C} \equiv \frac{4\pi m}{\hbar^2} \frac{dH}{d(-1/a)}$	(1a)	$\hat{C} \equiv \frac{2\pi m}{\hbar^2} \frac{dH}{d(\ln a)}$	(1b)
$H_{\rm int} = \frac{\hbar^4}{m^2} \frac{\hat{C}}{g_0}$	(2)		
$H - H_{\rm trap} = \frac{\hbar^2 \hat{C}}{4\pi m a} + \sum_\sigma \int_D \frac{d^3k}{(2\pi)^3} \epsilon_{\mathbf{k}} \left[\hat{n}_\sigma(\mathbf{k}) - \hat{C} \left(\frac{\hbar^2}{2m\epsilon_{\mathbf{k}}} \right)^2 \right]$	(3a)	$H - H_{\rm trap} = \lim_{q \to 0} \left\{ -\frac{\hbar^2 \hat{C}}{2\pi m} \ln \left(\frac{aqe^\gamma}{2} \right) + \sum_\sigma \int_D \frac{d^2k}{(2\pi)^2} \epsilon_{\mathbf{k}} \left[\hat{n}_\sigma(\mathbf{k}) - \hat{C} \frac{\hbar^2}{2m\epsilon_{\mathbf{k}}} \mathrm{P} \frac{\hbar^2}{2m(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{q}})} \right] \right\}$	(3b)
$C = (4\pi)^2 (A, A)$	(4a)	$C = (2\pi)^2 (A, A)$	(4b)
$\frac{dE}{d(-1/a)} = \frac{\hbar^2 C}{4\pi m}$	(5a)	$\frac{dE}{d(\ln a)} = \frac{\hbar^2 C}{2\pi m}$	(5b)
$\frac{1}{2} \frac{d^2 E_n}{dg_0^2} = \lvert \phi(\mathbf{0}) \rvert^4 \sum_{n', E_{n'} \neq E_n} \frac{\lvert (A^{(n')}, A^{(n)}) \rvert^2}{E_n - E_{n'}}$	(6)		
$\left(\frac{d^2 F}{dg_0^2} \right)_T < 0, \quad \left(\frac{d^2 E}{dg_0^2} \right)_S < 0$	(7)		
$\sum_{\mathbf{R}} b^3 (\psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\downarrow \psi_\uparrow)(\mathbf{R}) = \frac{\hat{C}}{(4\pi)^2} \lvert \phi(\mathbf{0}) \rvert^2$	(8a)	$\sum_{\mathbf{R}} b^2 (\psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\downarrow \psi_\uparrow)(\mathbf{R}) = \frac{\hat{C}}{(2\pi)^2} \lvert \phi(\mathbf{0}) \rvert^2$	(8b)
In the zero-range regime $k_{\rm typ} b \ll 1$			
$\sum_{\mathbf{R}} b^3 g_{\uparrow\downarrow}^{(2)} (\mathbf{R} + \frac{\mathbf{r}}{2}, \mathbf{R} - \frac{\mathbf{r}}{2}) \simeq \frac{C}{(4\pi)^2} \lvert \phi(\mathbf{r}) \rvert^2$ for $r \ll k_{\rm typ}^{-1}$	(9a)	$\sum_{\mathbf{R}} b^2 g_{\uparrow\downarrow}^{(2)} (\mathbf{R} + \frac{\mathbf{r}}{2}, \mathbf{R} - \frac{\mathbf{r}}{2}) \simeq \frac{C}{(2\pi)^2} \lvert \phi(\mathbf{r}) \rvert^2$ for $r \ll k_{\rm typ}^{-1}$	(9b)
$n_\sigma(\mathbf{k}) \simeq C \left(\frac{\hbar^2}{2m\epsilon_{\mathbf{k}}} \right)^2$ for $k \gg k_{\rm typ}$	(10)		

a regular part $A_{ij}^{(2)}$. Then, as shown in Appendix B using the divergence theorem, the following lemma holds:

$$\langle \psi_1, H\psi_2 \rangle - \langle H\psi_1, \psi_2 \rangle = \frac{4\pi\hbar^2}{m} \left(\frac{1}{a_1} - \frac{1}{a_2} \right) (A^{(1)}, A^{(2)}), \tag{33}$$

where the scalar product between regular parts is defined by Table I, Eq. (2). We then apply Eq. (33) to the case where ψ_1 and ψ_2 are N-body stationary states of energy E_1 and E_2. The left-hand side of Eq. (33) then reduces to $(E_2 - E_1)\langle \psi_1 | \psi_2 \rangle$. Taking the limit $a_2 \to a_1$ gives

$$\frac{dE}{d(-1/a)} = \frac{4\pi\hbar^2}{m} (A, A) \tag{34}$$

for any stationary state. Expressing (A, A) in terms of C thanks to Table II, Eq. (2a) finally yields Table II, Eq. (4a). This result as well as Eq. (34) is contained in Ref. [97,98].[8] We recall that here and in what follows, the wave function is normalized: $\langle \psi | \psi \rangle = 1$.

Two dimensions. The 2D version of the lemma (33) is

$$\langle \psi_1, H\psi_2 \rangle - \langle H\psi_1, \psi_2 \rangle = \frac{2\pi\hbar^2}{m} \ln(a_2/a_1)(A^{(1)}, A^{(2)}), \tag{35}$$

as shown in Appendix B. As in 3D, we deduce that

$$\frac{dE}{d(\ln a)} = \frac{2\pi\hbar^2}{m} (A, A), \tag{36}$$

which gives the desired Table II, Eq. (4b) by using Table II, Eq. (2b).

[8] Our derivation is similar to the one given in the two-body case and sketched in the many-body case in Sec. 3 of Ref. [98].

D. Expression of energy in terms of momentum distribution

Three dimensions. As shown in Ref. [97], the mean total energy E minus the mean trapping-potential energy $E_{\rm trap} \equiv \langle H_{\rm trap} \rangle$ has the simple expression in terms of the momentum distribution given in Table II, Eq. (5a) for any pure state $|\psi\rangle$ satisfying the contact condition [Table I, Eq. (1a)]. We give a simple rederivation of this result by using the lattice model (defined in Sec. III B).

We first treat the case where $|\psi\rangle$ is an eigenstate of the zero-range model. Let $|\psi_b\rangle$ be the eigenstate of the lattice model that tends to $|\psi\rangle$ for $b \to 0$. We first note that $C_b \equiv \langle \psi_b | \hat{C} | \psi_b \rangle$, where $\hat{C}$ is defined by Table III, Eqs. (1a) and (1b), tends to the contact C of the state ψ [defined in Table II, Eq. (1)] when $b \to 0$, as shown in Appendix C. Then, the key step is to use Table III, Eq. (3a), which, after taking the expectation value in the state $|\psi_b\rangle$, yields the desired result [Table II, Eq. (5a)] in the zero-range limit since $D \to \mathbb{R}^3$ and $\epsilon_{\mathbf{k}} \to \hbar^2 k^2/(2m)$ for $b \to 0$.

To generalize Table II, Eq. (5a) to any pure state $|\psi\rangle$ satisfying the contact condition Table I, Eq. (1a), we use the state $|\psi_b\rangle$ defined in Sec. 2 of Appendix C. As shown in that Appendix, the expectation value of $\hat{C}$ taken in this state $|\psi_b\rangle$ tends to the contact C of $|\psi\rangle$ defined in Table II, Eq. (1). Moreover, the expectation values of $H - H_{\rm trap}$ and of $\hat{n}_\sigma(\mathbf{k})$, taken in this state $|\psi_b\rangle$, should tend to the corresponding expectation values taken in the state $|\psi\rangle$. This yields the desired relation.

Finally, we mention the equivalent form of the relation Table II, Eq. (5a):

$$E - E_{\rm trap} = \lim_{\Lambda \to \infty} \left[\frac{\hbar^2 C}{4\pi m} \left(\frac{1}{a} - \frac{2\Lambda}{\pi} \right) + \sum_\sigma \int_{k<\Lambda} \frac{d^3k}{(2\pi)^3} \frac{\hbar^2 k^2}{2m} n_\sigma(\mathbf{k}) \right]. \tag{37}$$

Two dimensions. The 2D version of Eq. (37) is Table II, Eq. (5b). This was shown for a homogeneous system in Ref. [105] and in the general case in Ref. [104].[9] This can easily be rewritten in the following forms, which resemble Table II, Eq. (5a):

$$E - E_{\rm trap} = -\frac{\hbar^2 C}{2\pi m}\ln\left(\frac{aqe^{\gamma}}{2}\right) + \sum_{\sigma}\int \frac{d^2k}{(2\pi)^2}\frac{\hbar^2k^2}{2m} \times\left[n_\sigma(\mathbf{k}) - \frac{C}{k^4}\theta(k-q)\right] \text{ for any } q>0, \tag{38}$$

where the Heaviside function θ ensures that the integral converges at small k or, equivalently,

$$E - E_{\rm trap} = -\frac{\hbar^2 C}{2\pi m}\ln\left(\frac{aqe^{\gamma}}{2}\right) + \sum_{\sigma}\int \frac{d^2k}{(2\pi)^2}\frac{\hbar^2k^2}{2m} \times\left[n_\sigma(\mathbf{k}) - \frac{C}{k^2(k^2+q^2)}\right] \text{ for any } q>0. \tag{39}$$

To derive this we again use the lattice model. We note that, if the limit $q\to 0$ is replaced by the limit $b\to 0$ taken for fixed a, Eq. (12) remains true (see Appendix A); repeating the reasoning of Sec. V B then shows that Table III, Eq. (3b) remains true; as in 3D we finally get in the limit $b\to 0$

$$E - E_{\rm trap} = -\frac{\hbar^2 C}{2\pi m}\ln\left(\frac{aqe^{\gamma}}{2}\right) + \sum_{\sigma}\int \frac{d^2k}{(2\pi)^2}\frac{\hbar^2k^2}{2m} \times\left[n_\sigma(\mathbf{k}) - \frac{C}{k^2}\mathrm{P}\frac{1}{k^2-q^2}\right] \tag{40}$$

for any $q>0$; this is easily rewritten as Table II, Eq. (5b).

E. One-body density matrix at short distances

The one-body density matrix is defined as $g^{(1)}_{\sigma\sigma}(\mathbf{r},\mathbf{r}') = \langle\hat\psi^\dagger_\sigma(\mathbf{r})\hat\psi_\sigma(\mathbf{r}')\rangle$ where $\hat\psi_\sigma(\mathbf{r})$ annihilates a particle of spin σ at point $\mathbf{r}$. Its spatially integrated version

$$G^{(1)}_{\sigma\sigma}(\mathbf{r}) \equiv \int d^dR\, g^{(1)}_{\sigma\sigma}\left(\mathbf{R}-\frac{\mathbf{r}}{2},\mathbf{R}+\frac{\mathbf{r}}{2}\right) \tag{41}$$

is a Fourier transform of the momentum distribution:

$$G^{(1)}_{\sigma\sigma}(\mathbf{r}) = \int \frac{d^dk}{(2\pi)^d}e^{i\mathbf{k}\cdot\mathbf{r}}n_\sigma(\mathbf{k}). \tag{42}$$

The expansion of $G^{(1)}_{\sigma\sigma}(\mathbf{r})$ up to first order in r is given by Table II, Eq. (6a) in 3D, as first obtained in Ref. [97], and by Table II, Eq. (6b) in 2D. The expansion can be pushed to second order if one sums over spin and averages over d orthogonal directions of $\mathbf{r}$, see Table II, Eqs. (7a) and (7b), where the $\mathbf{u_i}$'s are an orthonormal basis.[10] Such a second-order expansion was first obtained in 1D in Ref. [91]; the following derivations however differ from the 1D case.[11]

Three dimensions. To derive Table II, Eqs. (6a) and (7a) we rewrite Eq. (42) as

$$G^{(1)}_{\sigma\sigma}(\mathbf{r}) = N_\sigma + \int\frac{d^3k}{(2\pi)^3}(e^{i\mathbf{k}\cdot\mathbf{r}}-1)\frac{C}{k^4} + \int\frac{d^3k}{(2\pi)^3}(e^{i\mathbf{k}\cdot\mathbf{r}}-1)\left(n_\sigma(\mathbf{k})-\frac{C}{k^4}\right). \tag{43}$$

The first integral equals $-(C/8\pi)r$. In the second integral, we use

$$e^{i\mathbf{k}\cdot\mathbf{r}} - 1 \underset{r\to 0}{=} i\mathbf{k}\cdot\mathbf{r} - \frac{(\mathbf{k}\cdot\mathbf{r})^2}{2} + o(r^2). \tag{44}$$

The first term of this expansion gives a contribution to the integral proportional to the total momentum of the gas, which vanishes since the eigenfunctions are real. The second term is $O(r^2)$, which gives Table II, Eq. (6a). Equation (7a) of Table II follows from the fact that the contribution of the second term, after averaging over the directions of $\mathbf{r}$, is given by the integral of $k^2[n_\sigma(\mathbf{k}) - C/k^4]$, which (after summation over spin) is related to the total energy by Table II, Eq. (5a).

Two dimensions. To derive Table II, Eqs. (6b) and (7b) we rewrite Eq. (42) as $G^{(1)}_{\sigma\sigma}(\mathbf{r}) = N_\sigma + I(\mathbf{r}) + J(\mathbf{r})$ with

$$I(\mathbf{r}) = \int\frac{d^2k}{(2\pi)^2}(e^{i\mathbf{k}\cdot\mathbf{r}}-1)\frac{C}{k^4}\theta(k-q), \tag{45}$$

$$J(\mathbf{r}) = \int\frac{d^2k}{(2\pi)^2}(e^{i\mathbf{k}\cdot\mathbf{r}}-1)\left(n_\sigma(\mathbf{k})-\frac{C}{k^4}\theta(k-q)\right), \tag{46}$$

where $q>0$ is arbitrary and the Heaviside function θ ensures that the integrals converge.

To evaluate $I(\mathbf{r})$ we use standard manipulations to rewrite it as $I(\mathbf{r}) = [Cr^2/(2\pi)]\int_{qr}^{+\infty}dx[J_0(x)-1]/x^3$, with J_0 being a Bessel function. Expressing this integral with MATHEMATICA in terms of an hypergeometric function and a logarithm leads for $r\to 0$ to $I(\mathbf{r}) = [Cr^2/(8\pi)][\gamma - 1 - \ln 2 + \ln(qr)] + O(r^4)$. To evaluate $J(\mathbf{r})$ we use the same procedure as in 3D: expanding the exponential [see Eq. (44)] yields an integral which can be related to the total energy thanks to Eq. (38).[12]

[9] This relation was written in Ref. [104] in a form containing a generalized function $\eta(\mathbf{k})$ (i.e., a distribution). We have checked that this form is equivalent to our Eq. (38), using Eq. (16b) of Ref. [104], $n_\sigma(\mathbf{k}) - (C/k^4)\theta(k-q) = O(1/k^5)$ at large k, and $\int d^2k\eta(\mathbf{k})f(\mathbf{k}) = \int d^2k f(\mathbf{k})$ for any $f(\mathbf{k}) = O(1/k^3)$. This last property is implied in Eq. (16a) in Ref. [104].

[10] These last relations also hold if one averages over all directions of $\mathbf{r}$ uniformly on the unit sphere or unit circle.

[11] Our result does not follow from the well-known fact that, for a finite-range interaction potential in continuous space, $-\frac{\hbar^2}{2m}\sum_\sigma \Delta G^{(1)}_{\sigma\sigma}(\mathbf{r}=\mathbf{0})$ equals the kinetic energy; indeed, the Laplacian does not commute with the zero-range limit in that case [cf. also the comment below Eq. (180)].

[12] As suggested by a referee, Table II, Eq. (7b) can be tested for the dimer wave function $\psi(\mathbf{r}_1,\mathbf{r}_2) = \phi_{\rm dim}(r_{12}) = -\kappa K_0(\kappa r)/\pi^{1/2}$ [113], which has the energy $E = -\hbar^2\kappa^2/m$ and the momentum distribution $n_\sigma(\mathbf{k}) = 4\pi\kappa^2/(k^2+\kappa^2)^2$, where $\kappa = 2/(ae^{\gamma})$ and K_0 is a Bessel function. From Eq. (42) we find $G^{(1)}_{\sigma\sigma}(\mathbf{r}) = \kappa r K_1(\kappa r)$. From $C/(4\pi) = -mE/\hbar^2 = \kappa^2$ and the known expansion of K_1 around zero, we get the same low-r expansion as in Table II, Eq. (7b). To calculate $G^{(1)}_{\sigma\sigma}(\mathbf{r})$, we used the fact that $K_0(\kappa r)$ is the 2D Fourier transform of $2\pi/(k^2+\kappa^2)$: it remains to take the derivative with respect to κ and to realize that $K_0' = -K_1$.

F. Second-order derivative of energy with respect to scattering length

We denote by $|\psi_n\rangle$ an orthonormal basis of N-body stationary states that vary smoothly with $1/a$, and by E_n the corresponding eigenenergies. We will derive Table II, Eqs. (8a) and (8b), where the sum is taken on all values of n' such that $E_{n'} \neq E_n$. This implies that, for the ground-state energy E_0,

$$\frac{d^2E_0}{d\,(-1/a)^2} < 0 \text{ in 3D}, \tag{47}$$

$$\frac{d^2E_0}{d\,(\ln a)^2} < 0 \text{ in 2D}. \tag{48}$$

Equation (47) was intuitively expected [124]: Eq. (31) shows that $dE_0/d(-1/a)$ is proportional to the probability of finding two particles very close to each other, and it is natural that this probability decreases when one goes from the BEC limit ($-1/a \to -\infty$) to the BCS limit ($-1/a \to +\infty$); that is, when the interactions become less attractive.[13] Equation (48) also agrees with intuition.[14]

For the derivation, it is convenient to use the lattice model (defined in Sec. III B): As shown in Sec. V F one easily obtains Eq. (60) and Table III, Eq. (6), from which the result is deduced as follows: $|\phi(\mathbf{0})|^2$ is eliminated using Eqs. (17) and (18). Then, in 3D, one uses

$$\frac{d^2E_n}{d(-1/a)^2} = \frac{d^2E_n}{dg_0{}^2}\left(\frac{dg_0}{d\,(-1/a)}\right)^2 + \frac{dE_n}{dg_0}\frac{d^2g_0}{d(-1/a)^2}, \tag{49}$$

where the second term equals $2g_0[dE_n/d(-1/a)]m/(4\pi\hbar^2)$ and thus vanishes in the zero-range limit. In 2D, similarly, one uses the fact that $d^2E_n/d(\ln a)^2$ is the zero-range limit of $(d^2E_n/dg_0{}^2)[dg_0/d(\ln a)]^2$.

G. Time derivative of energy

We now consider the case where the scattering length $a(t)$ and the trapping potential $U(\mathbf{r},t)$ are varied with time. The time-dependent version of the zero-range model (see, e.g., Ref. [125]) is given by Schrödinger's equation

$$i\hbar\frac{\partial}{\partial t}\psi\,(\mathbf{r}_1,\ldots,\mathbf{r}_N;t) = H\,(t)\,\psi\,(\mathbf{r}_1,\ldots,\mathbf{r}_N;t) \tag{50}$$

when all particle positions are distinct, with

$$H\,(t) = \sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}_i} + U\,(\mathbf{r}_i,t)\right], \tag{51}$$

and by the contact condition Table I, Eq. (1a) in 3D or by Table I, Eq. (1b) in 2D for the scattering length $a = a(t)$. One then has the relations Table II, Eqs. (12a) and (12b), where $E(t) = \langle\psi(t)|H(t)|\psi(t)\rangle$ is the total energy and $H_{\text{trap}}(t) = \sum_{i=1}^{N} U(\mathbf{r}_i,t)$ is the trapping-potential part of the Hamiltonian. In 3D, this relation was obtained in Ref. [98]. A very simple derivation of these relations using the lattice model is given in Sec. V G. Here, we give a derivation within the zero-range model.

Three dimensions. We first note that the generalization of the lemma (33) to the case of two Hamiltonians H_1 and H_2 with corresponding trapping potentials $U_1(\mathbf{r})$ and $U_2(\mathbf{r})$ reads

$$\begin{aligned}&\langle\psi_1,H_2\psi_2\rangle - \langle H_1\psi_1,\psi_2\rangle\\ &\quad= \frac{4\pi\hbar^2}{m}\left(\frac{1}{a_1}-\frac{1}{a_2}\right)(A^{(1)},A^{(2)})\\ &\qquad+\langle\psi_1|\sum_{i=1}^{N}[U_2(\mathbf{r}_i,t)-U_1(\mathbf{r}_i,t)]|\psi_2\rangle.\end{aligned} \tag{52}$$

Applying this relation for $|\psi_1\rangle = |\psi(t)\rangle$ and $|\psi_2\rangle = |\psi(t+\delta t)\rangle$ [and correspondingly $a_1 = a(t), a_2 = a(t+\delta t)$, and $H_1 = H(t)$, $H_2 = H(t+\delta t)$] gives

$$\begin{aligned}&\langle\psi\,(t)\,,H\,(t+\delta t)\,\psi\,(t+\delta t)\rangle - \langle H\,(t)\,\psi\,(t)\,,\psi\,(t+\delta t)\rangle\\ &\quad= \frac{4\pi\hbar^2}{m}\left(\frac{1}{a\,(t)}-\frac{1}{a\,(t+\delta t)}\right)(A\,(t)\,,A\,(t+\delta t))\\ &\qquad+\langle\psi(t)|\sum_{i=1}^{N}[U(\mathbf{r}_i,t+\delta t)-U(\mathbf{r}_i,t)]|\psi(t+\delta t)\rangle.\end{aligned} \tag{53}$$

Dividing by δt, taking the limit $\delta t \to 0$, and using the expression Table II, Eq. (1a) of (A,A) in terms of C, the right-hand side of Eq. (53) reduces to the right-hand side of Table II, Eq. (12a). Using twice Schrödinger's equation, one rewrites the left-hand side of Eq. (53) as $i\hbar\frac{d}{dt}\langle\psi(t)|\psi(t+\delta t)\rangle$ and one Taylor expands this last expression to obtain Table II, Eq. (12a).

Two dimensions. Table II, Eq. (12b) is derived similarly from the lemma

$$\begin{aligned}&\langle\psi_1,H_2\psi_2\rangle - \langle H_1\psi_1,\psi_2\rangle\\ &\quad= \frac{2\pi\hbar^2}{m}\ln\,(a_2/a_1)\,(A^{(1)},A^{(2)})\\ &\qquad+\langle\psi_1|\sum_{i=1}^{N}[U_2(\mathbf{r}_i,t)-U_1(\mathbf{r}_i,t)]|\psi_2\rangle.\end{aligned} \tag{54}$$

V. RELATIONS FOR LATTICE MODELS

In this section, it will prove convenient to introduce an *operator* $\hat{C}$ by Table III, Eqs. (1a) and (1b) and to *define* C by its expectation value in the state of the system,

$$C = \langle\hat{C}\rangle. \tag{55}$$

In the zero-range limit, this new definition of C coincides with the definition Table II, Eq. (1), as shown in Appendix C.

A. Interaction energy and $\hat{C}$

The interaction part H_{int} of the lattice model's Hamiltonian is obviously equal to $g_0 dH/dg_0$ [see Eqs. (2)–(4)]. Rewriting

[13] In the lattice model in 3D, the coupling constant g_0 is always negative in the zero-range limit $|a| \gg b$, and is an increasing function of $-1/a$, as seen from Eq. (11).

[14] Equation (32) shows that $dE_0/d(\ln a)$ is proportional to the probability of finding two particles very close to each other, and it is natural that this probability decreases when one goes from the BEC limit ($\ln a \to -\infty$) to the BCS limit ($\ln a \to +\infty$); that is, when the interactions become less attractive [in the lattice model in 2D, the coupling constant g_0 is always negative in the zero-range limit $a \gg b$, and is an increasing function of $\ln a$, as can be seen from Eq. (12)].

this as $(1/g_0)[dH/d(-1/g_0)]$, and using the simple expressions (13) and (14) for $d(1/g_0)$, we get the relation Table III, Eq. (2) between $H_{\rm int}$ and $\hat{C}$, both in 3D and in 2D.

B. Total energy minus trapping potential energy in terms of momentum distribution and $\hat{C}$

Here we derive Table III, Eqs. (3a) and (3b). We start from the expression Table III, Eq. (2) of the interaction energy and eliminate $1/g_0$ thanks to Eqs. (11) and (12). The desired expression of $H - H_{\rm trap} = H_{\rm int} + H_{\rm kin}$ then simply follows from the expression (5) of the kinetic energy.

C. Interaction energy and regular part

In the forthcoming subsections V D–V F, we will use the following lemma: For any wave functions ψ and ψ',

$$\langle\psi'|H_{\rm int}|\psi\rangle = g_0|\phi(\mathbf{0})|^2(A',A), \tag{56}$$

where A and A' are the regular parts related to ψ and ψ' through Eq. (19), and the scalar product between regular parts is naturally defined as the discrete version of Table I, Eq. (2):

$$\begin{aligned}(A',A) \equiv \sum_{i<j}\sum_{(\mathbf{r}_k)_{k\neq i,j}}\sum_{\mathbf{R}_{ij}} b^{(N-1)d} A'^{*}_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}) \\ \times A_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}).\end{aligned} \tag{57}$$

The lemma simply follows from

$$\begin{aligned}\langle\psi'|H_{\rm int}|\psi\rangle = g_0\sum_{i<j}\sum_{(\mathbf{r}_k)_{k\neq i,j}} b^{(N-2)d}\sum_{\mathbf{r}_j} b^d \\ \times(\psi'^{*}\psi)(\mathbf{r}_1,\ldots,\mathbf{r}_i=\mathbf{r}_j,\ldots,\mathbf{r}_j,\ldots,\mathbf{r}_N).\end{aligned} \tag{58}$$

D. Relation between $\hat{C}$ and (A,A)

Lemma (56) with $\psi' = \psi$ writes

$$\langle\psi|H_{\rm int}|\psi\rangle = g_0|\phi(\mathbf{0})|^2(A,A). \tag{59}$$

Expressing $\langle\psi|H_{\rm int}|\psi\rangle$ in terms of $C = \langle\psi|\hat{C}|\psi\rangle$ thanks to Table III, Eq. (2) and using expressions (17) and (18) of $|\phi(\mathbf{0})|^2$, we get Table III, Eqs. (4a) and (4b).

E. First-order derivative of eigenenergy with respect to coupling constant

For any stationary state, the Hellmann-Feynman theorem, together with the definition [Table III, Eqs. (1a) and (1b)] of $\hat{C}$ and the relations Table III, Eqs. (4a) and (4b) between C and (A,A), immediately yields Table III, Eqs. (5a) and (5b).

F. Second-order derivative of eigenenergy with respect to coupling constant

We denote by $|\psi_n\rangle$ an orthonormal basis of N-body stationary states which vary smoothly with g_0, and by E_n the corresponding eigenenergies. We apply second-order perturbation theory to determine how an eigenenergy varies for an infinitesimal change of g_0. This gives

$$\frac{1}{2}\frac{d^2E_n}{dg_0^{\,2}} = \sum_{n',E_{n'}\neq E_n}\frac{|\langle\psi_{n'}|H_{\rm int}/g_0|\psi_n\rangle|^2}{E_n - E_{n'}}, \tag{60}$$

where the sum is taken over all values of n' such that $E_{n'} \neq E_n$. Lemma (56) then yields Table III, Eq. (6).

G. Time derivative of energy

The relations Table II, Eqs. (12a) and (12b) remain exact for the lattice model. Indeed, dE/dt equals $\langle dH/dt\rangle$ from the Hellmann-Feynman theorem. In 3D, we can rewrite this quantity as $\langle dH_{\rm trap}/dt\rangle + d(-1/a)/dt\,\langle dH/d(-1/a)\rangle$, and the desired result follows from the definition Table III, Eq. (1a) of $\hat{C}$. The derivation of the 2D relation Table II, Eq. (12b) is analogous.

H. On-site pair distribution operator

Let us define a spatially integrated pair distribution operator

$$\hat{G}^{(2)}_{\uparrow\downarrow}(\mathbf{r}) \equiv \sum_{\mathbf{R}} b^d(\psi^\dagger_\uparrow\psi_\uparrow)\left(\mathbf{R}+\frac{\mathbf{r}}{2}\right)(\psi^\dagger_\downarrow\psi_\downarrow)\left(\mathbf{R}-\frac{\mathbf{r}}{2}\right). \tag{61}$$

Using the relation Table III, Eq. (2) between $\hat{C}$ and $H_{\rm int}$, expressing $H_{\rm int}$ in terms of $\hat{G}^{(2)}_{\uparrow\downarrow}(\mathbf{0})$ thanks to the second-quantized form (6), and expressing g_0 in terms of $\phi(\mathbf{0})$ thanks to Eqs. (15) and (16), we immediately get

$$\hat{G}^{(2)}_{\uparrow\downarrow}(\mathbf{0}) = \frac{\hat{C}}{(4\pi)^2}|\phi(\mathbf{0})|^2 \text{ in 3D}, \tag{62}$$

$$\hat{G}^{(2)}_{\uparrow\downarrow}(\mathbf{0}) = \frac{\hat{C}}{(2\pi)^2}|\phi(\mathbf{0})|^2 \text{ in 2D}. \tag{63}$$

Here, $|\phi(\mathbf{0})|^2$ may of course be eliminated using (15) and (16). These relations are analogous to the one obtained previously within a different field-theoretical model [see Eq. (12) in Ref. [99]].

I. Pair distribution function at short distances

The last result can be generalized to finite but small r [see Table III, Eqs. (9a) and (9b)] where the zero-range regime $k_{\rm typ}b \ll 1$ was introduced at the end of Sec. III B. Here, we justify this for the case where the expectation values $g^{(2)}_{\uparrow\downarrow}(\mathbf{R}+\frac{\mathbf{r}}{2},\mathbf{R}-\frac{\mathbf{r}}{2}) = \langle(\psi^\dagger_\uparrow\psi_\uparrow)(\mathbf{R}+\frac{\mathbf{r}}{2})(\psi^\dagger_\downarrow\psi_\downarrow)(\mathbf{R}-\frac{\mathbf{r}}{2})\rangle$ and $C = \langle\hat{C}\rangle$ are taken in an arbitrary stationary state ψ in the zero-range regime; this implies that the same result holds for a thermal equilibrium state in the zero-range regime (see Sec. IX). We first note that the expression (28) of $g^{(2)}_{\uparrow\downarrow}$ in terms of the wave function is valid for the lattice model with the obvious replacement of the integrals by sums, so that

$$\begin{aligned}G^{(2)}_{\uparrow\downarrow}(\mathbf{r}) &\equiv \langle\hat{G}^{(2)}_{\uparrow\downarrow}(\mathbf{r})\rangle \\ &= \sum_{\mathbf{R}} b^d\sum_{i=1}^{N_\uparrow}\sum_{j=N_\uparrow+1}^{N}\sum_{(\mathbf{r}_k)_{k\neq i,j}} b^{(N-2)d}\left|\psi\left(\mathbf{r}_1,\ldots,\right.\right. \\ &\qquad \left.\left.\mathbf{r}_i=\mathbf{R}+\frac{\mathbf{r}}{2},\ldots,\mathbf{r}_j=\mathbf{R}-\frac{\mathbf{r}}{2},\ldots,\mathbf{r}_N\right)\right|^2.\end{aligned} \tag{64}$$

For $r \ll 1/k_{\rm typ}$, we can replace ψ by the short-distance expression (20), assuming that the multiple sum is dominated by the configurations where all the distances $|\mathbf{r}_k - \mathbf{R}|$ and $r_{kk'}$ are much larger than b and r:

$$G^{(2)}_{\uparrow\downarrow}(\mathbf{r}) \simeq (A,A)\,|\phi(\mathbf{r})|^2. \tag{65}$$

TABLE IV. Relations for spin-1/2 fermions with a finite-range interaction potential $V(r)$ in continuous space, for any stationary state. C is defined in line 1. All relations remain valid at thermal equilibrium in the canonical ensemble; the derivatives of the energy in line 1 then have to be taken at constant entropy. Equations (1a), (2a), and (4a) are contained in Ref. [101] (for $k_{\rm typ}b \ll 1$). The functions $\phi'(r)$ and $\phi'_R(r)$ are given by Eqs. (73) and (78) and $\tilde{\phi}'(k)$, $\tilde{\phi}'_R(k)$ are their Fourier transforms.

Three dimensions		Two dimensions	
$C \equiv \frac{4\pi m}{\hbar^2}\frac{dE}{d(-1/a)}$	(1a)	$C \equiv \frac{2\pi m}{\hbar^2}\frac{dE}{d(\ln a)}$	(1b)
$E_{\rm int} = \frac{C}{(4\pi)^2}\int d^3r\, V(r)\lvert\phi(r)\rvert^2$	(2a)	$E_{\rm int} = \frac{C}{(2\pi)^2}\int d^2r\, V(r)\lvert\phi(r)\rvert^2$	(2b)
$E - E_{\rm trap} = \frac{\hbar^2 C}{4\pi m a} + \sum_\sigma \int \frac{d^3k}{(2\pi)^3}\frac{\hbar^2k^2}{2m}\left[n_\sigma(\mathbf{k}) - \frac{C}{(4\pi)^2}\lvert\tilde{\phi}'(k)\rvert^2\right]$	(3a)	$E - E_{\rm trap} = \lim_{R\to\infty}\left\{\frac{\hbar^2 C}{2\pi m}\ln\left(\frac{R}{a}\right) + \sum_\sigma \int \frac{d^2k}{(2\pi)^2}\frac{\hbar^2k^2}{2m}\left[n_\sigma(\mathbf{k}) - \frac{C}{(2\pi)^2}\lvert\tilde{\phi}'_R(k)\rvert^2\right]\right\}$	(3b)
In the zero-range regime $k_{\rm typ}b \ll 1$			
$\int d^3R\, g^{(2)}_{\uparrow\downarrow}\left(\mathbf{R}+\frac{\mathbf{r}}{2},\mathbf{R}-\frac{\mathbf{r}}{2}\right) \simeq \frac{C}{(4\pi)^2}\lvert\phi(\mathbf{r})\rvert^2$ for $r \ll k_{\rm typ}^{-1}$	(4a)	$\int d^2R\, g^{(2)}_{\uparrow\downarrow}\left(\mathbf{R}+\frac{\mathbf{r}}{2},\mathbf{R}-\frac{\mathbf{r}}{2}\right) \simeq \frac{C}{(2\pi)^2}\lvert\phi(\mathbf{r})\rvert^2$ for $r \ll k_{\rm typ}^{-1}$	(4b)
$n_\sigma(\mathbf{k}) \simeq \frac{C}{(4\pi)^2}\lvert\tilde{\phi}(\mathbf{k})\rvert^2$ for $k \gg k_{\rm typ}$	(5a)	$n_\sigma(\mathbf{k}) \simeq \frac{C}{(2\pi)^2}\lvert\tilde{\phi}(\mathbf{k})\rvert^2$ for $k \gg k_{\rm typ}$	(5b)

Expressing (A,A) in terms of C thanks to Table III, Eqs. (4a) and (4b) gives the desired Table III, Eqs. (9a) and (9b).

J. Momentum distribution at large momenta

Assuming again that we are in the zero-range regime $k_{\rm typ}b \ll 1$, we will justify Table III, Eq. (10) both in 3D and in 2D. We start from

$$n_\sigma(\mathbf{k}) = \sum_{i:\sigma}\sum_{(\mathbf{r}_l)_{l\neq i}} b^{d(N-1)}\left|\sum_{\mathbf{r}_i} b^d e^{-i\mathbf{k}\cdot\mathbf{r}_i}\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)\right|^2. \tag{66}$$

We are interested in the limit $k \gg k_{\rm typ}$. Since $\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is a function of $\mathbf{r}_i$ which varies on the scale of $1/k_{\rm typ}$, except when $\mathbf{r}_i$ is close to another particle $\mathbf{r}_j$ where it varies on the scale of b, we can replace ψ by its short-distance form (20):

$$\sum_{\mathbf{r}_i} b^d e^{-i\mathbf{k}\cdot\mathbf{r}_i}\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) \simeq \tilde{\phi}(\mathbf{k})\sum_{j,j\neq i} e^{-i\mathbf{k}\cdot\mathbf{r}_j} A_{ij}(\mathbf{r}_j,(\mathbf{r}_l)_{l\neq i,j}), \tag{67}$$

where $\tilde{\phi}(\mathbf{k}) = \langle\mathbf{k}|\phi\rangle = \sum_{\mathbf{r}} b^d e^{-i\mathbf{k}\cdot\mathbf{r}}\phi(\mathbf{r})$. Here, we excluded the configurations where more than two particles are at distances $\lesssim b$, which are expected to have a negligible contribution to Eq. (66). Inserting Eq. (67) into Eq. (66), expanding the modulus squared, and neglecting the cross-product terms in the limit $k \gg k_{\rm typ}$, we obtain

$$n_\sigma(\mathbf{k}) \simeq |\tilde{\phi}(\mathbf{k})|^2(A,A). \tag{68}$$

Finally, $\tilde{\phi}(\mathbf{k})$ is easily computed for the lattice model: for $k \neq 0$, the two-body Schrödinger equation (A1) directly gives $\tilde{\phi}(\mathbf{k}) = -g_0\phi(\mathbf{0})/(2\epsilon_{\mathbf{k}})$, and $\phi(\mathbf{0})$ is given by Eqs. (15) and (16), which yields Table III, Eq. (10).

VI. RELATIONS FOR A FINITE-RANGE INTERACTION IN CONTINUOUS SPACE

In this Sec. VI, we restrict ourselves for simplicity to the case of a stationary state. It is then convenient to define C by Table IV, Eqs. (1a) and (1b).

A. Interaction energy

As for the lattice model, we find that the interaction energy is proportional to C, see Table IV, Eqs. (2a) and (2b). It was shown in Ref. [101] that the 3D relation is asymptotically valid in the zero-range limit. Here, we show that it remains exact for any finite value of the range and we generalize it to 2D.

For the derivation, we set

$$V(r) = g_0 W(r), \tag{69}$$

where g_0 is a dimensionless coupling constant which allows us to tune a. The Hellmann-Feynman theorem then gives $E_{\rm int} = g_0 dE/dg_0$. The result then follows by writing $dE/dg_0 = [dE/d(-1/a)][d(-1/a)/dg_0]$ in 3D and $dE/dg_0 = [dE/d(\ln a)][d(\ln a)/dg_0]$ in 2D, and by using the definition Table IV, Eqs. (1a) and (1b) of C as well as the following lemmas:

$$g_0\frac{d(-1/a)}{dg_0} = \frac{m}{4\pi\hbar^2}\int d^3r\, V(r)|\phi(r)|^2 \text{ in 3D}, \tag{70}$$

$$g_0\frac{d(\ln a)}{dg_0} = \frac{m}{2\pi\hbar^2}\int d^2r\, V(r)|\phi(r)|^2 \text{ in 2D}. \tag{71}$$

To derive these lemmas, we consider two values of the scattering length a_i, $i = 1,2$, and the corresponding scattering states ϕ_i and coupling constants $g_{0,i}$. The corresponding two-particle relative-motion Hamiltonians are $H_i = -(\hbar^2/m)\Delta_{\mathbf{r}} + g_{0,i}W(r)$. Since $H_i\phi_i = 0$, we have

$$\lim_{R\to\infty}\int_{r<R} d^dr\,(\phi_1 H_2\phi_2 - \phi_2 H_1\phi_1) = 0. \tag{72}$$

The contribution of the kinetic energies can be computed from the divergence theorem and the large-distance form of ϕ.[15] The contribution of the potential energies is proportional to $g_{0,2} - g_{0,1}$. Taking the limit $a_2 \to a_1$ gives the results (70) and (71). Lemma (70) was also used in Ref. [101] and the above derivation is essentially identical to the one of Ref. [101]. For

[15]To facilitate the derivation, we assume that $V(r) = 0$ for $r > b$, but the result is expected to hold for any $V(r)$ which vanishes quickly enough at infinity.

this 3D lemma, there also exists an alternative derivation based on the two-body problem in a large box.[16]

B. Relation between energy and momentum distribution

Three dimensions. For a finite-range interaction potential, the natural counterpart of the zero-range-model expression of the energy as a functional of the momentum distribution [Table II, Eq. (5a)] is given by Table IV, Eq. (3a), where $\tilde{\phi}'(k)$ is the zero-energy scattering state in momentum space with the incident wave contribution $\propto\delta(\mathbf{k})$ subtracted out: $\tilde{\phi}'(k) = \tilde{\phi}(k) + a^{-1}(2\pi)^3\delta(\mathbf{k}) = \int d^3r e^{-i\mathbf{k}\cdot\mathbf{r}}\phi'(r)$ with

$$\phi'(r) = \phi(r) + \frac{1}{a}. \tag{73}$$

This is simply obtained by adding the kinetic energy to Table IV, Eq. (2a) and by using the lemma

$$\int d^3r\, V(r)|\phi(r)|^2 = \frac{4\pi\hbar^2}{ma} - \int \frac{d^3k}{(2\pi)^3}\frac{\hbar^2k^2}{m}|\tilde{\phi}'(k)|^2. \tag{74}$$

To derive this lemma, we start from Schrödinger's equation $-(\hbar^2/m)\Delta\phi + V(r)\phi = 0$, which implies

$$\int d^3r\, V(r)|\phi(r)|^2 = \frac{\hbar^2}{m}\int d^3r\,\phi\Delta\phi. \tag{75}$$

Applying the divergence theorem over the sphere of radius R, using the asymptotic expression (9) of ϕ and taking the limit $R\to\infty$ then yields

$$\int d^3r\,\phi\Delta\phi = \frac{4\pi}{a} - \int d^3r\,(\nabla\phi)^2. \tag{76}$$

We then replace $\nabla\phi$ by $\nabla\phi'$. Applying the Parseval-Plancherel relation to $\partial_i\phi'$ and using the fact that $\phi'(r)$ vanishes at infinity, we get

$$\int d^3r(\nabla\phi')^2 = \int \frac{d^3k}{(2\pi)^3}k^2|\tilde{\phi}'(k)|^2. \tag{77}$$

The desired result (74) follows.

Two dimensions. An additional regularization procedure for small momenta is required in 2D, as was the case for the zero-range model [Table II, Eq. (5b)] and for the lattice model [Table III, Eq. (3b)]. One obtains Table IV, Eq. (3b), where $\tilde{\phi}'_R(k) = \int d^2r e^{-i\mathbf{k}\cdot\mathbf{r}}\phi'_R(r)$ with

$$\phi'_R(r) = [\phi(r) - \ln(R/a)]\,\theta(R-r). \tag{78}$$

This follows from Table IV, Eq. (2b) and from the lemma

$$\int d^2r\, V(r)|\phi(r)|^2 = \lim_{R\to\infty}\left\{\frac{2\pi\hbar^2}{m}\ln\left(\frac{R}{a}\right) - \int\frac{d^2k}{(2\pi)^2}\frac{\hbar^2k^2}{m}|\tilde{\phi}'_R(k)|^2\right\}. \tag{79}$$

The derivation of this lemma again starts with the 2D version of (75). The divergence theorem then gives[15]

$$\int d^2r\,\phi\Delta\phi = \lim_{R\to\infty}\left\{2\pi\ln\left(\frac{R}{a}\right) - \int_{r<R} d^2r(\nabla\phi)^2\right\}. \tag{80}$$

We can then replace $\int_{r<R} d^2r(\nabla\phi)^2$ by $\int d^2r(\nabla\phi'_R)^2$, since $\phi'_R(r)$ is continuous at $r = R$ [15] so that $\nabla\phi'_R$ does not contain any delta distribution. The Parseval-Plancherel relation can be applied to $\partial_i\phi'_R$, since this function is square-integrable. Then, using the fact that $\phi'_R(r)$ vanishes at infinity, we get

$$\int d^2r(\nabla\phi'_R)^2 = \int\frac{d^2k}{(2\pi)^2}k^2|\tilde{\phi}'_R(k)|^2, \tag{81}$$

and the lemma (79) follows.

C. Pair distribution function at short distances

In the zero-range regime $k_{\rm typ}b \ll 1$, the short-distance behavior of the pair distribution function is given by the same expressions [Table III, Eqs. (9a) and (9b)] as for the lattice model. Indeed, Eq. (65) is derived in the same way as for the lattice model; one can then use the zero-range model's expressions [Table II, Eqs. (2a) and (2b)] of (A,A) in terms of C, since the finite-range model's quantities C and A tend to the zero-range model's ones in the zero-range limit. In 3D, the result [Table III, Eq. (9a)] is contained in Ref. [101].

D. Momentum distribution at large momenta

In the zero-range regime $k_{\rm typ}b \ll 1$ the momentum distribution at large momenta $k \gg k_{\rm typ}$ is given by

$$n_\sigma(\mathbf{k}) \simeq \frac{C}{(4\pi)^2}|\tilde{\phi}(\mathbf{k})|^2 \text{ in 3D}, \tag{82}$$

$$n_\sigma(\mathbf{k}) \simeq \frac{C}{(2\pi)^2}|\tilde{\phi}(\mathbf{k})|^2 \text{ in 2D}. \tag{83}$$

Indeed, Eq. (68) is derived as for the lattice model, and (A,A) can be expressed in terms of C as in the previous subsection VI C.

VII. DERIVATIVE OF ENERGY WITH RESPECT TO EFFECTIVE RANGE

Assuming that the zero-range model is solved, we first show that the first correction to the energy due to a finite range of the interaction potential $V(r)$ can be explicitly obtained and only depends on the s-wave effective range of the interaction. We then enrich the discussion using the many-body diagrammatic point of view, where the central object is the full two-body T matrix, to recall in particular that the situation is more subtle for lattice models [116]. Finally, we relate $\partial E/\partial r_e$ to a subleading term of the short-distance behavior of the pair distribution function in Sec. VII D and to the coefficient of the $1/k^6$ subleading tail of $n_\sigma(\mathbf{k})$ in Sec. VII E.

[16] We consider two particles of opposite spin in a cubic box of side L with periodic boundary conditions, and we work in the limit where L is much larger than $|a|$ and b. In this limit, there exists a "weakly interacting" stationary state ψ whose energy is given by the "mean-field" shift $E = g/L^3$ with $g = 4\pi\hbar^2a/m$. The Hellmann-Feynman theorem gives $g_0 dE/dg_0 = E_{\rm int}[\psi]$. But the wave function $\psi(\mathbf{r}_1,\mathbf{r}_2) \simeq \Phi(r_{12})/L^3$ where Φ is the zero-energy scattering state normalized by $\Phi\to 1$ at infinity. Thus $E_{\rm int} = \int d^3r\, V(r)|\Phi(r)|^2/L^3$. The desired Eq. (70) then follows, since $\Phi = -a\phi$.

TABLE V. For spin-1/2 fermions, derivative of the energy with respect to the effective range r_e, or to its square in 2D, taken at $r_e = 0$ for a fixed value of scattering length. The functions A (assumed to be real) are the ones of the zero-range regime. The compact notations for the scalar products and the matrix elements are defined in Table I. $\bar{n}_\sigma(k)$ is the average of $n_\sigma(\mathbf{k})$ over the direction of $\mathbf{k}$. $\bar{G}^{(2)}_{\uparrow\downarrow}(\mathbf{r})$ is the pair distribution function integrated over the center of mass of the pair and averaged over the direction of $\mathbf{r}$.

Three dimensions		Two dimensions	
$\left(\frac{\partial E}{\partial r_e}\right)_a = 2\pi\langle A,(E-\mathcal{H})A\rangle$	(1a)	$\left(\frac{\partial E}{\partial (r_e^2)}\right)_a = \pi\langle A,(E-\mathcal{H})A\rangle$	(1b)
$\mathcal{H}_{ij} \equiv -\frac{\hbar^2}{4m}\Delta_{\mathbf{R}_{ij}} - \frac{\hbar^2}{2m}\sum_{k\neq i,j}\Delta_{\mathbf{r}_k} + 2U(\mathbf{R}_{ij}) + \sum_{k\neq i,j}U(\mathbf{r}_k)$			(2)
$\bar{G}^{(2)}_{\uparrow\downarrow}(\mathbf{r}) \underset{r\to 0}{=} \frac{C}{(4\pi)^2}\left(\frac{1}{r}-\frac{1}{a}\right)^2 - \frac{m}{2\pi\hbar^2}\frac{\partial E}{\partial r_e} + O(r)$	(3a)	$\bar{G}^{(2)}_{\uparrow\downarrow}(\mathbf{r}) \underset{r\to 0}{=} \frac{C}{(2\pi)^2}\ln^2(r/a) - \frac{m}{2\pi\hbar^2}\frac{\partial E}{\partial (r_e^2)} r^2\ln^2 r + O(r^2\ln r)$	(3b)
$\bar{n}_\sigma(k) - \frac{C}{k^4} \underset{k\to\infty}{\sim} \frac{1}{k^6}\left[\frac{16\pi m}{\hbar^2}\frac{\partial E}{\partial r_e} - 8\pi^2\langle A,\Delta_{\mathbf{R}}A\rangle\right]$	(4a)	$\bar{n}_\sigma(k) - \frac{C}{k^4} \underset{k\to\infty}{\sim} \frac{1}{k^6}\left[\frac{8\pi m}{\hbar^2}\frac{\partial E}{\partial (r_e^2)} - 4\pi^2\langle A,\Delta_{\mathbf{R}}A\rangle\right]$	(4b)

A. Derivation of explicit formulas

Three dimensions. In 3D, the leading order finite-range correction to the zero-range model's spectrum depends on the interaction potential $V(r)$ only *via* its effective range r_e, and is given by the expression Table V, Eq. (1a), where the derivative is taken in $r_e = 0$ for a fixed value of the scattering length, the function A is assumed to be real without loss of generality. As a first way to obtain this result we use a modified version of the zero-range model, where the boundary condition [Table I, Eq. (1a)] is replaced by

$$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) \underset{r_{ij}\to 0}{=} \left(\frac{1}{r_{ij}} - \frac{1}{a} + \frac{m}{2\hbar^2}\mathcal{E}r_e\right) A_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}) + O(r_{ij}), \tag{84}$$

where

$$\mathcal{E} = E - 2U(\mathbf{R}_{ij}) - \left(\sum_{k\neq i,j}U(\mathbf{r}_k)\right) + \frac{1}{A_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j})} \times\left[\frac{\hbar^2}{4m}\Delta_{\mathbf{R}_{ij}} + \frac{\hbar^2}{2m}\sum_{k\neq i,j}\Delta_{\mathbf{r}_k}\right]A_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}). \tag{85}$$

Equations (84) and (85) generalize the ones already used for three bosons in free space in Refs. [126,127] (the predictions of Refs. [126] and [127] have been confirmed using different approaches; see Ref. [128] and references therein, and [129, 130], respectively; moreover, a derivation of these equations was given in Ref. [126]). Such a model was also used in the two-body case (see, e.g., [131–133]), and the modified scalar product that makes it Hermitian was constructed in Ref. [134].

For the derivation of Table V, Eq. (1a), we consider a stationary state ψ_1 of the zero-range model, satisfying the boundary condition Table I, Eq. (1a) with a scattering length a and a regular part $A^{(1)}$, and the corresponding finite-range stationary state ψ_2 satisfying Eqs. (84) and (85) with the same scattering length a and a regular part $A^{(2)}$. As in Appendix B we get Eq. (B3), as well as Eq. (B6) with $1/a_1 - 1/a_2$ replaced by $m\mathcal{E}r_e/(2\hbar^2)$. This yields Table V, Eq. (1a).

A deeper physical understanding and a more self-contained derivation may be achieved by going back to the actual finite-range model $V(r;b)$ for the interaction potential, such that the scattering length remains fixed when the range b tends to zero. The Hellmann-Feynman theorem gives

$$\frac{dE}{db} = \sum_{i=1}^{N_\uparrow}\sum_{j=N_\uparrow+1}^{N}\int d^3r_1\ldots d^3r_N|\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)|^2\partial_b V(r_{ij};b). \tag{86}$$

We need to evaluate $|\psi|^2$ for a typical configuration with two atoms i and j within the potential range b; in the limit $b\to 0$ one may then assume that the other atoms are separated by much more than b and are at distances from $\mathbf{R}_{ij} = (\mathbf{r}_i + \mathbf{r}_j)/2$ much larger than b. This motivates the factorized ansatz

$$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) \simeq \chi(r_{ij})A_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}). \tag{87}$$

We take a rotationally invariant χ, because we assume the absence of scattering resonance in the partial waves other than s wave:[17] The p-wave scattering amplitude, which vanishes quadratically with the relative wave number k, is then $O(b^3k^2)$, resulting in an energy contribution $O(b^3)$ negligible at the present order.

Inserting the ansatz (87) into Schrödinger's equation $H\psi = E\psi$, and neglecting the trapping potential within the interaction range $r_{ij} \leqslant b$, as justified in the Appendix D, gives[18]

$$\mathcal{E}\chi(r_{ij}) \simeq \left[-\frac{\hbar^2}{m}\Delta_{\mathbf{r}_{ij}} + V(r_{ij};b)\right]\chi(r_{ij}), \tag{88}$$

where $\mathcal{E}$ is given by (85). For $\mathcal{E} > 0$, we set $\mathcal{E} = \hbar^2k^2/m$ with $k > 0$, and χ is a finite-energy scattering state; to match the normalization of the zero-energy scattering state ϕ used in this

[17] More precisely, one first takes a general, nonrotationally invariant function $\chi(\mathbf{r})$, that one then expands in partial waves of angular momentum l; that is, in spherical harmonics. Performing the reasoning to come for each l, one finds at the end that the $l = 0$ channel finite-range correction dominates for small b, in the absence of l-wave resonance for $l \neq 0$. Furthermore, for three bosons, the ansatz (87) was justified in [81] and used in [126].

[18] Since $\mathcal{E}$ depends on $\mathbf{R}_{ij}$ and the $(\mathbf{r}_k)_{k\neq i,j}$, χ actually depends on these variables and not only on r_{ij}. This dependence however rapidly vanishes in the limit $b\to 0$, if one restricts to the distances $r_{ij} \lesssim b$, for the normalization (89): $\partial_{\mathcal{E}}\chi/\chi = O(mb^2/\hbar^2)$.

article [see Eq. (9)], we take out of the interaction potential

$$\chi(r) \underset{r\to\infty}{=} \frac{1}{f_k}\frac{\sin(kr)}{kr} + \frac{e^{ikr}}{r}, \tag{89}$$

where f_k is the scattering amplitude. The optical theorem, implying that

$$f_k = -\frac{1}{ik + u(k)}, \tag{90}$$

where $u(k) \in \mathbb{R}$, ensures that χ is real.[19]

Inserting the ansatz (87) into the Hellmann-Feynman expression (86) gives

$$\frac{dE}{db} \simeq \sum_{i<j} \int d^3R_{ij} \int \left(\prod_{k\neq i,j} d^3r_k\right) A_{ij}^2(\mathbf{R}_{ij}, (\mathbf{r}_k)_{k\neq i,j}) \times \int d^3r_{ij}\ \chi^2(r_{ij})\partial_b V(r_{ij};b). \tag{91}$$

To evaluate the integral of $\chi^2\partial_b V$, we use the following lemma (whose derivation is given in the next paragraph):

$$\frac{4\pi\hbar^2}{m}[u_2(k) - u_1(k)] = \int_{\mathbb{R}^3} d^3r\,\chi_1(r)\chi_2(r)[V(r;b_1) - V(r;b_2)], \tag{92}$$

where χ_1 and χ_2 are the same energy $\mathcal{E}$ scattering states for two different values b_1 and b_2 of the potential range. Then dividing this expression by $b_1 - b_2$, taking the limit $b_1 \to b_2$, and afterwards the limit $b_2 \to 0$ for which the low-k expansion holds:

$$u(k) = \frac{1}{a} - \frac{1}{2}r_e k^2 + O(b^3k^4), \tag{93}$$

r_e being the effective range of the interaction potential of range b, we obtain Table V, Eq. (1a).[20]

As a side result of this physical approach, the modified contact conditions (84) may be rederived. One performs an analytical continuation of the out-of-potential wave function (89) to the interval $r \leqslant b$ [105] and one takes the zero-r limit of that continuation.[21] In simple words, this amounts to expanding Eq. (89) in powers of r:

$$\chi(r) = \frac{1}{r} - \frac{1}{a} + \frac{1}{2}k^2 r_e + O(r). \tag{94}$$

Inserting this expansion in Eq. (87) and using $k^2 = m\mathcal{E}/\hbar^2$ gives Eq. (84).

The lemma (92) is obtained by multiplying Schrödinger's equations for χ_1 (respectively for χ_2) by χ_2 (respectively by χ_1), taking the difference of the two resulting equations, integrating this difference over the sphere $r < R$, and using the divergence theorem to convert the volume integral of $\chi_2\Delta_{\mathbf{r}}\chi_1 - \chi_1\Delta_{\mathbf{r}}\chi_2$ into a surface integral, where the asymptotic forms (89) for $r = R \to +\infty$ may be used. When $\mathcal{E} < 0$, we set $\mathcal{E} = -\hbar^2\kappa^2/m$ with $\kappa > 0$ and we perform analytic continuation of the $\mathcal{E} > 0$ case by replacing k with $i\kappa$. From Eq. (89) it appears that $\chi(r)$ now diverges exponentially at large distances, as $e^{\kappa r}/r$, if $1/f(i\kappa) \neq 0$. If the interaction potential is a compact support potential, or simply tends to zero more rapidly than $\exp(-2\kappa r)$, the lemma and the final conclusion [Table V, Eq. (1a)] still hold; the functions $u_1(i\kappa)$ and $u_2(i\kappa)$ remain real, since the series expansion of $u(k)$ has only even powers of k.

Two dimensions. The above physical reasoning may be directly generalized to 2D,[22] giving Table V, Eq. (1b), where the derivative is taken for a fixed scattering length in $r_e = 0$. The main difference with the 3D case [Table V, Eq. (1a)] is that the energy E now varies quadratically with the effective range r_e, as already observed numerically for three-boson-bound states in Ref. [138]. In the derivation, the first significant difference with the 3D case occurs in the normalization of the two-body scattering state: (89) is replaced with

$$\chi(r) \underset{r\to\infty}{=} \frac{\pi}{2i}\left[\frac{1}{f_k}J_0(kr) + H_0^{(1)}(kr)\right], \tag{95}$$

where $H_0^{(1)} = J_0 + iN_0$ is a Hankel function, and J_0 and N_0 are Bessel functions of the first and second kinds. The optical theorem implies $|f_k|^2 + \mathrm{Re}\, f_k = 0$ so that

$$f_k = \frac{-1}{1 + iu(k)} \quad \text{with} \quad u(k) \in \mathbb{R}, \tag{96}$$

and χ is real. The low-k expansion for a potential of range b takes the form [139,140]

$$u(k) = \frac{2}{\pi}\left[\ln(e^\gamma ka/2) + \frac{1}{2}(kr_e)^2 + \cdots\right], \tag{97}$$

where $\gamma = 0.577\,216\ldots$ is Euler's constant, the logarithmic term being obtained in the zero-range Bethe-Peierls model and the k^2 term corresponding to finite effective-range corrections (with the sign convention of Ref. [139] such that $r_e^2 > 0$ for a hard-disk potential). The subsequent calculations are similar to the 3D case, also for the negative-energy case where analytic continuation gives rises to the special functions $I_0(\kappa r)$ and $K_0(\kappa r)$. For example, at positive energy, the lemma (92) takes

[19] $u(k)$ is related to the s-wave collisional phase shift $\delta_0(k)$ by $u(k) = -k/\tan\delta_0(k)$.

[20] In general, when $N_\uparrow \geqslant 2$ and $N_\downarrow \geqslant 2$, the functions A_{ij} have $1/r_{kl}$ divergences when $r_{kl} \to 0$. This is apparent in the dimer-dimer scattering problem [135]. As a consequence, in the integral of [Table V, Eq. (1a)], one has to exclude the manifold where at least two particles are at the same location. The same exclusion has to be performed in 2D.

[21] The wave function is not an analytic function of r for a compact support interaction potential, since a nonzero compact support function is not analytic.

[22] We consider here a truly 2D gas. In experiments, quasi-2D gases are produced by freezing the z motion in a harmonic oscillator ground state of size $a_z = [\hbar/(m\omega_z)]^{1/2}$: At zero temperature, a 2D character appears for $\hbar^2k_F^2/(2m) \ll \hbar\omega_z$. From the quasi-2D scattering amplitude given in Ref. [136] (see also Ref. [137]) we find the effective-range squared, $r_e^2 = -(\ln 2)a_z^2$. Anticipating on subsection VII B we also find $\rho_e = R_1 = 0$. It would be interesting to see if the finite-range energy corrections dominate over the corrections due to the 3D nature of the gas, both effects being controlled by the same small parameter $(k_F r_e)^2$.

in 2D the form

$$\frac{\pi^2\hbar^2}{m}\left[u_1(k)-u_2(k)\right] = \int_{\mathbb{R}^2} d^2r\,\chi_1(r)\chi_2(r)\left[V(r;b_1)-V(r;b_2)\right]. \quad (98)$$

The fact that one can neglect the trapping potential within the interaction range is again justified in Appendix D. Finally, we note that the expansion of the asymptotic form (95) for $r \to 0$ and for $k \to 0$,

$$\chi(r) = \ln(r/a) - \tfrac{1}{2}(kr_e)^2 + O(r^2 \ln r), \quad (99)$$

allows us to determine the 2D version of the modified zero-range model (84),

$$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) \underset{r_{ij}\to 0}{=} \left(\ln(r_{ij}/a) - \frac{m}{2\hbar^2}\mathcal{E}r_e^2\right) A_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}) + O(r_{ij}), \quad (100)$$

where $\mathcal{E}$ is defined as in 3D by Eq. (85). To complete this 2D derivation, one has to check that the p-wave interaction brings a negligible contribution to the energy. The p-wave scattering amplitude at low relative wave number k vanishes as $k^2R_1^2$ where R_1^2 is the p-wave scattering surface [141]. One could believe that $r_e \approx R_1 \approx b$, one would then conclude that the p-wave contribution to the energy, scaling as R_1^2, cannot be neglected as compared to the s-wave finite-range correction, scaling as r_e^2. Fortunately, as shown in subsection VII B, this expectation is too naive, and Table V, Eq. (1b) is saved by a logarithm, r_e being larger than R_1 by a factor $\ln(a/b) \gg 1$ in the zero-range limit.[23]

B. What we learn from diagrammatic formalism

In the many-body diagrammatic formalism [142,143], the equation of state of the homogeneous gas (in the thermodynamic limit) is accessed from the single-particle Green's function, which can be expanded in powers of the interaction potential, each term of the expansion being represented by a Feynman diagram. The internal momenta of the diagrams can however be as large as $\hbar/b$, where b is the interaction range. A standard approach to improve the convergence of the perturbative series for strong interaction potentials is to perform the so-called *ladder* resummation. The resulting Feynman diagrams then involve the two-body T matrix of the interaction, rather than the bare interaction potential V. For the spin-1/2 Fermi gas, where there is *a priori* no Efimov effect, one then expects that the internal momenta of the Feynman diagrams are on the order of $\hbar k_{\text{typ}}$ only, where the typical wave number k_{typ} was defined in subsection III B. As put forward in Ref. [116], the interaction parameters controlling the first deviation of the gas energy from its zero-range limit are then the ones appearing in the first deviations of the two-body T-matrix element $\langle \mathbf{k}_1,\mathbf{k}_2|T(E+i0^+)|\mathbf{k}_3,\mathbf{k}_4\rangle$ from its zero-range limit, where all the $\mathbf{k}_i$ are on the order of k_{typ} and E is on the order of $\hbar^2k_{\text{typ}}^2/m$. The single-particle Green's function is indeed a sum of integrals of products of T-matrix elements and of ideal-gas Green's functions.

We explore this idea in this subsection. For an interaction potential $V(r)$, we confirm the results of subsection VII A. In addition to the effective range r_e characterizing the on-shell T-matrix elements (that is the scattering amplitude), the diagrammatic point of view introduces a length ρ_e characterizing the s-wave low-energy *off-shell* T-matrix elements, and a length R_1 characterizing the p-wave on-shell scattering; we will show that the contributions of ρ_e and R_1 are negligible as compared to the one of the effective range r_e. Moreover, in the case of lattice models, a length R_e characterizing the breaking of the Galilean invariance appears [116]. Its contribution is in general of the same order as the one of r_e. Both contributions can be zeroed for appropriately tuned matterwave dispersion relations on the lattice. Finally, in the case of a continuous space model with a δ interaction potential plus a spherical cutoff in momentum space, and in the case of a lattice model with a spherical momentum cutoff, we show that the breaking of Galilean invariance does not disappear in the infinite-cutoff limit.

1. For continuous space interaction $V(r)$

When each pair of particles i and j interact in continuous space *via* the potential $V(r_{ij})$, one can use Galilean invariance to restrict the T matrix to the center-of-mass frame, where $\mathbf{k}' \equiv \mathbf{k}_1 = -\mathbf{k}_2$ and $\mathbf{k} \equiv \mathbf{k}_3 = -\mathbf{k}_4$. Further using rotational invariance, one can restrict this internal T matrix to fixed total angular momentum l, with matrix elements characterized by the function $t_l(k',k;E)$ whose low-energy behavior was extensively studied [141,144]. This function is said to be *on shell* if and only if $k = k' = (mE)^{1/2}/\hbar$, in which case it is simply noted as $t_l(E)$, otherwise it is said to be *off shell*.

Three dimensions. We assume that the interaction potential, of compact support of range b, is everywhere nonpositive (or infinite). We recall that we are here in the *resonant* regime, with a s-wave scattering length a such that $|a| \gg b$. The potential is assumed to have the *minimal* depth leading to the desired value of a, so as to exclude deeply bound dimers. In particular, at resonance ($1/a = 0$), there is no two-body bound state. To invalidate the usual variational argument [115,145–147] (which shows, for a nonpositive interaction potential, that the spin-1/2 fermions have deep N-body bound states in the large-N limit), we allow that $V(r)$ has a hard core of range $b_{\text{hard}} < b$. We directly restrict to the s-wave case ($l = 0$), since the nonresonant p-wave interaction brings a negligible $O(b^3)$ contribution, as already discussed in Sec. VII A.

The first deviation of the on-shell s-wave T matrix from its zero-range limit is characterized by the effective range r_e, already introduced in Eq. (93). The effective range is given by the well-known Smorodinski formula [140]

$$\frac{1}{2}r_e = \int_0^{+\infty} dr\left[(1-r/a)^2 - u_0^2(r)\right], \quad (101)$$

in terms of the zero-energy scattering state $\phi(r)$, with $u_0(r) = r\phi(r)$ and where ϕ is normalized as in Eq. (9). Note that $u_0(r)$ is zero for $r \leqslant b_{\text{hard}}$. As r_e deviates from its resonant ($|a| \to \infty$)

[23] As in 3D one may also be worried by the dependence of χ with $\mathbf{R}_{ij}$ and the $(\mathbf{r}_k)_{k\neq i,j}$ *via* its dependence with the energy $\mathcal{E}$. We reach the estimate $\partial_{\mathcal{E}}\chi(b)/\chi(b) \approx mr_e^2/[\hbar^2\ln(a/b)]$ that vanishes more rapidly than r_e^2 in the zero-range limit.

value by terms $O(b^2/a)$, the discussion of its $1/a = 0$ value is sufficient here. The function u_0 then solves

$$0 = -\frac{\hbar^2}{m}u_0''(r) + V(r)u_0(r), \tag{102}$$

with the boundary conditions $u_0(b_{\text{hard}}) = 0$ and $u_0(r) = 1$ for $r > b$. Due to the absence of two-body bound states, u_0 is the ground two-body state and it has a constant sign, $u_0(r) \geqslant 0$ for all r. Since $V \leqslant 0$, Eq. (102) implies that $u_0'' \leqslant 0$; the function u_0 is concave. Combined with the boundary conditions, this leads to $0 \leqslant u_0(r) \leqslant 1$ for all r. Then, from Eq. (101),

$$2b_{\text{hard}} \leqslant r_e \leqslant 2b. \tag{103}$$

For the considered model, this proves that $k_{\text{typ}}r_e \to 0$ in the zero-range limit $b \to 0$, which is a key property for the present work. Note that the absence of two-body bound states at resonance is the crucial hypothesis ensuring that $r_e \geqslant 0$; it was not explicitly stated in the solution of problem 1 in Sec. 131 of Ref. [148]. Without this hypothesis, r_e at resonance can be arbitrarily large and negative even for $V(r) \leqslant 0$ for all r (see an explicit example in Ref. [122]).

In the s-wave channel, the first deviations of the *off-shell* T matrix from its zero-range value introduces, in addition to r_e, another length that we call ρ_e, such that [144][24]

$$\begin{aligned}\tfrac{t_0(k,k';E)}{t_0(E)} - 1 &\underset{k,k',E\to 0}{\sim} \left(\frac{2mE}{\hbar^2} - k^2 - k'^2\right)\frac{1}{2}\rho_e^2,\\ \frac{1}{2}\rho_e^2 &= \int_0^{+\infty} dr\, r[(1 - r/a) - u_0(r)].\end{aligned} \tag{104}$$

For our minimal-depth model at resonance, we conclude that $0 \leqslant \rho_e^2 \leqslant b^2$, so it appears in the finite-range correction to the energy at a higher order than r_e and it cannot contribute to Table V, Eq. (1a).

Two dimensions. The specific feature of the 2D case is that the minimal-depth attractive potential ensuring the desired scattering length a only weakly dephases the matterwave over its range, when $\ln(a/b) \gg 1$. This is apparent, for example, if $V(r)$ is a square-well potential of range b, $V(r) = -\frac{\hbar^2 k_0^2}{m}\theta(b - r)$: One has $-k_0 b J_0'(k_0 b)/J_0(k_0 b) = 1/\ln(a/b)$, where J_0 is a Bessel function, which shows that, for the minimal-depth solution, the matterwave phase shift $k_0 b$ vanishes as $[2/\ln(a/b)]^{1/2}$ in the zero-range limit. This property allows to treat the potential perturbatively.

There are three relevant parameters describing the low-energy behavior of the T matrix beyond the zero-range limit. The first one is the effective range r_e for the s-wave on-shell T matrix, see Eq. (97). It is given by the bidimensional Smorodinski formula [139,140]:

$$\frac{1}{2}r_e^2 = \int_0^{+\infty} dr\, r[\ln^2(r/a) - \phi^2(r)] \tag{105}$$

where the zero-energy scattering state $\phi(r)$ is normalized as in Eq. (10). The second parameter is the length ρ_e associated with the s-wave off-shell T matrix: The 2D equivalent of Eq. (104) is [141]

$$\begin{aligned}\tfrac{t_0(k,k';E)}{t_0(E)} - 1 &\underset{k,k',E\to 0}{\sim} \left(\frac{2mE}{\hbar^2} - k^2 - k'^2\right)\frac{1}{2}\rho_e^2,\\ \frac{1}{2}\rho_e^2 &= \int_0^{+\infty} dr\, r\,[\phi(r) - \ln(r/a)]\,.\end{aligned} \tag{106}$$

The third parameter is the length R_1 characterizing the low-energy p-wave scattering. For the l-wave scattering state of energy $E = \hbar^2 k^2/m$, $k > 0$, we generalize Eq. (95) as

$$\chi^{(l)}(r) \underset{r\to\infty}{=} \frac{\pi}{2i}k^l\left[\frac{1}{f_k^{(l)}}J_l(kr) + H_l^{(1)}(kr)\right]. \tag{107}$$

The l-wave scattering amplitude then vanishes as

$$f_k^{(l)} \underset{k\to 0}{\sim} i\frac{\pi}{2}k^{2l}R_l^{2l}, \tag{108}$$

and the leading behavior of the off-shell l-wave T matrix is characterized by the same length R_l as the on-shell one [141].

The situation thus looks critical in 2D: Three lengths squared characterize the low-energy T matrix, one may naively expect that they are of the same order $\approx b^2$ and that they all three contribute to the finite-range correction to the gas energy at the same level, whereas Table V, Eq. (1b) singles out the effective range r_e. By a perturbative treatment of the minimal-depth finite-range potential $V(r)$ of fixed scattering length a, we however obtain in the zero-range limit the following hierarchy (see Appendix E):

$$r_e^2 \underset{b\to 0}{\sim} 2\rho_e^2\ln(a/b), \tag{109}$$

$$\rho_e^2 \underset{b\to 0}{=} \frac{1}{2}\frac{\int_{\mathbb{R}^2} d^2r\, r^2 V(r)}{\int_{\mathbb{R}^2} d^2r\, V(r)}\left[1 + O\left(\frac{1}{\ln(a/b)}\right)\right], \tag{110}$$

$$R_1^2 \underset{b\to 0}{\sim} \frac{\rho_e^2}{2\ln(a/b)}. \tag{111}$$

This validates Table V, Eq. (1b) when $\ln(a/b) \gg 1$.

2. *Lattice models*

We restrict here for simplicity to the 3D case. To obtain a nonzero T-matrix element $\langle \mathbf{k}_1,\mathbf{k}_2|T(E + i0^+)|\mathbf{k}_3,\mathbf{k}_4\rangle$, due to the conservation of the total quasimomentum, we have to restrict to $\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4 \equiv \mathbf{K}$ (modulo a vector of the reciprocal lattice). As the interactions in the lattice model are purely on site, the matrix element only depends on the total quasimomentum $\mathbf{K}$ and the energy E and is noted as $t(\mathbf{K},E)$ in what follows. We recall that the bare coupling constant g_0 is adjusted to have a fixed scattering length a on the lattice [see Eq. (11)], which leads to

$$g_0 = \frac{4\pi\hbar^2 a/m}{1 - K_3 a/b}, \tag{112}$$

where the numerical constant K_3 depends on the lattice dispersion relation $\epsilon_{\mathbf{k}}$. One then gets [116]

$$\begin{aligned}\frac{1}{t(\mathbf{K},E)} = \frac{m}{4\pi\hbar^2 a}\\ - \int_D \frac{d^3q}{(2\pi)^3}\left(\frac{1}{2\epsilon_{\mathbf{q}}} + \frac{1}{E + i0^+ - \epsilon_{\frac{1}{2}\mathbf{K}+\mathbf{q}} - \epsilon_{\frac{1}{2}\mathbf{K}-\mathbf{q}}}\right),\end{aligned} \tag{113}$$

[24] We have checked that the hypothesis of a nonresonant interaction in Ref. [144] is actually not necessary to obtain (C16) and (C18) of that reference, that lead to Eq. (104).

where a is the s-wave scattering length and the dispersion relation $\epsilon_{\mathbf{q}}$ is extended by periodicity from the first Brillouin zone D to the whole space. The low-$\mathbf{K}$ and low-energy limit of that expression was worked out in Ref. [116], it involves the effective range r_e and an extra length R_e quantifying the breaking of Galilean invariance:

$$\frac{1}{t\,(\mathbf{K},E)} = \frac{m}{4\pi\hbar^2}\left(\frac{1}{a} + ik - \frac{1}{2}r_e k^2 - \frac{1}{2}R_e K^2\right) + \cdots \quad (114)$$

where the relative wave number k such that $E - \frac{\hbar^2 K^2}{4m} = \frac{\hbar^2 k^2}{m}$ is either real nonnegative or purely imaginary with a positive imaginary part. The two lengths are given by

$$r_e = \int_{\mathbb{R}^3\setminus D} \frac{d^3q}{\pi^2 q^4} + \int_D \frac{d^3q}{\pi^2}\left[\frac{1}{q^4} - \left(\frac{\hbar^2}{2m\epsilon_{\mathbf{q}}}\right)^2\right], \quad (115)$$

$$R_e = -\int_{\mathring{D}} \frac{d^3q}{4\pi^2}\left(\frac{\hbar^2}{2m\epsilon_{\mathbf{q}}}\right)^2\left[1 - \frac{m}{\hbar^2}\frac{\partial^2\epsilon_{\mathbf{q}}}{\partial q_x^2}\right] - \int_{-\frac{\pi}{b}}^{\frac{\pi}{b}}\int_{-\frac{\pi}{b}}^{\frac{\pi}{b}} \frac{dq_y dq_z}{8\pi^2}\frac{\hbar^2}{m\epsilon^2_{(\frac{\pi}{b},q_y,q_z)}}\frac{\partial\epsilon_{(\frac{\pi}{b},q_y,q_z)}}{\partial q_x}, \quad (116)$$

where the dispersion relation $\epsilon_{\mathbf{k}}$ was supposed to be twice differentiable on the interior $\mathring{D}$ of the first Brillouin zone and to be invariant under permutation of the coordinate axes. As compared to Ref. [116] we have added the second term (a surface term) in Eq. (116) to include the case where the dispersion relation has cusps at the border of the first Brillouin zone.[25] As mentioned in the introduction of the present section, we then expect that, in the lattice model, the first deviation of any many-body eigenenergy E from the zero-range limit is a linear function of the *two* parameters r_e and R_e with model-independent coefficients:

$$E(b) \underset{b\to 0}{=} E(0) + \frac{\partial E}{\partial r_e}r_e + \frac{\partial E}{\partial R_e}R_e + o(b). \quad (117)$$

This feature was overlooked in the early version [90] of this work. It invalidates the discussion of $\partial T_c/\partial r_e$ given in Ref. [90].

We illustrate this discussion with a few relevant examples. For a parabolic dispersion relation $\epsilon_{\mathbf{k}} = \hbar^2 k^2/(2m)$, the constant $K_3 = 2.442\,749\,607\,806\,335\ldots$ [15,149] and the effective range [114,122] were already calculated, first numerically then analytically; in the quantity R_e, the first term vanishes but there is still breaking of Galilean invariance due to the nonzero surface term that can be deduced from Eq. (F6):

$$r_e = b\frac{12\sqrt{2}}{\pi^3}\arcsin\frac{1}{\sqrt{3}} \simeq 0.337b \quad \text{and} \quad R_e = -\frac{1}{12}r_e. \quad (118)$$

[25]This term is obtained by distinguishing three integration zones before taking the limit $K_x \to 0$, so as to fold back the vectors $\mathbf{q} \pm \frac{1}{2}\mathbf{K}$ inside the first Brillouin zone: the left zone $-\frac{\pi}{b} < q_x < -\frac{\pi}{b} + \frac{1}{2}K_x$ where $\epsilon_{\mathbf{q}-\frac{1}{2}\mathbf{K}}$ is written as $\epsilon_{\mathbf{q}+\frac{2\pi}{b}\mathbf{e}_x-\frac{1}{2}\mathbf{K}}$, the right zone $\frac{\pi}{b} - \frac{1}{2}K_x < q_x < \frac{\pi}{b}$ where $\epsilon_{\mathbf{q}+\frac{1}{2}\mathbf{K}}$ is written as $\epsilon_{\mathbf{q}-\frac{2\pi}{b}\mathbf{e}_x+\frac{1}{2}\mathbf{K}}$, and the central zone. The surface term can also be obtained by interpreting $\partial^2_{q_x}$ in the sense of distributions, after having shifted the integration domain D by $\frac{\pi}{b}\mathbf{e}_x$ for mathematical convenience. The second-order derivative in the first term of Eq. (116) is of course taken in the sense of functions.

A popular model for quantum Monte Carlo simulations is the Hubbard model, which leads to the dispersion relation $\epsilon_{\mathbf{k}}^{\text{Hub}} = [\hbar^2/(mb^2)][3 - \cos(k_x b) - \cos(k_y b) - \cos(k_z b)]$ (as already mentioned in subsection III B). This leads to $K_3 \simeq 3.175\,911\,6$. Again, both r_e and R_e differ from zero:

$$r_e \simeq -0.305\,718b \quad \text{and} \quad R_e \simeq -0.264\,659b. \quad (119)$$

In an attempt to reduce the dependence of the Monte Carlo results on the grid spacing b, a zero-effective-range dispersion relation was constructed [122,150],

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}[1 - C(kb/\pi)^2], \quad (120)$$

with $C \simeq 0.257\,022$ and used in real simulations [150]. The corresponding $K_3 \simeq 2.899\,952$. Unfortunately, this leads to a sizable R_e:

$$R_e \simeq -0.168b. \quad (121)$$

As envisioned in Ref. [116] one may look for dispersion relations with $r_e = R_e = 0$. We have found an example of such a *magic* dispersion relation:

$$\epsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}}^{\text{Hub}}[1 + \alpha X + \beta X^2] \quad \text{with} \quad X = \frac{\epsilon_{\mathbf{k}}^{\text{Hub}}}{6\hbar^2/(mb^2)}. \quad (122)$$

Two sets of parameters are possible. The first choice is

$$\alpha \simeq 1.470\,885 \quad \text{and} \quad \beta \simeq -2.450\,725, \quad (123)$$

which leads to $K_3 \simeq 3.137\,788$. The second choice is

$$\alpha \simeq -1.728\,219 \quad \text{and} \quad \beta \simeq 12.838\,540, \quad (124)$$

which leads to $K_3 \simeq 1.949\,671$. Other examples of magic dispersion relation can be found [151].

3. *Single-particle momentum-cutoff model*

A continuous-space model used in particular in Ref. [57] takes a Dirac δ interaction potential $g_0\delta(\mathbf{r}_i - \mathbf{r}_j)$ between particles i and j and regularizes the theory by introducing a cutoff Λ on all the single-particle wave vectors. Due to the conservation of momentum one needs to evaluate the T matrix only between states with the same total momentum $\hbar\mathbf{K}$. Due to the contact interaction the resulting matrix element depends only on $\mathbf{K}$ and on E and is noted as $t(\mathbf{K},E)$. Expressing g_0 in terms of the s-wave scattering length as in Ref. [57], one gets

$$\frac{1}{t\,(\mathbf{K},E)} = \frac{m}{4\pi\hbar^2 a} - \int_{\mathbb{R}^3}\frac{d^3q}{(2\pi)^3}\left[\frac{\theta\,(\Lambda - q)}{2\epsilon_{\mathbf{q}}} + \frac{\theta\big(\Lambda - \big|\frac{1}{2}\mathbf{K}+\mathbf{q}\big|\big)\theta\big(\Lambda - \big|\frac{1}{2}\mathbf{K}-\mathbf{q}\big|\big)}{E + i0^+ - \epsilon_{\frac{1}{2}\mathbf{K}+\mathbf{q}} - \epsilon_{\frac{1}{2}\mathbf{K}-\mathbf{q}}}\right], \quad (125)$$

where $\epsilon_{\mathbf{q}} = \hbar^2 q^2/(2m)$ for all $\mathbf{q}$. Introducing the relative wave number k such that $E - \hbar^2 K^2/(4m) = \hbar^2 k^2/m$, $k \in \mathbb{R}^+$, or $k \in i\mathbb{R}^+$, we obtain the low-wave-numbers expansion

$$\frac{1}{t\,(\mathbf{K},E)} = \frac{m}{4\pi\hbar^2}\left(\frac{1}{a} + ik - \frac{K}{2\pi} - \frac{1}{2}r_e k^2 - \frac{1}{2}R_e K^2\right) + \cdots. \quad (126)$$

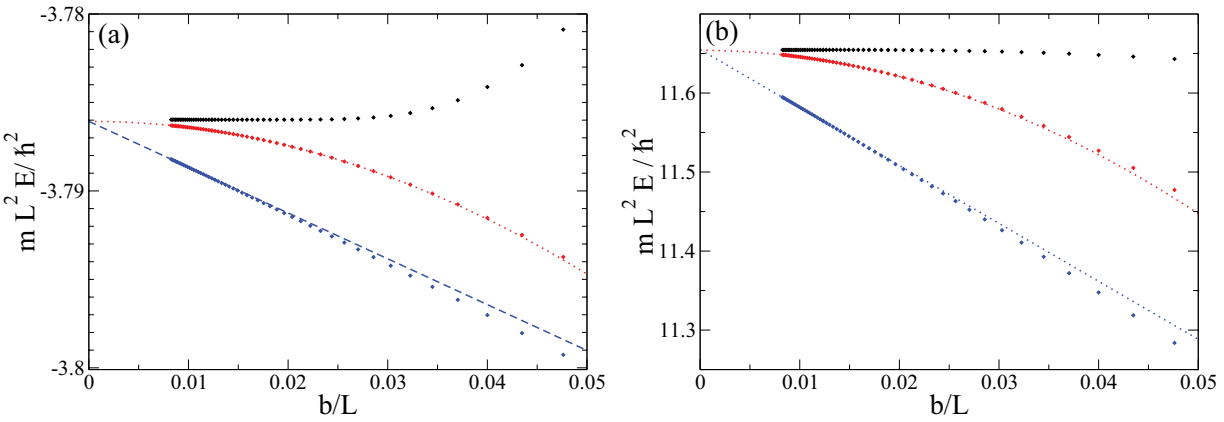

FIG. 1. (Color online) Illustration of Juillet effect for lattice model: In the cubic box $[0,L]^3$ with periodic boundary conditions, ground-state energy of two opposite spin fermions as a function of the grid spacing b, for an infinite scattering length ($1/a = 0$), for a total momentum equal to $\mathbf{0}$ in (a) and equal to $(2\pi\hbar/L)\mathbf{e}_z$ in (b). Three dispersion relations $\epsilon_{\mathbf{k}}$ are considered, the quartic one of Eq. (120) with zero effective range $r_e = 0$ (in blue, lower set), and the magic one (122) with $r_e = R_e = 0$ with the parameters of Eq. (123) (in black, upper set) and of Eq. (124) (in red, middle set). The fact that the energy varies linearly in b for the $r_e = 0$ quartic dispersion relation at zero total momentum is the Juillet effect explained in Sec. VII C, and the corresponding dashed line is the analytical result (134). At nonzero total momentum the quartic dispersion relation leads to an energy variation linear in b as expected, for example, from the fact that it has a nonzero R_e (the dotted line is a linear fit for $b/L \leqslant 0.01$). The magic dispersion relations lead to a $O(b^2)$ variation of the energy both at zero and nonzero total momentum (the dotted lines are purely quadratic fits performed for $b/L \leqslant 0.02$).

The effective range is given by $r_e = 4/(\pi\Lambda)$ and the length $R_e = r_e/12$.[26] The unfortunate feature of this model is the occurrence of a term linear in K, that does not disappear even if $\Lambda \to +\infty$: The model thus does *not* reproduce the universal zero-range model in the large-cutoff limit, as soon as pairs of particles have a nonzero total momentum. Note that, here, one cannot exchange the order of the integration over $\mathbf{q}$ and the $\Lambda \to \infty$ limit. As a concrete illustration of the breaking of the Galilean invariance, for $a > 0$ and in the limit $\Lambda \to +\infty$, it is found (e.g., by calculating the pole of the T matrix) that the total energy of a free-space dimer of total momentum $\hbar\mathbf{K}$ is

$$E_{\mathrm{dim}}^{\mathrm{model}}(\mathbf{K}) = \frac{\hbar^2 K^2}{4m} - \frac{\hbar^2}{m}\left(\frac{1}{a} - \frac{K}{2\pi}\right)^2 \qquad (127)$$

and that this dimer state exists only for $K < 2\pi/a$.[27]

4. *Single-particle momentum-cutoff lattice model*

A spherical momentum cutoff was also introduced for a lattice model in Refs. [53,56,155,156]. Our understanding is that this amounts to taking the following dispersion relation inside the first Brillouin zone: $\epsilon_{\mathbf{k}} = \hbar^2 k^2/(2m)$ for $k < \pi/b$, $\epsilon_{\mathbf{k}} = +\infty$ otherwise. The T matrix is then given by Eq. (113), where for $\mathbf{K} \neq \mathbf{0}$ one extends $\epsilon_{\mathbf{k}}$ by periodicity out of the first Brillouin zone. By distinguishing three zones within the integration domain for $\mathbf{q}$, similarly to the note,[25] and restricting for simplicity to $E = \hbar^2 K^2/(4m)$, we find the same undesired term $-K/(2\pi)$ as in Eq. (126), implying that the model does not reproduce the unitary gas even for $b \to 0$.

C. Juillet effect for lattice models

With the lattice dispersion relation $\epsilon_{\mathbf{k}}$ of Eq. (120), adjusted to have a zero effective range $r_e = 0$, Juillet numerically observed, for two particles in the cubic box $[0,L]^3$ with periodic boundary conditions and zero total momentum, that the first energy correction to the zero-range limit $b \to 0$ is linear in b [151], which seems to contradict Table V, Eq. (1a). This is illustrated in Fig. 1. This cannot be explained by a nonzero R_e [defined in Eq. (116)] because the two opposite-spin fermions have here a zero total momentum.

This Juillet effect, as we shall see, is due to the fact that the *integral* of $1/\epsilon_{\mathbf{k}}$ over $\mathbf{k}$ in the first Brillouin zone and the corresponding *discrete sum* for the finite-size quantization box differ for $b/L \to 0$ not only by a constant term but also by a term linear in b, when the dispersion relation has a cusp at the surface of the first Brillouin zone, such as Eq. (120). The Juillet effect thus disappears in the thermodynamic limit. This explains why it does not show up in the diagrammatic point of view of Sec. VII B, which was considered in the thermodynamic limit, so that only momentum integrals appeared. This also shows that the Juillet effect does not invalidate Table V, Eq. (1a) since it was derived for an interaction that is smooth in momentum space.

In Ref. [149] it was shown that the lattice model spectrally reproduces the zero-range model when the grid spacing $b \to 0$. We now simply extend the reasoning of Ref. [149] for two particles to first order in b included. For an eigenenergy E which does not belong to the noninteracting spectrum, the

[26] The integration can be performed in spherical coordinates of polar axis the direction of $\mathbf{K}$.

[27] This problem does not show up in recent studies of the fermionic polaron problem [152,153] since the momentum cutoff is introduced only for the majority atoms and not for the impurity (see Ref. [154]).

exact implicit equation is

$$\frac{1}{g_0}+\frac{1}{L^3}\sum_{\mathbf{k}\in D}\frac{1}{2\epsilon_{\mathbf{k}}-E}=0, \tag{128}$$

where the notation with a discrete sum over $\mathbf{k}$ implicitly restricts $\mathbf{k}$ to $(2\pi/L)\mathbb{Z}^3$. By adding and subtracting terms and using expressions (11) and (115) for the bare coupling constant g_0 and the effective range r_e, one obtains the useful form

$$\frac{1}{g}-\frac{m^2Er_e}{8\pi\hbar^4}+\frac{1}{L^3}\left[-\frac{1}{E}+\sum_{\mathbf{k}\in D^*}F(\epsilon_{\mathbf{k}})+\sum_{\mathbf{k}\in\mathbb{R}^{3*}}\frac{E}{(\hbar^2k^2/m)^2}\right] = R_1+ER_2-ER_3 \tag{129}$$

with $g=4\pi\hbar^2a/m$ and $F(\epsilon)=(2\epsilon-E)^{-1}-(2\epsilon)^{-1}-E/(2\epsilon)^2$. We have defined

$$R_1\equiv\int_D\frac{d^3k}{(2\pi)^3}\frac{1}{2\epsilon_{\mathbf{k}}}-\frac{1}{L^3}\sum_{\mathbf{k}\in D^*}\frac{1}{2\epsilon_{\mathbf{k}}}, \tag{130}$$

proportional to the function $C(b)$ introduced in Ref. [149]. The quantities R_2 and R_3 have the same structure: R_2 is obtained by replacing in R_1 the function $1/(2\epsilon_{\mathbf{k}})$ by $1/(2\epsilon_{\mathbf{k}})^2-1/(\hbar^2k^2/m)^2$, in the integral and in the sum; R_3 is obtained by replacing in R_1 the function $1/(2\epsilon_{\mathbf{k}})$ by $1/(\hbar^2k^2/m)^2$ and the set D by $\mathbb{R}^3\setminus D$, both for the integration and for the summation.

We now take $b\to 0$ in Eq. (129), keeping terms up to $O(b)$ included. Since $F(\epsilon)=O(1/\epsilon^3)$ at large ϵ, we can replace $F(\epsilon_{\mathbf{k}})$ by its $b\to 0$ limit $F(\hbar^2k^2/(2m))$, and the summation set D^* by its $b\to 0$ limit:[28]

$$\sum_{\mathbf{k}\in D^*}F(\epsilon_{\mathbf{k}})\underset{b\to 0}{=}\sum_{\mathbf{k}\in\mathbb{R}^{3*}}F\left(\frac{\hbar^2k^2}{2m}\right)+O(b^2). \tag{131}$$

In the quantities R_i, we perform the change of variables $\mathbf{k}=2\pi\mathbf{q}/b$, and we write the dispersion relation as

$$\epsilon_{\mathbf{k}}=\frac{(2\pi\hbar)^2}{mb^2}\eta_{\mathbf{k}b/(2\pi)}, \tag{132}$$

where the dimensionless $\eta_{\mathbf{q}}$ does not depend on the lattice spacing b. We then find that bR_1, R_2/b, and R_3/b are differences between a converging integral and a three-dimensional Riemann sum with a vanishing cell volume $(b/L)^3$. As these differences vanish as $O(b)$, we conclude that $R_2=O(b^2)$ and $R_3=O(b^2)$ can be neglected in Eq. (129). This however leads only to $R_1=O(1)$, so that more mathematical work needs to be done, as detailed in Appendix F, to obtain

$$\frac{\hbar^2}{m}LR_1\underset{b\to 0}{=}\frac{\mathcal{C}}{4\pi^2}+\frac{\pi R_e^{\rm surf}}{2L}+O\left(b/L\right)^2. \tag{133}$$

The numerical constant $\mathcal{C}\simeq 8.913\,63$ was calculated and called $C(0)$ in Ref. [149]. $R_e^{\rm surf}$ remarkably is the surface contribution to the quantity R_e in Eq. (116), it scales as b. It is nonzero only when the dispersion relation has a cusp at the surface of the first Brillouin zone. In this case, R_1 varies to first order in b, which comes in addition to the expected linear contribution of the Er_e term in Eq. (129): This leads to the Juillet effect. More quantitatively, the first deviation of the eigenenergy from its zero-range limit E^0, shown as a dashed line in Fig. 1(a), is[29]

$$E-E^0\underset{b\to 0}{\sim}\frac{\frac{m^2E^0r_e}{8\pi\hbar^4}+\frac{m\pi R_e^{\rm surf}}{2\hbar^2L^2}}{\frac{1}{L^3}\sum_{\mathbf{k}\in\mathbb{R}^3}\frac{1}{(\frac{\hbar^2k^2}{m}-E^0)^2}}. \tag{134}$$

D. Link between $\partial E/\partial r_e$ and subleading short-distance behavior of pair distribution function

As shown by Table II, Eqs. (3a) and (3b), the short-distance behavior of the pair distribution function (averaged over the center-of-mass position of the pair) diverges as $1/r^2$ in 3D and as $\ln^2 r$ in 2D, with a coefficient proportional to C; that is, related to the derivative of the energy with respect to the scattering length a. Here, we show that a subleading term in this short-distance behavior is related to the derivative of the energy with respect to the effective range r_e. To this end, we explicitly write the next-order term in the contact conditions Table I, Eqs. (1a) and (1b).

Three dimensions. Including the next-order term in Table I, Eq. (1a) gives

$$\begin{aligned}\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)&\underset{r_{ij}\to 0}{=}\left(\frac{1}{r_{ij}}-\frac{1}{a}\right)A_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j})+r_{ij}\;B_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j})\\&+\sum_{\alpha=1}^{3}r_{ij,\alpha}L_{ij}^{(\alpha)}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j})+O\left(r_{ij}^2\right),\end{aligned} \tag{135}$$

where we have distinguished between a *singular* part linear with the interparticle distance r_{ij} and a *regular* part linear in the relative coordinates of i and j ($r_{ij,\alpha}$ is the component along axis α of the vector $\mathbf{r}_{ij}$). Injecting this form into Schrödinger's equation, keeping the resulting $\propto 1/r_{ij}$ terms and using the notation of Table V, Eq. (2) gives

$$B_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j})=-\frac{m}{2\hbar^2}(E-\mathcal{H}_{ij})A_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}). \tag{136}$$

Table V, Eq. (1a) thus becomes

$$\frac{\partial E}{\partial r_e}=-\frac{4\pi\hbar^2}{m}(A,B). \tag{137}$$

We square Eq. (135) and, as in Sec. IV B, we integrate over $\mathbf{R}_{ij}$, the $\mathbf{r}_k$, and we sum over $i<j$. We further average $G^{(2)}_{\uparrow\downarrow}(\mathbf{r})$ over the direction of $\mathbf{r}$ to eliminate the contribution of the regular term L_{ij}, defining $\bar{G}^{(2)}_{\uparrow\downarrow}(\mathbf{r})=[G^{(2)}_{\uparrow\downarrow}(\mathbf{r})+G^{(2)}_{\uparrow\downarrow}(-\mathbf{r})]/2$. We obtain Table V, Eq. (3a).

[28] One has $\epsilon_{\mathbf{k}}=[\hbar^2k^2/(2m)][1+O(k^2b^2)]$. For the finite number low-energy terms, we directly use this fact. For the other terms, such that $\epsilon_{\mathbf{k}}\gg|E|$ and $\gg(2\pi\hbar)^2/(mL^2)$, we use $F(\epsilon_{\mathbf{k}})-F(\frac{\hbar^2k^2}{2m})\simeq(\epsilon_{\mathbf{k}}-\frac{\hbar^2k^2}{2m})F'(\frac{\hbar^2k^2}{2m})=O(b^2/k^4)$ which is integrable at large k in 3D and leads to a total error $O(b^2)$.

[29] The contribution proportional to r_e in Eq. (134) can also be obtained from Table V, Eq. (1a) and from the fact that $\sum_{\mathbf{k}\neq\mathbf{0}}e^{i\mathbf{k}\cdot\mathbf{r}}/k^2\sim L^3/(4\pi r)$ for $r\to 0$.

Two dimensions. Including next-order terms in Table I, Eq. (1b) gives[30]

$$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) \underset{r_{ij}\to 0}{=} \ln(r_{ij}/a)A_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}) + r_{ij}^2 \ln r_{ij}\ B_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}) + \sum_{\alpha=1}^{2} r_{ij,\alpha} L_{ij}^{(\alpha)}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}) + O\left(r_{ij}^2\right). \tag{138}$$

Proceeding as in 3D we obtain

$$B_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}) = -\frac{m}{4\hbar^2}(E-\mathcal{H}_{ij})A_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}). \tag{139}$$

Table V, Eq. (1b) thus becomes

$$\frac{\partial E}{\partial\left(r_e^2\right)} = -\frac{4\pi\hbar^2}{m}(A,B). \tag{140}$$

These equations finally leads to Table V, Eq. (3b).

E. Link between $\partial E/\partial r_e$ and $1/k^6$ subleading tail of momentum distribution

A general idea given in Ref. [91] is that singular terms in the dependence of ψ on the interparticle distance r_{ij} (at short distances) reflect into power-law tails in the momentum distribution $n_\sigma(\mathbf{k})$ given by Eq. (23). In Sec. IV A, we restricted to the leading order. Here, we include the subleading term and we follow the same reasoning as in Sec. IV A to obtain[31,32]

$$\bar{n}_\sigma(k) \underset{k\to\infty}{=} \frac{C}{k^4} + \frac{D}{k^6} + \cdots, \tag{141}$$

where $\bar{n}_\sigma(k) = \frac{1}{d}\sum_{i=1}^{d} n_\sigma(k\mathbf{u}_i)$ and D is the linear combination of $\partial E/\partial r_e$ and $(A,\Delta_{\mathbf{R}}A)$ given in Table V, Eqs. (4a) and (4b). Physically, the extra term $(A,\Delta_{\mathbf{R}}A)$ results from the fact that the wave vector $\mathbf{k}_1$ of a particle in an $\uparrow\downarrow$ colliding pair is a linear combination of the relative wave vector $\mathbf{k}_{\rm rel}$ and of the center-of-mass wave vector $\mathbf{K}$ of the pair, so that, even if the probability distribution of $\mathbf{k}_{\rm rel}$ was exactly scaling as $1/k_{\rm rel}^4$, a nonzero $\mathbf{K}$ would generate a subleading $1/k_1^6$ contribution in the single-particle momentum distribution.

This is apparent for the simple case of a free-space dimer: When the dimer is at rest, $\psi(\mathbf{r}_1,\mathbf{r}_2) = \phi_{\rm dim}(r_{12})$, $A_{12}(\mathbf{R}_{12})$ is uniform and the extra term vanishes. When it has a momentum $\mathbf{K}$, $\psi(\mathbf{r}_1,\mathbf{r}_2) = e^{i\mathbf{K}\cdot\mathbf{R}_{12}}\phi_{\rm dim}(r_{12})$, which shifts the single-particle momentum distribution, $n_\uparrow^{\rm mov}(\mathbf{k}) = n_\uparrow^{\rm rest}(\mathbf{k}-\mathbf{K}/2)$. Applying this shift to the momentum tail C/k^4 gives, after continuous average over the direction of $\mathbf{k}$, a subleading $\delta D^{\rm mov}/k^6$ contribution, with $\delta D^{\rm mov} = CK^2/2$ in 3D and $\delta D^{\rm mov} = CK^2$ in 2D. Remarkably, the ratio of the extra term to C is proportional to the pair–center-of-mass kinetic energy.

In the N-body case, one can generalize this property by defining the mean center-of-mass kinetic energy of a $\uparrow\downarrow$ pair at *vanishing* pair diameter, which is allowed in quantum mechanics since the center-of-mass operators and the relative-particle operators commute.[33] By a direct generalization of the pair distribution function of Sec. IV B, one has for the opposite-spin pair density operator $\langle\mathbf{r}_\uparrow,\mathbf{r}_\downarrow|\hat{\rho}^{(2)}_{\uparrow\downarrow}|\mathbf{r}'_\uparrow,\mathbf{r}'_\downarrow\rangle = \langle\hat{\psi}^\dagger_\uparrow(\mathbf{r}'_\uparrow)\hat{\psi}^\dagger_\downarrow(\mathbf{r}'_\downarrow)\hat{\psi}_\downarrow(\mathbf{r}_\downarrow)\hat{\psi}_\uparrow(\mathbf{r}_\uparrow)\rangle$. Whereas the usual pair–center-of-mass density operator is obtained by taking the trace over the relative coordinates $\mathbf{r} = \mathbf{r}_\uparrow - \mathbf{r}_\downarrow$, we rather define it here by taking the limit of vanishing relative coordinates,

$$\langle\mathbf{R}|\hat{\rho}^{(2)}_{\rm CoM}|\mathbf{R}'\rangle = \mathcal{N}\lim_{r\to 0}\frac{\left\langle\mathbf{R}+\frac{\mathbf{r}}{2},\mathbf{R}-\frac{\mathbf{r}}{2}\middle|\hat{\rho}^{(2)}_{\uparrow\downarrow}\middle|\mathbf{R}'+\frac{\mathbf{r}}{2},\mathbf{R}'-\frac{\mathbf{r}}{2}\right\rangle}{\phi^2(\mathbf{r})}, \tag{142}$$

where the factor $\mathcal{N}$ is such that $\hat{\rho}^{(2)}_{\rm CoM}$ has a unit trace and $\phi(\mathbf{r})$ is the zero-energy scattering state of Eqs. (9) and (10). Proceeding as in Sec. IV B we obtain

$$\langle\mathbf{R}|\hat{\rho}^{(2)}_{\rm CoM}|\mathbf{R}'\rangle = \mathcal{N}\sum_{i<j}\int\left(\prod_{k\neq i,j} d^d r_k\right) A^*_{ij}(\mathbf{R}',(\mathbf{r}_k)_{k\neq i,j}) \times A_{ij}(\mathbf{R},(\mathbf{r}_k)_{k\neq i,j}). \tag{143}$$

By taking the expectation value of $-(\hbar^2/4m)\Delta_{\mathbf{R}}$ within $\hat{\rho}^{(2)}_{\rm CoM}$, we finally obtain for the mean pair–center-of-mass kinetic energy at vanishing diameter:

$$E^{r_{\uparrow\downarrow}\to 0}_{\rm kin\ pair-CoM} = -\frac{\hbar^2}{4m}\frac{(A,\Delta_{\mathbf{R}}A)}{(A,A)}, \tag{144}$$

where the denominator is $\propto C$ [see Table II, Eqs. (2a) and (2b)].

VIII. GENERALIZATION TO ARBITRARY STATISTICAL MIXTURES

In this section, we generalize some of the relations derived in the previous sections for pure states to the case of arbitrary statistical mixtures. Let us first discuss zero-range interactions. We consider a statistical mixture of pure states ψ_n with occupation probabilities p_n, which is arbitrary, but nonpathological in the following sense [97]: Each ψ_n satisfies the contact condition [Table I, Eqs. (1a) and (1b)]; moreover, p_n decays sufficiently quickly at large n so that we have $C = \sum_n p_n C_n$, where C_n (resp. C) is defined by Table II, Eq. (1) with $n_\sigma(\mathbf{k}) = \langle c^\dagger_\sigma(\mathbf{k})c_\sigma(\mathbf{k})\rangle$ and $\langle\cdot\rangle = \langle\psi_n|\cdot|\psi_n\rangle$ (respectively,

[30] From Schrödinger's equation, $\Delta_{\mathbf{r}_{ij}}\psi$ diverges at most as ψ itself; that is, as $\ln r_{ij}$, for $r_{ij}\to 0$. The particular solution $f(r) = \frac{1}{4}r^2(\ln r - 1)$ of $\Delta_{\mathbf{r}} f(r) = \ln r$ fixes the form of the subleading term in ψ.

[31] In 3D we used the identity $\int d^3r e^{i\mathbf{k}\cdot\mathbf{r}}/r = 4\pi/k^2$ and its derivatives with respect to k_α; for example, taking the Laplacian with respect to $\mathbf{k}$ gives $\int d^3r e^{i\mathbf{k}\cdot\mathbf{r}} r = -8\pi/k^4$. Equivalently, one can use the relation $\int d^3r e^{i\mathbf{k}\cdot\mathbf{r}}\frac{u(r)}{r} = \frac{4\pi}{k^2}u(0) - \frac{4\pi}{k^4}u^{(2)}(0) + O(1/k^6)$ and its derivatives with respect to k_α; this relations holds for any $u(r)$ which has a series expansion in $r=0$ and rapidly decreases at ∞. In 2D for $k>0$ we used the identity $\int d^2r e^{i\mathbf{k}\cdot\mathbf{r}}\ln r = -2\pi/k^2$ and its derivatives with respect to k_α. The regular terms involving $L_{ij}^{(\alpha)}$ have (as expected) a negligible contribution to the tail of $n_\sigma(\mathbf{k})$.

[32] The configurations with three close particles contribute to the tail of $n_\sigma(\mathbf{k})$ as $1/k^{5+2s}$, see a note of Ref. [98], with s defined in Sec. X B, which is negligible for $s > 1/2$.

[33] Similarly, a "contact current" was recently introduced in Ref. [157], whose spatial integral is proportional to $(A,\nabla_{\mathbf{R}}A)$.

$\langle\cdot\rangle = \sum_n p_n \langle\psi_n|\cdot|\psi_n\rangle$). Then, the relations in lines 3, 5, 6, and 7 of Table II, which were derived in Sec. IV for any pure state satisfying the contact conditions, obviously generalize to such a statistical mixture. The relations for the time derivative of E (Table II line 12) hold for any time-evolving pure state satisfying the contact conditions for a time-dependent $a(t)$, and thus also for any statistical mixture of such time-evolving pure states.

For lattice models, one can obviously take an average of the definition of $\hat{C}$ [Table III, Eqs. (1a) and (1b)] to define $C = \langle\hat{C}\rangle$ for in any statistical mixture; taking averages of the relations between operators [Table III, lines 2, 3, and 8] then gives relations valid for any statistical mixture.

IX. THERMODYNAMIC EQUILIBRIUM IN CANONICAL ENSEMBLE

We now turn to the case of thermal equilibrium in the canonical ensemble. We use the notation

$$\lambda \equiv \begin{cases} -1/a & \text{in} \quad 3\text{D} \\ \frac{1}{2}\ln a & \text{in} \quad 2\text{D}. \end{cases} \tag{145}$$

A. First-order derivative of E

The thermal average in the canonical ensemble $\overline{dE/d\lambda}$ can be rewritten in the following more familiar way, as detailed in Appendix G:

$$\overline{\left(\frac{dE}{d\lambda}\right)} = \left(\frac{dF}{d\lambda}\right)_T = \left(\frac{d\bar{E}}{d\lambda}\right)_S, \tag{146}$$

where $\overline{(\cdots)}$ is the canonical thermal average, F is the free energy, and S is the entropy. Taking the thermal average of Table II, Eqs. (4a) and (4b) (which was shown above for any stationary state) thus gives Table II, Eqs. (9a) and (9b).

B. Second-order derivative of E

Taking a thermal average of the line 8 in Table II we get, after a simple manipulation,

$$\frac{1}{2}\overline{\left(\frac{d^2E}{d\lambda^2}\right)} = \left(\frac{4\pi\hbar^2}{m}\right)^2 \frac{1}{2Z} \sum_{n,n';E_n\neq E_{n'}} \frac{e^{-\beta E_n} - e^{-\beta E_{n'}}}{E_n - E_{n'}} \times |(A^{(n')}, A^{(n)})|^2, \tag{147}$$

where $Z = \sum_n \exp(-\beta E_n)$. This implies

$$\overline{\left(\frac{d^2E}{d\lambda^2}\right)} < 0. \tag{148}$$

Moreover, one can check that

$$\left(\frac{d^2F}{d\lambda^2}\right)_T - \overline{\left(\frac{d^2E}{d\lambda^2}\right)} = -\beta\left[\overline{\left(\frac{dE}{d\lambda}\right)^2} - \overline{\left(\frac{dE}{d\lambda}\right)}^2\right] < 0, \tag{149}$$

which implies Table II, Eqs. (10a) and (10b). In usual cold-atom experiments, however, there is no thermal reservoir imposing a fixed temperature to the gas; one rather can achieve adiabatic transformations by a slow variation of the scattering length of the gas [158–160] where the entropy is fixed [161–163]. One also more directly accesses the mean energy $\bar{E}$ of the gas rather than its free energy, even if the entropy is also measurable [38,39]. The second-order derivative of $\bar{E}$ with respect to λ for a fixed entropy is thus the relevant quantity to consider. As shown in Appendix G one has in the canonical ensemble

$$\left(\frac{d^2\bar{E}}{d\lambda^2}\right)_S = \overline{\left(\frac{d^2E}{d\lambda^2}\right)} + \frac{\left[\mathrm{Cov}\left(E, \frac{dE}{d\lambda}\right)\right]^2 - \mathrm{Var}(E)\mathrm{Var}\left(\frac{dE}{d\lambda}\right)}{k_B T \mathrm{Var}(E)}, \tag{150}$$

where $\mathrm{Var}(X)$ and $\mathrm{Cov}(X,Y)$ stand for the variance of the quantity X and the covariance of the quantities X and Y in the canonical ensemble, respectively. From the Cauchy-Schwarz inequality $[\mathrm{Cov}(X,Y)]^2 \leqslant \mathrm{Var}(X)\mathrm{Var}(Y)$, and from the inequality (148), we thus obtain Table II, Eqs. (11a) and (11b).

For lattice models, the inequalities Table III, Eq. (7) are derived in the same way, by taking λ now equal to g_0 and starting from the expression Table III, Eq. (6) of d^2E_n/dg_0^2. For the case of a finite-range interaction potential $V(r)$ in continuous space, the relations Table IV, lines 1–3 which were derived for an arbitrary stationary state are generalized to the thermal equilibrium case in the same way. Finally, the relations which asymptotically hold in the zero-range regime [Table III lines 9 and 10] for lattice models and Table IV lines 4 and 5 for finite-range interaction-potential models, which were justified for any eigenstate in the zero-range regime $k_{\mathrm{typ}}b \ll 1$ where the typical relative wave vector k_{typ} is defined in terms of the considered eigenstate as described in Sec. III, remain true at thermal equilibrium with k_{typ} now defined as the typical density- and temperature-dependent wave vector described in Sec. III, since all the eigenstates which are thermally populated with a non-negligible weight are expected to have a typical wave vector smaller or on the order of the thermal-equilibrium typical wave vector.

C. Quantum-mechanical adiabaticity

To be complete, we also consider the process where λ is varied so slowly that there is adiabaticity in the many-body quantum-mechanical sense: The adiabatic theorem of quantum mechanics [164] implies that, in the limit where λ is changed infinitely slowly, the occupation probabilities of each eigenspace of the many-body Hamiltonian do not change with time, even in presence of level crossings [165]. We note that this may require macroscopically long evolution times for a large system. For an initial equilibrium state in the canonical ensemble, the mean energy then varies with λ as

$$E_{\mathrm{adiab}}^{\mathrm{quant}}(\lambda) = \sum_n \frac{e^{-\beta_0 E_n(\lambda_0)}}{Z_0} E_n(\lambda), \tag{151}$$

where the subscript 0 refers to the initial state. Taking the second-order derivative of Eq. (151) with respect to λ in $\lambda = \lambda_0$ gives

$$\frac{d^2 E_{\mathrm{adiab}}^{\mathrm{quant}}}{d\lambda^2} = \overline{\left(\frac{d^2E}{d\lambda^2}\right)} < 0. \tag{152}$$

Note that the sign of the second-order derivative of $E^{\rm quant}_{\rm adiab}$ remains negative at all λ provided one assumes that there is no level crossing in the many-body spectrum when λ is varied: $E_n(\lambda) - E_{n'}(\lambda)$ has the same sign as $E_n(\lambda_0) - E_{n'}(\lambda_0)$ for all indices n,n', which allows us to conclude on the sign with the same manipulation as that which led to Eq. (147).

Thermodynamic vs quantum adiabaticity. The result of the isentropic transformation [Eq. (150)] and the one of the adiabatic transformation in the quantum sense (152) differ by the second term on the right-hand side of Eq. (150). *A priori* this term is extensive and thus not negligible compared to the first term. We have explicitly checked this expectation for the Bogoliubov model Hamiltonian of a weakly interacting Bose gas, which is however not really relevant since this Bogoliubov model corresponds to the peculiar case of an integrable dynamics.

For a quantum ergodic system we now show that the second term in the right-hand side of Eq. (150) is negligible in the thermodynamic limit, as a consequence of the eigenstate thermalization hypothesis [166–169]. This hypothesis was tested numerically for several interacting quantum systems [170–172]. It states that, for a large system, the expectation value $\langle\psi_n|\hat{O}|\psi_n\rangle$ of a few-body observable $\hat{O}$ in a single eigenstate $|\psi_n\rangle$ of energy E_n can be identified with the microcanonical average $O_{\rm mc}(E_n)$ of $\hat{O}$ at that energy. Here, the relevant operator $\hat{O}$ is the two-body observable (the so-called *contact operator*) such that $\frac{d}{d\lambda}E_n = \langle\psi_n|\hat{O}|\psi_n\rangle$. In the canonical ensemble, the energy fluctuations scale as $\mathcal{V}^{1/2}$ where $\mathcal{V}$ is the system volume. We can thus expand the microcanonical average around the mean energy $\bar{E}$:

$$O_{\rm mc}(E) = O_{\rm mc}(\bar{E}) + (E-\bar{E})O'_{\rm mc}(\bar{E}) + O(1). \qquad (153)$$

To leading order, we then find that $\mathrm{Cov}(E,\frac{dE}{d\lambda}) \sim O'_{\rm mc}(\bar{E})\mathrm{Var}E$ and $\mathrm{Var}(\frac{dE}{d\lambda}) \sim [O'_{\rm mc}(\bar{E})]^2\mathrm{Var}E$, so that the second term in the right-hand side of Eq. (150) is $O(\mathcal{V}^{1/2})$ which is negligible as compared to the first term on that right-hand side. For the considered quantity, this shows the equivalence of the thermodynamic adiabaticity and of the quantum adiabaticity for a large system.

A microcanonical detour. We now argue that the quantum adiabatic expression (151) for the mean energy as a function of the slowly varying parameter λ can be obtained by a purely thermodynamic reasoning. This implies that the exponentially long evolution times *a priori* required to reach the quantum adiabatic regime for a large system are actually not necessary to obtain Eq. (151). The first step is to realize that the initial canonical ensemble (for $\lambda = \lambda_0$) can be viewed as a statistical mixture of microcanonical ensembles [173]. These microcanonical ensembles correspond to nonoverlapping energy intervals of width Δ, each interval contains many eigenstates, but Δ is much smaller than the width of the probability distribution of the system energy in the canonical ensemble. For further convenience, we take $\Delta \ll k_BT$. One can label each energy interval by its central energy value, or more conveniently by its entropy S. If the eigenenergies $E_n(\lambda)$ are numbered in ascending order, the initial microcanonical ensemble of entropy S contains the eigenenergies with $n_1(S) \leqslant n < n_2(S)$ and $S = k_B\ln[n_2(S) - n_1(S)]$. When λ is slowly varied, the entropy is conserved for our isolated system, and the microcanonical ensemble simply follows the evolution of the initial $n_2(S) - n_1(S)$ eigenstates, which cannot cross for an ergodic system and remain bunched in energy space. Furthermore, according to the eigenstate thermalization hypothesis, the energy width $E_{n_2} - E_{n_1}$ remains close to its initial value Δ: Each eigenenergy varies with a macroscopically large slope $dE_n/d\lambda$ but all the eigenenergies in the microcanonical ensemble have essentially the same slope.[34] The mean microcanonical energy for this isentropic evolution is thus

$$E_{\rm mc}(S,\lambda) = \frac{1}{n_2(S) - n_1(S)}\sum_{n=n_1(S)}^{n_2(S)-1} E_n(\lambda). \qquad (154)$$

Finally, we take the appropriate statistical mixture of the microcanonical ensembles (so as to reconstruct the initial $\lambda = \lambda_0$ canonical ensemble): The microcanonical ensemble of entropy S has an initial central energy $E_{\rm mc}(S,\lambda_0)$; it is weighted in the statistical mixture by the usual expression $P(S) = e^{S/k_B}e^{-\beta E_{\rm mc}(S,\lambda_0)}$. Since $\Delta \ll k_BT$, one can identify $e^{-\beta E_{\rm mc}(S,\lambda_0)}$ with $e^{-\beta E_n(\lambda_0)}$, for $n_1(S) \leqslant n < n_2(S)$. The corresponding statistical average of Eq. (154) with the weight $P(S)$ gives Eq. (151).

X. APPLICATIONS

In this section, we apply some of the above relations in three dimensions, first to the two-body and three-body problems and then to the many-body problem. Except for the two-body case, we restrict to the infinite-scattering length case $a = \infty$ in three dimensions.

A. Two-body problem in harmonic trap: finite-range corrections

Two particles interact with the compact-support potential $V(r_{12};b)$ of range b and scattering length a in an isotropic harmonic potential $U(\mathbf{r}_i) = \frac{1}{2}m\omega^2r_i^2$. One separates out the center of mass in an eigenstate of energy $E_{\rm c.m.}$. The relative motion is taken with zero angular momentum; its wave function $\psi(r)$ is an eigenstate of energy $E_{\rm rel} = E - E_{\rm c.m.}$ for a particle of mass $\mu = m/2$ in the potential $V(r;b) + \mu\omega^2r^2/2$. We take in this subsection $\hbar\omega$ as the unit of energy and $[\hbar/(\mu\omega)]^{1/2}$ as the unit of length. For $r \geqslant b$ the solution may be expressed in terms of the Whittaker function W or, equivalently, of the Kummer function U (see Sec. 13 in Ref. [174]):

$$\frac{\psi(r)}{C_3} \overset{\rm 3D}{=} \frac{W_{\frac{E_{\rm rel}}{2},\frac{1}{4}}(r^2)}{r^{3/2}} = e^{-\frac{r^2}{2}}U\left(\frac{3}{4} - \frac{E_{\rm rel}}{2},\frac{3}{2},r^2\right), \qquad (155)$$

$$\frac{\psi(r)}{C_2} \overset{\rm 2D}{=} \frac{W_{\frac{E_{\rm rel}}{2},0}(r^2)}{r} = e^{-\frac{r^2}{2}}U\left(\frac{1-E_{\rm rel}}{2},1,r^2\right), \qquad (156)$$

where the factors C_2 and C_3 ensure that ψ is normalized to unity. The zero-range limit, where $V(r;b)$ is replaced by the Bethe-Peierls contact conditions at the origin, is exactly

[34] One has $\frac{d}{d\lambda}(E_{n_2} - E_{n_1}) = O_{\rm mc}(E_{n_2}) - O_{\rm mc}(E_{n_1}) \simeq (E_{n_2} - E_{n_1})O'_{\rm mc}(E_{\rm mc}) = O(\Delta)$, where $O_{\rm mc}$ is the microcanonical expectation value of the contact operator.

solvable; it gives eigenenergies $E^0_{\rm rel}$. We give here the finite-range corrections to the energy in terms of r_e.

Three dimensions. Imposing the contact condition $\psi(r) = A[r^{-1} - a^{-1}] + O(r)$ to Eq. (155) gives an implicit equation for the spectrum in the zero-range limit, obtained in Ref. [175] with a different technique:

$$f\left(E^0_{\rm rel}\right) = -\frac{1}{a} \quad \text{with} \quad f(E) \equiv -\frac{2\Gamma\left(\frac{3}{4} - \frac{E}{2}\right)}{\Gamma\left(\frac{1}{4} - \frac{E}{2}\right)}. \quad (157)$$

We calculated the finite-range corrections up to order two in b included; they remarkably involve only the effective range:

$$E_{\rm rel} = E^0_{\rm rel} + \frac{E^0_{\rm rel} r_e}{f'} + \left(\frac{E^0_{\rm rel} r_e}{f'}\right)^2 \left(\frac{1}{E^0_{\rm rel}} - \frac{f''}{2f'}\right) + O\left(b^3\right), \quad (158)$$

where the first- and second-order derivatives f' and f'' of $f(E)$ are taken in $E = E^0_{\rm rel}$. To obtain this expansion, we have used the result of Appendix D that one can neglect, at this order, the effect of the trapping potential for $r \leqslant b$, so that the wave function is proportional to the free-space scattering state at energy $E_{\rm rel} = \hbar^2 k^2/(2\mu)$, $\psi(r) = \mathcal{A}\chi(r)$. Such an approximation was already proposed in Refs. [133,176,177], without analytical control on the resulting spectral error.[35] We have checked that the term of Eq. (158) linear in r_e coincides with the prediction of Table V, Eq. (1a), due to the fact that, from relation 7.611(4) in Ref. [178], the normalization factor in the zero-range limit obeys $(C^0_3)^2 2\pi^2 f'(E^0_{\rm rel})/\Gamma^2(\frac{3}{4} - \frac{E^0_{\rm rel}}{2}) = 1$.

The term in Eq. (158) linear in r_e was already written explicitly in Ref. [115]. This corresponds to the first-order perturbative use of the modified version of the zero-range model, as put forward in Ref. [126]. It can also be obtained by solving to first order in r_e the self-consistent equation considered in Ref. [131] obtained by replacing a_0 by a_E [see Eq. (5) of Ref. [131]] into Eq. (6) of Ref. [131]. This self-consistent equation was also introduced in Refs. [176] and [177] [see Eqs. (11), (12), and (30) of that reference] with more elaborate forms for a_E. With our notations and units this self-consistent equation is simply

$$f(E) = -u(k = \sqrt{2E}), \quad (159)$$

where $u(k)$ is related to the s-wave scattering amplitude by Eq. (90). The self-consistent equation of Ref. [131] corresponds to the choice $u(k) = 1/a - k^2 r_e/2$ in Eq. (159). We have checked that solving that equation to second order in r_e then exactly gives the term of Eq. (158) that is quadratic in r_e. Our result of Appendix D shows that going to order three in r_e with the self-consistent equation should not give the correct result, since one can then no longer neglect the effect of harmonic trapping within the interaction range. This clarifies the status of that self-consistent equation.

To ascertain this statement, we have calculated the ground-state relative energy up to third order included in b, restricting ourselves for simplicity to an infinite-scattering length, $1/a = 0$.[36] We find

$$E_{\rm rel} = \frac{1}{2} + \frac{r_e}{2\pi^{1/2}} + \frac{2 - \ln 2}{4\pi} r_e^2 + \left[\frac{(1 - \ln 2)(2 - \ln 2)}{4\pi^{3/2}} - \frac{\pi^2 + 12\ln^2 2}{192\pi^{3/2}}\right] r_e^3 - \frac{\lambda_2 + \Lambda_2}{\pi^{1/2}} + O(b^4). \quad (160)$$

Here λ_2 is the coefficient of k^4 in the low-k expansion of $u(k)$, $u(k) = 1/a - k^2 r_e/2 + \lambda_2 k^4 + O(k^6)$, it can be evaluated by a generalized Smorodinski relation [179]. On the contrary, Λ_2 is a new coefficient containing the effect of the trapping potential within the interaction range. It can be expressed in terms of the zero-energy free-space scattering state $\phi(r)$, normalized as in Eq. (9):

$$\Lambda_2 = \int_0^{+\infty} dr r^2 \left[1 - u_0^2(r)\right], \quad (161)$$

with $u_0(r) = r\phi(r)$. Although our derivation is for a compact support potential, we expect that our result is applicable as long as λ_2 and Λ_2 are finite. For both quantities, this requires (for $1/a = 0$) that the interaction potential drops faster than $1/r^5$ [179]. Interestingly, if one expands the self-consistent Eq. (159) up to order b^3 included, one exactly recovers Eq. (160), except for the term Λ_2. This was expected from the fact that the derivation of Eq. (159) in Ref. [177] indeed neglects the trapping potential within the interaction range.

This discussion is illustrated for the particular case of the square-well potential (182) in Fig. 2, with the exact spectrum obtained by matching the logarithmic derivative of a Whittaker M function for $r = b^-$ with the logarithmic derivative of a Whittaker W function for $r = b^+$ as in Eqs. (6.16, 6.17, 6.18) of Ref. [115].[37] In this case, one finds $r_e = b$ [114] and, remarkably, $\Lambda_2 = -2\lambda_2$ so that the difference between the

[35] We employed two equivalent techniques. The first is to match in $r = b$ the logarithmic derivatives of Eqs. (155) and (89) and to expand their inverses up to order b^4 included. Due to Eq. (93) this involves only r_e. The second is to use relation (D6): The matching of $\mathcal{A}\chi$ with Eq. (155) in $r = b$ gives $\mathcal{A}/C_3 = [\pi^{1/2}/\Gamma(3/4 - E_{\rm rel}/2)][1 + O(b^2)]$, and the normalization of ψ to unity, from relation 7.611(4) in Ref. [178] together with the Smorodinski relation (101), gives $dE_{\rm rel}/dr_e$ up to order one in b included, which one integrates to get the result.

[36] The result is based on Appendix D. The simplest calculation is as follows: One first neglects the trapping potential for $r \leqslant b$, one matches the inverse of the logarithmic derivative of the scattering state (89) for $r = b^-$ with the inverse of the logarithmic derivative of Eq. (155) for $r = b^+$, and one expands the resulting equation up to order b^5 included, using relations 13.1.2 and 13.1.3 in Ref. [174] for $r = b^+$. Then one includes the $r < b$ trapping effect by applying the usual first-order perturbation theory to the operator $\frac{1}{2}\mu\omega^2 r^2 \theta(b - r)$; at this order the wave function for $r < b$ may be identified with the zero-energy scattering state $\phi(r)$. An alternative, more complicated technique is to use $\psi^{(1)}$ of Appendix D. One finds that, up to order b^4 included, $\psi(b)/[-b\psi'(b)] = u(1)/[-u'(1)] + f(1)/u(1) - f'(1)/u'(1)$, where we used the fact that $u(1)/[-u'(1)] = 1$ to zeroth order in b and $f(x)$ solves (D8). Then from relations (D10) and (D11) and from the expression of $v(x)$ in terms of $u(y)$, given above Eq. (D9), one finds $\psi(b)/[-b\psi'(b)] = u(1)/[-u'(1)] + \beta(1)/u^2(1) + O(b^5)$. Matching this to the $r > b$ solution gives (160).

[37] In Ref. [180] a similar calculation was performed, except that the harmonic trap was neglected within the interaction range.

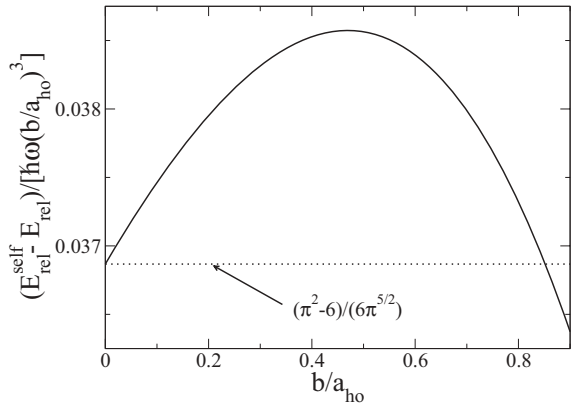

FIG. 2. For two opposite spin fermions interacting in 3D *via* a potential of short range b in an isotropic harmonic trap, the self-consistent equation (159), derived, for example, in Ref. [177], gives the eigenenergies with an error of order b^3, due to the fact that it neglects the effect of the harmonic trap within the interaction range (see Appendix D). This is illustrated with the ground-state relative energy for a square-well potential of infinite scattering length: The deviation (solid line) between the approximate energy $E_{\rm rel}^{\rm self}$ [solving Eq. (159)] and the exact one $E_{\rm rel}$ (calculated as in Ref. [115]) vanishes as b^3, with a coefficient given by Eq. (162) (dotted line). μ is the reduced mass, ω is the angular oscillation frequency in the trap, and $a_{\rm ho} = [\hbar/(\mu\omega)]^{1/2}$.

ground-state energy of Eq. (159) and the exact ground-state energy obeys

$$E_{\rm rel}^{\rm self} - E_{\rm rel} = \frac{\Lambda_2}{\pi^{1/2}} + O(b^4) = \left(\frac{1}{6} - \frac{1}{\pi^2}\right)\frac{b^3}{\pi^{1/2}} + O(b^4). \tag{162}$$

Note that the case of two fermions with a square-well interaction in a harmonic trap was numerically studied in Ref. [181], for the s-wave and also for the p-wave case, with the exact spectrum compared to the self-consistent equation (159) or to its p-wave equivalent. No conclusion was given on the scaling with b of the difference between the exact and the approximate spectrum.

Two dimensions. Imposing the contact condition $\psi(r) = A\ln(r/a) + O(r)$ to Eq. (156) gives an implicit equation for the spectrum in the zero-range limit [122,175]:

$$\psi\left(\frac{1 - E_{\rm rel}^0}{2}\right) - 2\psi(1) = -2\ln a, \tag{163}$$

where ψ is the digamma function. We have obtained the finite-range correction

$$E_{\rm rel} = E_{\rm rel}^0 + \frac{4r_e^2 E_{\rm rel}^0}{\psi'\left(\frac{1-E_{\rm rel}^0}{2}\right)} + O(b^4 \ln^4 b) \tag{164}$$

by neglecting the trapping potential for $r \leqslant b$, as justified by Appendix D, and by matching in $r = b$ the scattering state $\mathcal{A}\chi(r)$ to Eq. (156). The bound on the error results in particular from the statement that the ellipses $(\cdots)$ in Eq. (97) are $O[(kb)^4 \ln(a/b)]$, that one can, for example, check for the square-well potential. As expected, the value of $\partial E_{\rm rel}/\partial(r_e^2)$ in $r_e = 0$ obtained from Eq. (164) coincides with Table V, Eq. (1b), knowing that the normalization factor in the zero-range limit, according to relation 7.611(5) in Ref. [178], obeys

$$\left(C_2^0\right)^2 \pi \frac{\psi'\left(\frac{1-E_{\rm rel}^0}{2}\right)}{\Gamma^2\left(\frac{1-E_{\rm rel}^0}{2}\right)} = 1.$$

B. Three-body problem: corrections to exactly solvable cases and comparison with numerics

In this subsection, we use the known analytical expressions for the three-body wave functions to compute the corrections to the spectrum to first order in the inverse scattering length $1/a$ and in the effective range r_e. We shall consider not only spin-1/2 fermions, but also spinless bosons restricting to the universal stationary states [182,183] which do not depend on the three-body parameter.

The problem of three identical spinless bosons [182,183] or spin-1/2 fermions (say $N_\uparrow = 2$ and $N_\downarrow = 1$) [182,184] is exactly solvable in the unitary limit in an isotropic harmonic trap $U(\mathbf{r}) = \frac{1}{2}m\omega^2 r^2$. Here, we restrict to zero total angular momentum (see, however, the last line of Appendix H) with a center of mass in its ground state, so that the normalization constants of the wave functions are also known analytically [115]. Moreover, we restrict to universal eigenstates.[38] The spectrum is then

$$E = E_{\rm c.m.} + (s + 1 + 2q)\hbar\omega, \tag{165}$$

where $E_{\rm c.m.}$ is the energy of the center-of-mass motion, s belongs to the infinite set of real positive solutions of

$$-s\cos\left(s\frac{\pi}{2}\right) + \eta\frac{4}{\sqrt{3}}\sin\left(s\frac{\pi}{6}\right) = 0, \tag{166}$$

with $\eta = +2$ for bosons and -1 for fermions, and q is a nonnegative integer quantum number describing the degree of excitation of an exactly decoupled bosonic breathing mode [125,185]. We restrict ourselves to states with $q = 0$. The case of a nonzero q is treated in Sec. X C.

a. Derivative of energy with respect to $1/a$. Injecting the expression of the regular part A of the normalized wave function [115] into Table II, Eqs. (2a) and (4a) or its bosonic version (Table V, line 1 in Ref. [106]), we obtain

$$\left.\frac{\partial E}{\partial(-1/a)}\right|_{a=\infty} = \frac{\sqrt{\frac{\hbar^3\omega}{m}}\Gamma\left(s+\frac{1}{2}\right)\sqrt{2}s\sin\left(s\frac{\pi}{2}\right)/\Gamma(s+1)}{-\cos\left(s\frac{\pi}{2}\right) + s\frac{\pi}{2}\sin\left(s\frac{\pi}{2}\right) + \eta\frac{2\pi}{3\sqrt{3}}\cos\left(s\frac{\pi}{6}\right)}. \tag{167}$$

For the lowest fermionic state, this gives $(\partial E/\partial(1/a))_{a=\infty} \simeq -1.1980\sqrt{\hbar^3\omega/m}$, in agreement with the value $-1.19\,(2)$ which we extracted from the numerical solution of a finite-range model presented in Fig. 4(a) of Ref. [120], where the error bar comes from our simple way of extracting the derivative from the numerical data of Ref. [120].

[38] For Efimovian eigenstates, computing the derivative of the energy with respect to the effective range would require to use a regularization procedure similar to the one employed in free space in Refs. [126, 128]. However, the derivative with respect to $1/a$ can be computed [115].

b. Derivative of energy with respect to effective range. Using relation [Table V, Eq. (1a)], which holds not only for fermions but also for bosonic universal states, we obtain

$$\left(\frac{\partial E}{\partial r_e}\right)_{a=\infty} = \frac{\sqrt{\frac{\hbar m\omega^3}{8}}\Gamma\left(s-\frac{1}{2}\right)s\left(s^2-\frac{1}{2}\right)\sin\left(s\frac{\pi}{2}\right)/\Gamma(s+1)}{-\cos\left(s\frac{\pi}{2}\right)+s\frac{\pi}{2}\sin\left(s\frac{\pi}{2}\right)+\eta\frac{2\pi}{3\sqrt{3}}\cos\left(s\frac{\pi}{6}\right).} \quad (168)$$

For bosons, this result was derived previously using the method of Ref. [126] and found to agree with the numerical solution of a finite-range separable potential model for the lowest state [115]. For fermions, Eq. (168) agrees with the numerical data from Fig. 3 of Ref. [120] to ∼0.3% for the two lowest states and 5% for the third-lowest state;[39] Eq. (168) also agrees to within 3% with the numerical data from p. 21 of Ref. [115] for the lowest state of a finite-range separable potential model. All these deviations are compatible with the estimated numerical accuracy.

C. *N*-body problem in isotropic trap: Non-zero $1/a$ and r_e corrections

We now generalize Sec. X B to the case of an arbitrary number N of spin-1/2 fermions (with an arbitrary spin configuration) at the unitary limit in an isotropic harmonic trap. Although one cannot calculate $\partial E/\partial(1/a)$ and $\partial E/\partial r_e$, some useful information can be obtained from the following remarkable property: For any initial stationary state, and after an arbitrary change of the isotropic trap curvature, the system experiences an undamped breathing at frequency 2ω, with ω being the single atom oscillation frequency in the final trapping potential [125]. From this one can conclude that, in the case of a time-independent trap, the system exhibits an SO(2,1) dynamical symmetry [185]: The spectrum is a collection of semi-infinite ladders indexed by the natural integer q. Another crucial consequence is that the eigenstate wave functions are separable in N-body hyperspherical coordinates, with a know expression for the dependence with the hyperradius [185]. This implies that the functions A_{ij} are also separable in $(N-1)$-body hyperspherical coordinates and that their hyperradial dependence is also known. As the eigenstates within a ladder have exactly the same hyperangular part, one can relate the energy derivatives (with respect to $1/a$ or r_e) for step q of a ladder to the derivative for the ground step of the *same* ladder, as detailed in Appendix H:

$$\left[\frac{\partial E}{\partial(1/a)}\right]_q = \left[\frac{\partial E}{\partial(1/a)}\right]_0 \frac{\Gamma(s+1)}{\Gamma(s+q+1)}\sum_{k=0}^{q}\left[\frac{\Gamma\left(k+\frac{1}{2}\right)}{\Gamma(k+1)\Gamma\left(\frac{1}{2}\right)}\right]^2 \times \frac{\Gamma\left(s+q-k+\frac{1}{2}\right)\Gamma(q+1)}{\Gamma\left(s+\frac{1}{2}\right)\Gamma(q-k+1)}, \quad (169)$$

with the eigenenergy of step q written as Eq. (165), s being now unknown for the general N-body problem. We have checked that this explicit result is consistent with the recursion relations derived in Ref. [187]. A similar type of result holds for the derivative with respect to r_e:

$$\left[\frac{\partial E}{\partial r_e}\right]_q = \left[\frac{\partial E}{\partial r_e}\right]_0 \frac{\Gamma(s+1)}{\Gamma(s+q+1)}\sum_{k=0}^{q}\left[\frac{\Gamma\left(k+\frac{3}{2}\right)}{\Gamma(k+1)\Gamma\left(\frac{3}{2}\right)}\right]^2 \times \frac{\Gamma\left(s+q-k-\frac{1}{2}\right)\Gamma(q+1)}{\Gamma\left(s-\frac{1}{2}\right)\Gamma(q-k+1)}. \quad (170)$$

For nonzero $1/a$ or r_e, the level spacing is not constant within a ladder, the system will not respond to a trap change by a monochromatic breathing mode. In a small system, a Fourier transform of the system response can give access to the Bohr frequencies $(E_q - E_{q-1})/\hbar$, which would allow an experimental test of Eqs. (169) and (170). In the large-N limit, for a system prepared in its ground state, we now show that the main effects of nonzero $1/a$ or r_e on the breathing mode are a frequency change and a collapse.

Let us take the macroscopic limit of Eqs. (169) and (170) for a fixed q: Using Stirling's formula for $s \to +\infty$ we obtain

$$\frac{[\partial E/\partial(1/a)]_q}{[\partial E/\partial(1/a)]_0} = 1 - \frac{q}{4s} + \frac{q(9q+7)}{64s^2} + \cdots, \quad (171)$$

$$\frac{[\partial E/\partial r_e]_q}{[\partial E/\partial r_e]_0} = 1 + \frac{3q}{4s} - \frac{3q(5q+11)}{64s^2} + \cdots. \quad (172)$$

The first deviations from unity are thus linear in q, and correspond to a shift of the breathing-mode frequency ω_{breath} to the new value $2\omega + \delta\omega_{\text{breath}}$, which can be obtained to leading order in $1/a$ and r_e from

$$\frac{\partial\omega_{\text{breath}}}{\partial(1/a)} = -\frac{\omega}{4E_0}\frac{\partial E_0}{\partial(1/a)} \quad \text{and} \quad \frac{\partial\omega_{\text{breath}}}{\partial r_e} = \frac{3\omega}{4E_0}\frac{\partial E_0}{\partial r_e}. \quad (173)$$

For a nonpolarized gas (with the same number $N/2$ of particles in each spin state) the local-density approximation gives $4s \sim (3N)^{4/3}\xi^{1/2}$ [119,184] and it allows us to obtain the derivative of the energy with respect to $1/a$ [102] or to r_e in terms of ξ, ζ, and ζ_e, defined in Eqs. (179) and (186), so that

$$\delta\omega_{\text{breath}} = \frac{256\omega}{525\pi\xi^{5/4}}\left[\frac{\xi^{1/2}\zeta}{k_F a} + 2\zeta_e k_F r_e\right], \quad (174)$$

where we have introduced the Fermi momentum k_F of the unpolarized trapped ideal gas with the same atom number N as the unitary gas, with $\hbar^2 k_F^2/(2m) = (3N)^{1/3}\hbar\omega$. For $r_e = 0$, we recover the superfluid hydrodynamic prediction of Refs. [188–190]. We have checked that the change of the mode frequency due to finite-range effects can also be obtained from hydrodynamics;[40] this change in typical experiments is of the order of 0.1% for lithium and 0.5% for potassium (see Sec. X E).

[39] Here, we used the value of the effective range $r_e = 1.435r_0$ [186] for the Gaussian interaction potential $V(r) = -V_0 e^{-r^2/r_0^2}$ with V_0 equal to the value where the first two-body bound state appears.

[40] The hydrodynamic frequencies Ω are given by the eigenvalue problem $-m\Omega^2\delta\rho = \text{div}[\rho_0\nabla(\mu'_{\text{hom}}[\rho_0]\delta\rho)]$ where $\delta\rho(\mathbf{r})$ is the infinitesimal deviation from the stationary density profile $\rho_0(\mathbf{r})$, $\mu_{\text{hom}}[\rho]$ is the ground state chemical potential of the homogeneous gas of density ρ and the apex $'$ indicates derivation. For the equation of state $\mu_{\text{hom}}[\rho] = A\rho^{2/3} + B\rho^{\gamma}$, where B is arbitrarily small, we treat the

Furthermore, due to the presence of q^2 terms in Eqs. (171) and (172), the Bohr frequencies $(E_q - E_{q-1})/\hbar$ depend on the excitation degree q of the mode: If many steps of the ground-state ladder are coherently populated, this can lead to a *collapse* of the breathing mode, which constitutes a mechanism for zero-temperature damping [191,192]. To coherently excite the breathing mode, we start with a ground-state gas, with wave function $\psi_{\rm old}$, and we abruptly change at $t = 0$ the trap frequency from $\omega_{\rm old}$ to $\omega = \lambda^2\omega_{\rm old}$. For the unitary gas, $\psi_{\rm old}$ is deduced from the $t = 0^+$ ground state ψ_0 by a dilation with scaling factor λ,

$$|\psi_{\rm old}\rangle = e^{-i\hat{D}\ln\lambda}|\psi_0\rangle, \tag{175}$$

where $\hat{D}$ is the generator of the dilations [122,185]. Using the representation of $\hat{D}$ in terms of the bosonic operator $\hat{b}$ [185], that annihilates an elementary excitation of the breathing mode ($\hat{b}|q\rangle = q^{1/2}|q-1\rangle$), and restricting to $|\epsilon| \ll 1$, where $\epsilon = \ln\lambda$, one has

$$\hat{D} \simeq -is^{1/2}(\hat{b}^\dagger - \hat{b}), \tag{176}$$

so that the trap change prepares the breathing mode in a Glauber coherent state with mean occupation number $\bar{q} = \epsilon^2 s$ and standard deviation $\Delta q = \bar{q}^{1/2}$. Similarly, the fluctuations of the squared radius of the gas $\sum_i r_i^2/N$, which can be measured, are given by $-\frac{\hbar s^{1/2}}{m\omega}(\hat{b} + \hat{b}^\dagger)$ for small ϵ. In the large system limit, one can have $\bar{q} \gg 1$ so that $1 \ll \Delta q \ll \bar{q}$. At times much shorter than the revival time $2\pi\hbar/|\partial_q^2 E_q|$, one then replaces the discrete sum over q by an integral to obtain

$$\left|\frac{\langle\hat{b}\rangle(t)}{\langle\hat{b}\rangle(0)}\right| = e^{-t^2/(2t_c^2)} \quad \text{with} \quad t_c = \frac{\hbar}{\Delta q\left|\partial_q^2 E_q\right|_{q=\bar{q}}}. \tag{177}$$

For an unpolarized gas, using Eqs. (171) and (172) and the local-density approximation, we obtain the inverse collapse time due to nonzero $1/a$ or r_e:

$$(\omega t_c)^{-1} = \frac{64|\epsilon|}{35\pi\xi\,(3N)^{2/3}}\left|\frac{3\zeta}{5k_F a} + \frac{2\zeta_e k_F r_e}{3\xi^{1/2}}\right|. \tag{178}$$

For lithium experiments, t_c is more than thousands of mode oscillation periods. To conclude with an exotic note, we recall that the q^2 terms in Eqs. (171) and (172) lead to the formation of a Schrödinger-cat–like state for the breathing mode at half the revival time [193].

D. Unitary Fermi gas: comparison with fixed-node Monte Carlo

For the homogeneous nonpolarized unitary gas (i.e., the spin-1/2 Fermi gas in 3D with $a = \infty$ and $N_\uparrow = N_\downarrow$) at zero temperature, we can compare our analytical expressions for the short-distance behavior of the one-body density matrix $g^{(1)}_{\sigma\sigma}$ and the pair distribution function $g^{(2)}_{\uparrow\downarrow}$ to the fixed-node Monte Carlo results in Refs. [107–109]. In this case, $g^{(1)}_{\sigma\sigma}(\mathbf{R} - \mathbf{r}/2, \mathbf{R} + \mathbf{r}/2)$ and $g^{(2)}_{\uparrow\downarrow}(\mathbf{R} - \mathbf{r}/2, \mathbf{R} + \mathbf{r}/2)$ depend only on r and not on σ, $\mathbf{R}$, and the direction of $\mathbf{r}$. Expanding the energy to first order in $1/(k_F a)$ around the unitary limit yields

$$E = E_{\rm ideal}\left(\xi - \frac{\zeta}{k_F a} + \cdots\right), \tag{179}$$

where $E_{\rm ideal}$ is the ground-state energy of the ideal gas, ξ and ζ are universal dimensionless numbers, and the Fermi wave vector is related to the density through $k_F = (3\pi^2 n)^{1/3}$. Expressing C in terms of ζ thanks to Table II, Eqs. (2a) and (4a) and Eq. (179), and inserting this into Table II, Eq. (7a), we get

$$g^{(1)}_{\sigma\sigma}(r) \simeq \frac{n}{2}\left[1 - \frac{3\zeta}{10}k_F r - \frac{\xi}{10}(k_F r)^2 + \cdots\right]. \tag{180}$$

For a finite interaction range b, this expression is valid for $b \ll r \ll k_F^{-1}$.[41] Table IV, Eq. (4a) yields

$$g^{(2)}_{\uparrow\downarrow}(r) \underset{k_F r \ll 1}{\simeq} \frac{\zeta}{40\pi^3}k_F^4|\phi(r)|^2. \tag{181}$$

The interaction potential used in the Monte Carlo simulations [107–109] is a square-well:

$$V(r) = -\left(\frac{\pi}{2}\right)^2\frac{\hbar^2}{mb^2}\theta(b - r). \tag{182}$$

The corresponding zero-energy scattering state is

$$\phi(r) = \frac{\sin\left(\frac{\pi r}{2b}\right)}{r} \text{ for } r < b, \quad \phi(r) = \frac{1}{r} \text{ for } r > b, \tag{183}$$

and the range b was taken such that $nb^3 = 10^{-6}$ (i.e., $k_F b = 0.030\,936\,7\ldots$). Thus we can assume that we are in the zero-range limit $k_F b \ll 1$, so that Eqs. (180) and (181) are applicable.

Figure 3 shows that the expression (181) for $g^{(2)}_{\uparrow\downarrow}$ fits well the Monte Carlo data of Ref. [109] if one adjusts the value of ζ to 0.95. This value is close to the value $\zeta \simeq 1.0$ extracted from (179) and the $E(1/a)$ data of Ref. [107].

Using $\zeta = 0.95$ we can compare the expression (180) for $g^{(1)}_{\sigma\sigma}$ with Monte Carlo data of [108] without adjustable parameters. Figure 4 shows that the first-order derivatives agree, while the second-order derivatives are compatible within the statistical noise. This provides an interesting check of the numerical results, even though any wave function satisfying the contact condition [Table I, Eq. (1a)] leads to $g^{(1)}_{\sigma\sigma}$ and $g^{(2)}_{\uparrow\downarrow}$ functions satisfying Table II, Eqs. (3a) and (6a) with values of C compatible with each other.

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term in B to first order in perturbation theory around the breathing mode to obtain $\Omega = 2\omega + \omega\frac{96}{\pi}(\gamma - \frac{2}{3})\frac{B}{\mu}(\frac{\mu}{A})^{3\gamma/2}\int_0^1 du u^2(1 - 2u^2)(1 - u^2)^{(3\gamma+1)/2}$ where $\mu = \omega N^{1/3}(2mA/\pi^{4/3})^{1/2}$ is the unperturbed chemical potential of the trapped gas. To zeroth order in B, scaling invariance gives $\delta\rho^{(0)}(\mathbf{r}) = \frac{d}{d\lambda}[\rho_0(\mathbf{r}/\lambda)/\lambda^3]_{\lambda=1}$. To use perturbation theory, we made the differential operator Hermitian with the change of function $\delta f(\mathbf{r}) = (\mu'_{\rm hom}[\rho_0(\mathbf{r})])^{1/2}\delta\rho(\mathbf{r})$. Hermiticity of the perturbation is guaranteed (i.e., surface terms coming from the divergence theorem vanish) for γ larger than 1/3. For finite-r_e corrections, $\gamma = 1$.

[41] For a finite-range potential one has $g^{(1)}_{\sigma\sigma}(r) = n/2 - r^2 m E_{\rm kin}/(3\hbar^2\mathcal{V}) + \cdots$ where $\mathcal{V}$ is the volume; the kinetic energy diverges in the zero-range limit as $E_{\rm kin} \sim -E_{\rm int}$, thus $E_{\rm kin} \sim -C/(4\pi)^2\int d^3r V(r)|\phi(r)|^2$ from Table IV, Eq. (2a), so that $E_{\rm kin} \sim C\pi\hbar^2/(32mb)$ for the square-well interaction. This behavior of $g^{(1)}(r)$ only holds at very short distance $r \ll b$ and is below the resolution of the Monte Carlo data.

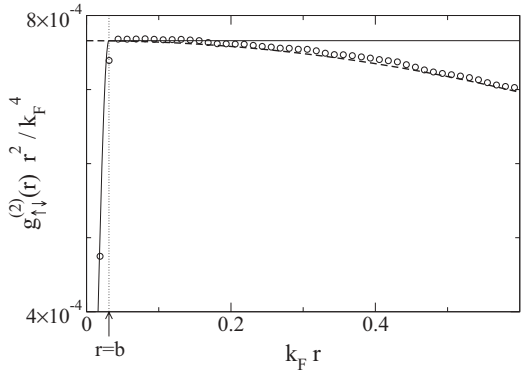

FIG. 3. Pair distribution function $g^{(2)}_{\uparrow\downarrow}(r) = \langle\hat{\psi}^\dagger_\uparrow(\mathbf{r})\hat{\psi}^\dagger_\downarrow(\mathbf{0})\hat{\psi}_\downarrow(\mathbf{0})\hat{\psi}_\uparrow(\mathbf{r})\rangle$ of the homogeneous nonpolarized unitary gas at zero temperature. Circles are for fixed-node Monte Carlo results from Ref. [109]. Solid line is for the analytic expression (181), where the value $\zeta = 0.95$ was taken to fit the Monte Carlo results. The arrow indicates the range b of the square-well interaction potential. Dashed line shows analytic expression (184), with $\zeta_e = 0.12$ [150].

A more interesting check is provided by our expression [Table V, Eq. (3a)] for the subleading term in the short-range behavior of $g^{(2)}_{\uparrow\downarrow}(r)$, which here reduces to

$$g^{(2)}_{\uparrow\downarrow}(r) = \frac{\zeta}{40\pi^3}\frac{k_F^4}{r^2} - \frac{\zeta_e}{20\pi^3}k_F^6 + O(r), \qquad (184)$$

where ζ_e is defined in Eq. (186). Remarkably, this expression is consistent with the fixed-node Monte Carlo results of Ref. [109] if one uses the value of ζ_e of Ref. [150] (see Fig. 3).

E. Finite-range correction in simulations and experiments

We recall that, as we have seen in Sec. VII, the finite-range corrections to eigenenergies are, to leading order, of the form $(\partial E/\partial r_e)r_e$ for continuous-space models or Eq. (117) for lattice models, where the coefficients $\partial E/\partial r_e$, and $\partial E/\partial R_e$ for lattice models are model independent. This can be used in practice by extracting the values of these coefficients from numerical simulations, done with some convenient continuous-space or lattice models (usually a dramatic simplification of the atomic physics reality); then, knowing the value of r_e in an experiment, one can compute the finite-range corrections present in the measurements, assuming that the universality of finite-range corrections, derived in Sec. VII for compact support potentials, also applies for multichannel $O(1/r^6)$ models. The value of r_e is predicted in Ref. [194] to be

$$r_e = -2R_*\left(1 - \frac{a_{\rm bg}}{a}\right)^2 + \frac{4\pi b}{3\Gamma^2(1/4)}\left[\left(\frac{\Gamma^2(1/4)}{2\pi} - \frac{b}{a}\right)^2 + \frac{b^2}{a^2}\right], \qquad (185)$$

where b is the van der Waals length $b = (mC_6/\hbar^2)^{1/4}$, $a_{\rm bg}$ is the background scattering length, and R_* is the so-called Feshbach length [127]. We recall that the magnetic-field dependence of a close to a Feshbach resonance reads $a(B) = a_{\rm bg}[1 - \Delta B/(B - B_0)]$ where B_0 is the resonance location and ΔB is the resonance width, and that $R_* = \hbar^2/(ma_{\rm bg}\mu_b\Delta B)$ where μ_b is the effective magnetic moment of the closed-channel molecule. We note that the a-dependent terms in the second term of Eq. (185) are $O(b^2)$ and thus do not contribute to the leading-order correction in b. In contrast, the a dependence of the first term of Eq. (185) can be significant since $a_{\rm bg}$ can be much larger than b (this is indeed the case for ^{6}Li).[42] A key assumption of Ref. [194] is that the open-channel interaction potential is well approximated by $-C_6/r^6$ down to interatomic distances $r \ll b$. This assumption is well satisfied for alkali-metal atoms [194,196]. Although we have not calculated the off-shell length ρ_e explicitly, we have checked that it is finite for a $-C_6/r^6$ potential [179].

As an illustration, we estimate the finite-range corrections to the nonpolarized unitary gas energy in typical experiments. Similarly to Eq. (179), we have the expansion

$$E = E_{\rm ideal}(\xi + \zeta_e k_F r_e + \cdots), \qquad (186)$$

where E and $E_{\rm ideal}$ are the ground-state energies of the homogeneous Fermi gas [of fixed density $n = k_F^3/(3\pi^2)$] for $1/a = 0$ and $a = 0$, respectively. The value of ζ_e was estimated both from fixed-node Monte Carlo and auxiliary field quantum Monte Carlo to be $\zeta_e = 0.12(3)$ [150].[43] The value of r_e as given by Eq. (185) is 4.7 nm for the $B_0 \simeq 834$ G resonance of ^{6}Li (in accordance with Ref. [197]) and 6.7 nm for the $B_0 \simeq 202.1$ G resonance of ^{40}K. The typical value of $1/k_F$ is $\simeq$400 nm in Ref. [48], while $1/k_F$ at the trap center is $\simeq$250 nm in Ref. [35] and $\simeq$100 nm in Ref. [198],

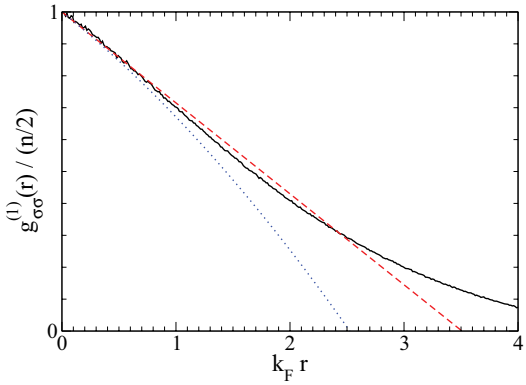

FIG. 4. (Color online) One-body density matrix $g^{(1)}_{\sigma\sigma}(r) = \langle\hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}_\sigma(\mathbf{0})\rangle$ of the homogeneous nonpolarized unitary gas at zero temperature: comparison between the fixed-node Monte Carlo results from Ref. [108] (black solid line) and the analytic expression (180) for the small-$k_F r$ expansion of $g^{(1)}_{\sigma\sigma}$ up to first order (red dashed straight line) and second order (blue dotted parabola) where we took the value $\zeta = 0.95$ extracted from the Monte Carlo data for $g^{(2)}_{\uparrow\downarrow}$ (see Fig. 3).

[42] The general structure of Eq. (185) already appeared for a simple separable two-channel model [102] with exactly the same expression for the first term, which explains why the a dependence is correctly reproduced by the simple expression of Ref. [102], as observed in Ref. [195] by comparison with a coupled-channel calculation, provided that the separable-potential range in Ref. [102] was adjusted to reproduce the correct value of r_e at resonance.

[43] As discussed around Eq. (117), one has to take into account not only r_e but also R_e for lattice models, which was not done in Ref. [150].

which respectively leads to a finite-range correction to the homogeneous gas energy of

$$\frac{\delta E}{E} \simeq 0.4\%,\ 0.6\% \text{ and } 2\%. \tag{187}$$

In the case of lithium, this type of analysis was used in Ref. [48] to estimate the resulting experimental uncertainty on ξ.

XI. CONCLUSION

We derived relations between various observables for N spin-1/2 fermions in an external potential with zero-range or short-range interactions, in continuous space or on a lattice, in two or three dimensions. Some of our results generalize the ones of Refs. [91,97,98,101,104,105]: Large-momentum behavior of the momentum distribution, short-distance behavior of the pair distribution function and of the one-body density matrix, derivative of the energy with respect to the scattering length or to time, norm of the regular part of the wave function (defined through the behavior of the wave function when two particles approach each other), and, in the case of finite-range interactions, interaction energy, are all related to the same quantity C; and the difference between the total energy and the trapping potential energy is related to C and to a functional of the momentum distribution (which is also equal to the second-order term in the short-distance expansion of the one-body density matrix). We also obtained the following relations: The second-order derivative of the energy with respect to the inverse scattering length (or to the logarithm of the scattering length in two dimensions) is related to the regular part of the wave functions and is negative at fixed entropy; and the derivative of the energy with respect to the effective range r_e of the interaction potential (or to r_e^2 in 2D) is also related to the regular part, to the subleading short-distance behavior of the pair distribution function, and to the subleading $1/k^6$ tail of the momentum distribution. We have found unexpected subtleties in the validity condition of the derived expression of this derivative in 2D: Our expression for $\partial E/\partial(r_e^2)$ applies because, for the class of interaction potentials that we have specified, the effective range squared r_e^2 is much larger than the true range squared b^2, than the length squared ρ_e^2 characterizing the low-energy s-wave off-shell T matrix, and than the length squared R_1^2 characterizing the low-energy p-wave scattering amplitude, by logarithmic factors that diverge in the zero-range limit. In 3D, for lattice models, our expression for $\partial E/\partial r_e$ applies only for magic dispersion relations where an extra parameter R_e quantifying the breaking of Galilean invariance (as predicted in Ref. [116]) vanishes; also, the magic dispersion relation should not have cusps at the border of the first Brillouin zone, otherwise the so-called Juillet effect compromises the validity of our $\partial E/\partial r_e$ expression for finite-size systems. We have explicitly constructed such a magic relation, which may be useful to reduce lattice discretization effects in quantum Monte Carlo simulations. We also considered models with a momentum cutoff used in quantum Monte Carlo calculations, either in continuous space [57] or on a lattice [53,56,155,156]: Surprisingly, in the infinite-cutoff limit, the breaking of Galilean invariance survives and one does not exactly recover the unitary gas.

Applications of general relations were presented in three dimensions. For two particles in an isotropic harmonic trap, finite-interaction-range corrections were obtained and were found to be universal up to order r_e^2 included in 3D; in particular, this clarifies analytically the validity of some approximation and self-consistent equation introduced in Refs. [131,133,176,177] that neglect the effect of the trapping potential within the interaction range. For the universal states of three particles with an infinite scattering length in an isotropic harmonic trap, the derivatives of the energy with respect to the inverse scattering length and with respect to the effective range were computed analytically and found to agree with available numerics. For the unitary gas in an isotropic harmonic trap, which has a SO(2,1) dynamical symmetry and an undamped breathing mode of frequency 2ω, we have determined the relative finite-$1/a$ and finite-range energy corrections within each SO(2,1) ladder, which allows in the large-N limit to obtain the frequency shift and the collapse time of the breathing mode. For the bulk unitary Fermi gas, existing fixed-node Monte Carlo data were checked to satisfy exact relations. Also, the finite-interaction-range correction to the unitary gas energy expected from our results to be (to leading order) model independent and thus extractable from quantum Monte Carlo results was estimated for typical experiments: This quantifies one of the experimental uncertainties on the Bertsch parameter ξ.

The relations obtained here may be used in various other contexts. For example, the result Table II, Eqs. (11a) and (11b) on the sign of the second-order derivative of E at constant entropy is relevant to adiabatic ramp experiments [38,39,160,162,198], and the relation Table III, Eq. (8a) allows us to directly compute C using determinantal diagrammatic Monte Carlo [199] and bold diagrammatic Monte Carlo [59,200,201]. C is directly related to the closed-channel fraction in a two-channel model [100,102], which allowed us to extract it [102] from the experimental photoassociation measurements in Ref. [35]. C was measured from the tail of the momentum distribution [52]. For the homogeneous gas C was extracted from measurements of the equation of state [45]. C also plays an important role in the theory of radiofrequency spectra [101,202–206] and in finite-a virial theorems [99,207,208], as verified experimentally [52]. C was also extracted from the momentum tail of the static structure factor $S(k)$, which is the Fourier transform of the spin-independent pair distribution function $\langle\hat{n}(\mathbf{r})\hat{n}(\mathbf{0})\rangle$ and was measured by Bragg spectroscopy [50,51]. In principle one can also measure *via* $S(k)$ the parameter ζ_e quantifying the finite-range correction to the unitary gas energy from the relation

$$\frac{\partial E}{\partial r_e} = -\frac{\pi\hbar^2}{m}\int\frac{d^3k}{(2\pi)^3}\left[S(k) - \frac{C}{4k}\right], \tag{188}$$

resulting from Table V, Eq. (3a). This procedure is not hampered by the small value of $k_F r_e$ in present experiments, contrarily to the extraction of ζ_e from a direct measurement of the gas relative energy correction $\propto\zeta_e k_F r_e \lesssim 10^{-2}$.

We can think of several generalizations of the relations presented here. All relations can be extended to the case of periodic boundary conditions. The techniques used here can be applied to the one-dimensional case to generalize the relations of Ref. [91]. For two-channel or multichannel models one

may derive relations other than the ones of Refs. [100–102]. Generalization of the present relations to arbitrary mixtures of atomic species, and to situations (such as indistinguishable bosons) where the Efimov effect takes place, was given in Ref. [106].

Note added. Table II, Eq. (4b), as well as Table II, Eq. (12b), were obtained independently by Tan [209] using the formalism of Ref. [104]. Recently, some of our 2D relations were tested in Ref. [65] and some of them were rederived in Ref. [210].

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APPENDIX A: TWO-BODY SCATTERING FOR LATTICE MODEL

For the lattice model defined in Sec. III B, we recall that $\phi(\mathbf{r})$ denotes the zero-energy two-body scattering state with the normalization (9) and (10). In this Appendix we derive the relation (11) and (12) between the coupling constant g_0 and the scattering length, as well as the expressions (15)–(18) of $\phi(\mathbf{0})$. Some of the calculation resemble the ones in Refs. [15,211].

We consider a low-energy scattering state $\Phi_{\mathbf{q}}(\mathbf{r})$ of wave vector $q \ll b^{-1}$ and energy $E = 2\epsilon_{\mathbf{q}} \simeq \hbar^2 q^2/m$; that is, the solution of the two-body Schrödinger equation (with the center of mass at rest):

$$(H_0 + V)\,|\Phi_{\mathbf{q}}\rangle = E|\Phi_{\mathbf{q}}\rangle, \tag{A1}$$

where $H_0 = \int_D d^dk/(2\pi)^d 2\epsilon_{\mathbf{k}}|\mathbf{k}\rangle\langle\mathbf{k}|$ and $V = g_0|\mathbf{r}=\mathbf{0}\rangle\langle\mathbf{r}=\mathbf{0}|$, with the asymptotic behavior

$$\Phi_{\mathbf{q}}(\mathbf{r}) \underset{r\to\infty}{=} e^{i\mathbf{q}\cdot\mathbf{r}} + f_{\mathbf{q}}\frac{e^{iqr}}{r} + \cdots \text{ in 3D}, \tag{A2}$$

$$\Phi_{\mathbf{q}}(\mathbf{r}) \underset{r\to\infty}{=} e^{i\mathbf{q}\cdot\mathbf{r}} + f_{\mathbf{q}}\sqrt{\frac{2}{i\pi qr}}e^{iqr} + \cdots \text{ in 2D}. \tag{A3}$$

Here, $f_{\mathbf{q}}$ is the scattering amplitude, which in the present case is independent of the direction of $\mathbf{r}$ as we will see. Note that, in 2D, the present definition corresponds to the convention (96), it differs, for example, from Ref. [212] by a factor $1/(4i)$. Also $\sqrt{i} \equiv e^{i\pi/4}$. We then have the well-known expression

$$|\Phi_{\mathbf{q}}\rangle = (1 + GV)\,|\mathbf{q}\rangle, \tag{A4}$$

where $G \equiv (E + i0^+ - H)^{-1}$. Since $G = G_0 + G_0VG$, with $G_0 \equiv (E + i0^+ - H_0)^{-1}$, Eq. (A4) is equivalent to

$$|\Phi_{\mathbf{q}}\rangle = (1 + G_0T)\,|\mathbf{q}\rangle, \tag{A5}$$

where the T matrix is $T = V + VGV$. Indeed, Eq. (A4) clearly solves Eq. (A1), and one can check [using the fact that $\langle\mathbf{r}|G_0|\mathbf{r}=\mathbf{0}\rangle$ behaves for $r \to \infty$ as $-[m/(4\pi\hbar^2)][e^{iqr}/r]$ in 3D and $-(m/\hbar^2)\sqrt{i/(8\pi qr)}e^{iqr}$ in 2D] that Eq. (A5) satisfies Eqs. (A2) and (A3) with

$$f_{\mathbf{q}} = -\frac{m}{4\pi\hbar^2}b^3\langle\mathbf{r}=\mathbf{0}|T|\mathbf{q}\rangle \text{ in 3D}, \tag{A6}$$

$$f_{\mathbf{q}} = \frac{m}{4i\hbar^2}b^2\langle\mathbf{r}=\mathbf{0}|T|\mathbf{q}\rangle \text{ in 2D}. \tag{A7}$$

Using $T = V + VGV$ and $G = G_0 + G_0VG$ one gets

$$\langle\mathbf{r}=\mathbf{0}|T|\mathbf{q}\rangle = b^{-d}\left[\frac{1}{g_0} - \int_D \frac{d^dk}{(2\pi)^d}\frac{1}{E + i0^+ - 2\epsilon_{\mathbf{k}}}\right]^{-1}. \tag{A8}$$

In 3D the scattering length in defined by $f_{\mathbf{q}} \underset{q\to0}{\to} -a$, which gives the relation (11) between a and g_0. In 2D,

$$f_{\mathbf{q}} \underset{q\to0}{=} \frac{i\pi/2}{\ln(qae^\gamma/2) - i\pi/2 + o(1)}, \tag{A9}$$

where a is by definition the 2D scattering length. Identifying the inverse of the right-hand-sides of Eqs. (A7) and (A9) and taking the real part gives the desired Eq. (12). We note that Eqs. (A9) and (12) remain true if $q \to 0$ is replaced by the limit $b \to 0$ taken for fixed a.

To derive Eqs. (15) and (16) we start from $V|\Phi_{\mathbf{q}}\rangle = T|\mathbf{q}\rangle$, which directly follows from Eq. (A4). Applying $\langle\mathbf{r}=\mathbf{0}|$ on the left and using Eqs. (A6) and (A7) yields

$$g_0\Phi_{\mathbf{q}}(\mathbf{0}) = -\frac{4\pi\hbar^2}{m}f_{\mathbf{q}} \text{ in 3D}, \tag{A10}$$

$$g_0\Phi_{\mathbf{q}}(\mathbf{0}) = \frac{4i\hbar^2}{m}f_{\mathbf{q}} \text{ in 2D}. \tag{A11}$$

In 3D, we simply have $\phi = -a^{-1}\lim_{q\to0}\Phi_{\mathbf{q}}$,[44] and the result (15) follows. In 2D, the situation is a bit more tricky because $\lim_{q\to0}\Phi_{\mathbf{q}}(\mathbf{0}) = 0$. We thus start with $q > 0$, and we will take the limit $q \to 0$ later on. At finite q, we define $\phi_{\mathbf{q}}(\mathbf{r})$ as being proportional to $\Phi_{\mathbf{q}}(\mathbf{r})$ and normalize it by imposing the same condition (10) as for zero energy, but only for $b \ll r \ll q^{-1}$. Inserting Eq. (A9) into Eq. (A11) gives an expression for $\Phi_{\mathbf{q}}(\mathbf{0})$. To deduce the value of $\phi(\mathbf{0})$, it remains to calculate the $\mathbf{r}$-independent ratio $\phi_{\mathbf{q}}(\mathbf{r})/\Phi_{\mathbf{q}}(\mathbf{r})$. But for $r \gg b$ we can replace $\phi_{\mathbf{q}}(\mathbf{r})$ and $\Phi_{\mathbf{q}}(\mathbf{r})$ by their values within the zero-range model (since we also have $b \ll q^{-1}$) which we denote by $\phi_{\mathbf{q}}^{\mathrm{ZR}}(\mathbf{r})$ and $\Phi_{\mathbf{q}}^{\mathrm{ZR}}(\mathbf{r})$. The two-body Schrödinger equation

$$-\frac{\hbar^2}{m}\Delta\Phi_{\mathbf{q}}^{\mathrm{ZR}} = E\Phi_{\mathbf{q}}^{\mathrm{ZR}}\ \forall\, r > 0 \tag{A12}$$

[44] In the case of an infinite scattering length, one has to take a finite a so that this expression makes sense, and only then take the limit $|a| \to \infty$ (this comes from the fact that the scattering amplitude at zero energy is infinite in this case).

implies that

$$\Phi_{\mathbf{q}}^{\mathrm{ZR}}(\mathbf{r}) = e^{i\mathbf{q}\cdot\mathbf{r}} + \mathcal{N} H_0^{(1)}(qr), \tag{A13}$$

where $\mathcal{N}$ is a constant and $H_0^{(1)}$ is an outgoing Hankel function. The contact condition

$$\exists\, A/\ \Phi_{\mathbf{q}}^{\mathrm{ZR}}(\mathbf{r}) \underset{r\to 0}{=} A \ln(r/a) + O(r), \tag{A14}$$

together with the known short-r expansion of the Hankel function [213] then gives

$$A = \frac{-1}{\ln(qae^{\gamma}/2) - i\pi/2}. \tag{A15}$$

Of course we also have $\Phi_{\mathbf{q}}^{\mathrm{ZR}}/\phi_{\mathbf{q}}^{\mathrm{ZR}} = A$, which gives Eq. (16).

Finally, Eqs. (17) and (18) are obtained from Eqs. (15) and (16) using the relations $d[m/(4\pi\hbar^2 a)]/d(1/g_0) = 1$ in 3D and $d(1/g_0)/d(\ln a) = -m/(2\pi\hbar^2)$ in 2D, which are direct consequences of the relations (11) and (12) between g_0 and a.

APPENDIX B: DERIVATION OF LEMMA

In this Appendix, we derive the lemma (33) in three dimensions, as well as its two-dimensional version (35).

Three dimensions. By definition we have

$$\langle\psi_1, H\psi_2\rangle - \langle H\psi_1, \psi_2\rangle = -\frac{\hbar^2}{2m}\int' d^3r_1\cdots d^3r_N \sum_{i=1}^{N}\left[\psi_1^*\Delta_{\mathbf{r}_i}\psi_2 - \psi_2\Delta_{\mathbf{r}_i}\psi_1^*\right]. \tag{B1}$$

Here the notation $\int'$ means that the integral is restricted to the set where none of the particle positions coincide.[45] We rewrite this as

$$\langle\psi_1, H\psi_2\rangle - \langle H\psi_1, \psi_2\rangle = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\int'\left(\prod_{k\neq i} d^3r_k\right)\lim_{\epsilon\to 0}\int_{\{\mathbf{r}_i/\forall\, j\neq i, r_{ij}>\epsilon\}} d^3r_i\left[\psi_1^*\Delta_{\mathbf{r}_i}\psi_2 - \psi_2\Delta_{\mathbf{r}_i}\psi_1^*\right]. \tag{B2}$$

We note that this step is not trivial to justify mathematically. The order of integration has been changed and the limit $\epsilon\to 0$ has been exchanged with the integral over $\mathbf{r}_i$. We expect that this is valid in the presently considered case of equal mass fermions and more generally provided the wave functions are sufficiently regular in the limit where several particles tend to each other.

Since the integrand is the divergence of $\psi_1^*\nabla_{\mathbf{r}_i}\psi_2 - \psi_2\nabla_{\mathbf{r}_i}\psi_1^*$, the divergence theorem gives

$$\langle\psi_1, H\psi_2\rangle - \langle H\psi_1, \psi_2\rangle = \frac{\hbar^2}{2m}\sum_{i=1}^{N}\int'\left(\prod_{k\neq i} d^3r_k\right)\lim_{\epsilon\to 0}\sum_{j,j\neq i}\oiint_{S_\epsilon(\mathbf{r}_j)}\left[\psi_1^*\nabla_{\mathbf{r}_i}\psi_2 - \psi_2\nabla_{\mathbf{r}_i}\psi_1^*\right]\cdot\mathbf{dS}, \tag{B3}$$

where the surface integral is for $\mathbf{r}_i$ belonging to the sphere $S_\epsilon(\mathbf{r}_j)$ of center $\mathbf{r}_j$ and radius ϵ, and the vector area $\mathbf{dS}$ points out of the sphere. We then expand the integrand by using the contact condition, in the limit $r_{ij} = \epsilon \to 0$ taken for fixed $\mathbf{r}_j$ and fixed $(\mathbf{r}_k)_{k\neq i,j}$. Using $\mathbf{R}_{ij} = \mathbf{r}_j + \epsilon\mathbf{u}/2$ with $\mathbf{u} \equiv (\mathbf{r}_i - \mathbf{r}_j)/r_{ij}$ we get

$$\psi_n \underset{\epsilon\to 0}{=} \left(\frac{1}{\epsilon} - \frac{1}{a_n}\right) A_{ij}^{(n)} + \frac{1}{2}\mathbf{u}\cdot\nabla_{\mathbf{R}_{ij}} A_{ij}^{(n)} + O(\epsilon), \tag{B4}$$

$$\nabla_{\mathbf{r}_i}\psi_n \underset{\epsilon\to 0}{=} -\frac{\mathbf{u}}{\epsilon^2}A_{ij}^{(n)} + \frac{1}{2\epsilon}\left[\nabla_{\mathbf{R}_{ij}} A_{ij}^{(n)} - \mathbf{u}\left(\mathbf{u}\cdot\nabla_{\mathbf{R}_{ij}} A_{ij}^{(n)}\right)\right] + O(1), \tag{B5}$$

where n equals 1 or 2, and the functions $A_{ij}^{(n)}$ and $\nabla_{\mathbf{R}_{ij}} A_{ij}^{(n)}$ are taken at $(\mathbf{r}_j, (\mathbf{r}_k)_{k\neq i,j})$. This simply gives

$$\oiint_{S_\epsilon(\mathbf{r}_j)}\left[\psi_1^*\nabla_{\mathbf{r}_i}\psi_2 - \psi_2\nabla_{\mathbf{r}_i}\psi_1^*\right]\cdot\mathbf{dS} \underset{\epsilon\to 0}{=} 4\pi\left(\frac{1}{a_1} - \frac{1}{a_2}\right) A_{ij}^{(1)*} A_{ij}^{(2)} + O(\epsilon) \tag{B6}$$

because the leading-order term cancels and most angular integrals vanish. Inserting this into Eq. (B3) gives the desired lemma (33).

Two dimensions. The derivation is analogous to the 3D case. In Eq. (B3), the double integral on the sphere of course has to be replaced by a simple integral on the circle. Instead of Eqs. (B4) and (B5), we now obtain, from the 2D contact condition [Table I, Eq. (1b)],

$$\psi_n \underset{\epsilon\to 0}{=} \ln(\epsilon/a_n)\ A_{ij}^{(n)} + O(\epsilon\ln\epsilon), \tag{B7}$$

$$\nabla_{\mathbf{r}_i}\psi_n \underset{\epsilon\to 0}{=} \frac{\mathbf{u}}{\epsilon}A_{ij}^{(n)} + O(\ln\epsilon), \tag{B8}$$

which gives

$$\oiint_{S_\epsilon(\mathbf{r}_j)}\left[\psi_1^*\nabla_{\mathbf{r}_i}\psi_2 - \psi_2\nabla_{\mathbf{r}_i}\psi_1^*\right]\cdot\mathbf{dS} \underset{\epsilon\to 0}{=} 2\pi\ln(a_2/a_1)\, A_{ij}^{(1)*} A_{ij}^{(2)} + O(\epsilon\ln^2\epsilon), \tag{B9}$$

and yields the lemma (35).

APPENDIX C: ZERO-RANGE LIMIT OF LATTICE MODEL'S CONTACT

In this Appendix, we show that our definition [Table III, Eqs. (1a) and (1b)] of the contact operator $\hat{C}$ within the lattice model agrees in the zero-range limit $b\to 0$ with the way [Table II, Eq. (1)] C is usually defined within the zero-range model.

[45] In other words, the Dirac distributions originating from the action of the Laplacian onto the $1/r_{ij}$ divergences can be ignored.

1. Stationary state

Let us first consider an eigenstate $|\psi\rangle$ of the zero-range model with an energy E. Let $|\psi_b\rangle$ denote the eigenstate of the lattice model which tends to $|\psi\rangle$ when $b \to 0$, and let E_b denote the corresponding eigenenergy. Then, $C_b \equiv \langle\psi_b|\hat{C}|\psi_b\rangle$ tends to the contact C of the state ψ [defined in Table II, Eq. (1)] when $b \to 0$. Indeed, C is related to $dE/d(-1/a)$ by Table II, Eq. (4a), C_b is related to $dE_b/d(-1/a)$ by Table II, Eq. (4a), and the function $E_b(1/a)$ should tend smoothly to $E(1/a)$ when $b \to 0$.

2. Arbitrary pure state

We now consider any pure state $|\psi\rangle$ satisfying the contact condition [Table I, Eq. (1a)]. We will show that $C_b \equiv \langle\psi_b|\hat{C}|\psi_b\rangle$ tends to the contact C of the state $|\psi\rangle$ [defined in Table II, Eq. (1)] when $b \to 0$, where $|\psi_b\rangle$ is defined as follows: Writing $|\psi\rangle$ as a linear combination $\sum_n c^{(n)}|\psi^{(n)}\rangle$ of the zero-range model's eigenstates $|\psi^{(n)}\rangle$, we define the linear combination $|\psi_b\rangle \equiv \sum_n c^{(n)}|\psi_b^{(n)}\rangle$ of the lattice-model's eigenstates $|\psi_b^{(n)}\rangle$.

We consider only the 3D case—the derivation being almost identical in 2D. Let A and $A^{(n)}$ denote the regular parts of ψ and $\psi^{(n)}$ [defined by the contact condition Table I, Eq. (1a)], and A_b and $A_b^{(n)}$ denote the regular parts of ψ_b and $\psi_b^{(n)}$ [defined by Eq. (19)]. Linearity immediately gives $A = \sum_n c^{(n)}A^{(n)}$ and $A_b = \sum_n c^{(n)}A_b^{(n)}$, as well as $C_b = \sum_{n,m}(c_b^{(n)})^* c_b^{(m)}\langle\psi_b^{(n)}|\hat{C}|\psi_b^{(m)}\rangle$. Expressing $\hat{C}$ in terms of $H_{\rm int}$ thanks to Table III, Eq. (2), and using the lemma (56) as well as Eq. (15), we get $\langle\psi_b^{(n)}|\hat{C}|\psi_b^{(m)}\rangle = (4\pi)^2(A_b^{(n)}, A_b^{(m)})$. When $b \to 0$, we expect that this last quantity tends to $(4\pi)^2(A^{(n)}, A^{(m)})$ because $A_b^{(n)} \to A^{(n)}$ [see Eq. (19) and the discussion thereafter]. Thus C_b indeed tends to C.

APPENDIX D: SPECTRAL EFFECT OF TRAPPING POTENTIAL WITHIN THE INTERACTION RANGE

The motivation of this Appendix is to justify the fact that, in Eq. (88) and in its equivalent form in 2D for an N-body problem, we have neglected the effect of the trapping potential within the interaction range. In the case of an isotropic harmonic trap, the exact form of Eq. (88) contains the external potential term $\frac{1}{4}m\omega^2 r_{ij}^2$. This issue is thus mappable to the two-body problem in a trap with a finite-range interaction, which was the object of numerous studies in 3D [131,133,176,177] that have, however, not analytically quantified the effect of the trapping potential within the interaction range. After elimination of the center-of-mass motion and restriction to a zero angular momentum, one faces the 3D or 2D eigenvalue problem

$$E\psi(r) = -\frac{\hbar^2}{m}\Delta\psi(r) + \left[\frac{1}{4}m\omega^2 r^2 + V(r;b)\right]\psi(r), \quad \text{(D1)}$$

with the conditions that ψ diverges neither in $r = 0$ nor at infinity. The rotationally invariant compact support potential $V(r;b)$ of range b is of the minimal depth ensuring a fixed scattering length a (as discussed in Sec. VII B). In the limit $b \to 0$, where E converges to a finite value, we show that neglecting the effect of the trapping potential *within* the interaction range $r \leqslant b$, as done in Sec. VII A, introduces on the eigenenergy E an error $O(b^3)$ in 3D and $O[b^4 \ln^2(a/b)]$ in 2D, which thus does not affect the results [Table V, Eqs. (1a) and (1b)].

The starting point is the Hellmann-Feynman theorem, with ψ real and normalized to unity:

$$\frac{dE}{db} = \int d^d r\, \psi^2(r)\partial_b V(r;b). \quad \text{(D2)}$$

To reexpress this integral in a more operational way, we introduce the solution $\tilde{\psi}(r)$ of Schrödinger's equation with the same eigenvalue E but for the interaction potential $V(r;\tilde{b})$ of a different range $\tilde{b}$. This solution $\tilde{\psi}(r)$ remains finite in $r = 0$ but it diverges at infinity and cannot be L^2 normalized. In what follows we take a convenient normalization of $\tilde{\psi}$ such that $\lim_{\tilde{b}\to b}\tilde{\psi} = \psi$.

We multiply Schrödinger's equation for ψ (respectively $\tilde{\psi}$) by $\tilde{\psi}$ (respectively ψ) and we integrate the difference of the two resulting equations over the domain $r < R$. Using the divergence theorem, the Wronskian $W(R)$ appears,

$$W(r) \equiv \tilde{\psi}(r)\psi'(r) - \psi(r)\tilde{\psi}'(r). \quad \text{(D3)}$$

For $r > b,\tilde{b}$, the Wronskian satisfies the differential equation

$$W'(r) = -\frac{d-1}{r^{d-1}}W(r),$$

so that, for large R, $W(R) = w/R^{d-1}$ and

$$w = \frac{m}{\hbar^2}\int_0^{+\infty} dr r^{d-1}[V(r;b) - V(r;\tilde{b})]\tilde{\psi}(r)\psi(r). \quad \text{(D4)}$$

Turning back to the Hellmann-Feynman formula (D2), we obtain the exact relation

$$\frac{dE}{db} = \frac{2(d-1)\pi\hbar^2}{m}\lim_{\tilde{b}\to b}\frac{w}{b-\tilde{b}}. \quad \text{(D5)}$$

It remains to calculate w treating perturbatively the trapping potential within the interaction range.

To zeroth order, one neglects the trapping potential for $r \leqslant b$ [or $r \leqslant \tilde{b}$ for $\tilde{\psi}$], so that $\psi^{(0)}(r) = \mathcal{A}\chi(r)$, where χ is the scattering state of energy E for $V(r;b)$. Taking for simplicity $E > 0$, we set $E = \hbar^2k^2/m$, $k > 0$, and χ is normalized as in Eqs. (89) and (95). Note that $\mathcal{A}$ is then fully specified by the continuous matching of $\psi^{(0)}$ in $r = b$ to the outer solution in the trapping potential (that can be expressed in terms of Whittaker functions, see Sec. X A) and by the fact that ψ is normalized to unity. We also have $\tilde{\psi}^{(0)}(r) = \mathcal{A}\tilde{\chi}(r)$ for $r \leqslant \tilde{b}$, where $\tilde{\chi}$ is the scattering state of energy E for $V(r;\tilde{b})$ and the same prefactor $\mathcal{A}$ was taken for convenience. The zeroth-order Wronskian $W^{(0)}$ can then be calculated explicitly, in particular using relations 8.477(1), 8.473(4), and 8.473 (5) of Ref. [178]. We use Eqs. (93) and (97), with $\cdots = O[(kb)^4\ln(a/b)]$ in Eq. (97) [as we have checked for the square well], to obtain

$$\left(\frac{dE}{db}\right)^{(0)} \overset{\rm 3D}{=} 2\pi E\mathcal{A}^2\frac{dr_e}{db} + O(b^2), \quad \text{(D6)}$$

$$\left(\frac{dE}{db}\right)^{(0)} \overset{\rm 2D}{=} \pi E\mathcal{A}^2\frac{d}{db}\left(r_e^2\right) + O[b^3\ln(a/b)]. \quad \text{(D7)}$$

We have checked that the $b \to 0$ limit of these relations coincide with Table V, Eqs. (1a) and (1b).

To first order, we treat the trapping potential perturbatively within the interaction range. We rescale the distance by b, so that $\psi^{(1)}(r) = f(x)$, and $\chi(r) = \mathcal{N}u(x)$, where $x = r/b$ and the function $u(x)$ is normalized by the condition $u(0) = 1$. The function f solves the inhomogeneous Schrödinger equation:

$$\mathcal{F}x^2u(x) = f''(x) + \frac{d-1}{x}f'(x) + \left[k^2b^2 - \frac{mb^2}{\hbar^2}V(bx;b)\right]f(x),$$
$$\mathcal{F} = \frac{1}{4}\mathcal{A}\mathcal{N}\frac{m^2\omega^2}{\hbar^2}b^4. \tag{D8}$$

The function $u(x)$ is a solution of the corresponding homogeneous equation. A second solution $v(x)$ can be constructed that diverges for $x \to 0$. It is of the form $v(x) = -u(x)/x + Z_3(x)$ with $Z_3(x) = O(x)$ for $x \to 0$ in 3D, and $v(x) = u(x)\ln x + Z_2(x)$ with $Z_2(x) = O(x^2)$ for $x \to 0$ in 2D. More precisely, one has $Z_d(x) = u(x)\int_0^x dy y^{1-d}[-1 + 1/u^2(y)]$. Since the expression between square brackets in Eq. (D8) is $O(1)$, $u(x)$ and $Z_d(x)$ are $O(1)$ for $x \leqslant 1$. A first consequence is that the factor $\mathcal{N}$ scales as $1/b$ in 3D and as $\ln(a/b)$ in 2D.[46] A second consequence is that, both in two and three dimensions,

$$\psi^{(1)}(b) \text{ and } b\psi^{(1)'}(b) = O(\mathcal{F}). \tag{D9}$$

This can be seen with the method of variation of constants, where one sets $(f(x), f'(x)) = \alpha(x)(u(x), u'(x)) + \beta(x)(v(x), v'(x))$, with the boundary conditions $\alpha(0) = 0$ (so that $\psi^{(1)}$ does not duplicate the zeroth-order solution) and $\beta(0) = 0$ (so that $\psi^{(1)}$ does not diverge in $r = 0$). This leads to

$$\alpha(x) = -\mathcal{F}\int_0^x dy y^{d+1}u(y)v(y), \tag{D10}$$
$$\beta(x) = \mathcal{F}\int_0^x dy y^{d+1}u^2(y). \tag{D11}$$

Similar results hold for $\tilde{\psi}^{(1)}$. From Eq. (D9) and its counterpart for $\tilde{\psi}^{(1)}(\tilde{b})$, $\tilde{\psi}^{(1)'}(\tilde{b})$, we can estimate the variation of the Wronskian $W(R)$ for R close to $b, \tilde{b}$, and thus the variation $w^{(1)}$ of w due to the trapping potential. Dividing by $b - \tilde{b}$ and taking the limit $\tilde{b} \to b$ as in Eq. (D5) amounts to taking a derivative with respect to $\tilde{b}$, which gives an additional factor $O(1/b)$. Finally, the error δE introduced on the eigenenergy by neglecting the trapping potential within the interaction range is bounded in the zero-range limit $b \to 0$ as

$$\delta E \overset{3D}{=} O(m\omega^2b^3\mathcal{A}^2), \tag{D12}$$
$$\delta E \overset{2D}{=} O[m\omega^2b^4\mathcal{A}^2\ln^2(a/b)], \tag{D13}$$

where the factor $\mathcal{A}$ converges to a finite, energy-dependent value for $b \to 0$.

APPENDIX E: LOW-ENERGY T MATRIX PARAMETERS IN 2D

We derive the hierarchy of Eqs. (109)–(111) for a 2D nonpositive minimal-depth potential of finite range b, $V(r) = [\hbar^2k_0^2/m]v(r/b)$, for $b \to 0$ and k_0 adjusted to have a constant s-wave scattering length a. The key point is then that $k_0b \to 0$ (differently from 3D).

In the s-wave channel, we write the zero-energy scattering wave function as $\psi(r) = f(x)$, with $x = r/b$. The function f solves $f''(x) + f'(x)/x = (k_0b)^2v(x)f(x)$ and it is normalized as $f(0) = 1$. We expand $f(x)$ in powers of $(k_0b)^2$. To zeroth order, $f_0(x) = 1$. To first order, $f_1'' + f_1'/x = (k_0b)^2v(x)$, with $f_1(0) = 0$. This is integrated with the method of variation of constants, $f_1(x) = \alpha(x) + \beta(x)\ln x$ and $f_1'(x) = \beta(x)/x$:

$$\alpha(x) = -(k_0b)^2\int_0^x dy y v(y)\ln y, \tag{E1}$$
$$\beta(x) = (k_0b)^2\int_0^x dy y v(y). \tag{E2}$$

Expressing that $f_1(x) \simeq \beta(+\infty)\ln(r/a)$ at infinity gives

$$-\frac{1}{\ln(a/b)} \simeq \frac{\beta(+\infty)}{1+\alpha(+\infty)} \simeq \frac{m}{\hbar^2}\int_0^{+\infty} dr r V(r), \tag{E3}$$

and further using Eq. (106) leads to

$$\frac{1}{2}\rho_e^2 \sim b^2\int_0^{+\infty} dx x\left[\frac{\beta(x)-\beta(+\infty)}{\beta(+\infty)}\ln x + \frac{\alpha(x)-\alpha(+\infty)}{\beta(+\infty)}\right]. \tag{E4}$$

Integration by parts then gives Eq. (110). Using Eqs. (105), (E3), and (E4) and realizing that $\phi(r) + \ln(r/a) = 2/\beta(+\infty) + O(1)$ for $b \to 0$ with $0 < r/b \leqslant 1$ fixed, gives Eq. (109). Reproducing this perturbative expansion with the same $v(x)$ in the l wave, one gets

$$R_l^{2l} \underset{b\to 0}{\sim} \left(\frac{b^l}{2^l l!}\right)^2 \frac{1}{\ln(a/b)}\frac{\int_0^\infty dx x^{2l+1}v(x)}{\int_0^\infty dx x v(x)}. \tag{E5}$$

This relation for $l = 1$, combined with Eq. (110), gives Eq. (111).

APPENDIX F: SOME MATH FOR JUILLET EFFECT

Here, in the context of the Juillet effect for lattice models, we justify the expansion (133). The quantity R_1 defined in Eq. (130) may be expressed in terms of the difference between an integral and a 3D Riemann sum. We are then guided by the following type of results: If $f(\mathbf{x})$ is a C^∞ function inside the cube $B = [-1/2, 1/2]^3$, then for $\varepsilon = 1/(2N+1)$, with the integer $N \to +\infty$:

$$\int_B d^3x f(\mathbf{x}) - \varepsilon^3\sum_{\mathbf{n}} f(\varepsilon\mathbf{n}) = \frac{\varepsilon^2}{24}\int_B d^3x \Delta f(\mathbf{x}) + O(\varepsilon^4), \tag{F1}$$

where Δf is the Laplacian of f and the sum over $\mathbf{n}$ ranges over $\{-N, \ldots, N\}^3$. To show this lemma, we introduce the short-hand notation $S[f]$ for the left-hand side of Eq. (F1) and we pave B with little cubes of volume ε^3 and of centers $\varepsilon\mathbf{n}$:

$$S[f] = \sum_{\mathbf{n}} \varepsilon^3\int_B d^3x [f(\varepsilon\mathbf{n} + \varepsilon\mathbf{x}) - f(\varepsilon\mathbf{n})]. \tag{F2}$$

Then we use the fourth-order Taylor-Lagrange formula for f restricted to the line connecting $\varepsilon\mathbf{n}$ to $\varepsilon\mathbf{n} + \varepsilon\mathbf{x}$: $f(\varepsilon\mathbf{n} + \varepsilon\mathbf{x}) -$

[46] This also results from the fact that $u(1)$ is not particularly close to zero: For $1/a = 0$ in 3D, $u(1)/u'(1) = -1$.

$f(\varepsilon\mathbf{n}) = (\varepsilon^2/2)\sum_{i,j} x_i x_j \partial_i \partial_j f(\varepsilon\mathbf{n}) + \text{odd} + O(\varepsilon^4)$ where "odd" stands for terms that are linear and cubic in the components of $\mathbf{x}$, and $O(\varepsilon^4)$ results from the fact that the fourth-order derivatives of f are uniformly bounded on B. Integration over $\mathbf{x}$ inside the cube B eliminates the odd terms, and the $i \neq j$ quadratic terms, so that

$$S[f] = \frac{\varepsilon^5}{24} \sum_{\mathbf{n}} [\Delta f(\varepsilon\mathbf{n}) + O(\varepsilon^2)]. \tag{F3}$$

A Riemann sum thus deviates from the integral by $O(\varepsilon^2)$ for a C^∞ integrand. Applying this conclusion to Eq. (F3), where Δf is C^∞, we obtain the desired Eq. (F1). This result, however, is not immediate to apply to the quantity R_1 because the integrand of R_1 is singular in $\mathbf{k} = \mathbf{0}$. We thus use several steps.

We first consider the quantity R_1 for a quadratic dispersion relation that is cut in a smooth way: One twice replaces $1/(2\epsilon_{\mathbf{k}})$ in Eq. (130) by $\phi(\mathbf{k}b/2\pi)/(\hbar^2k^2/m)$ where $\phi(\mathbf{x})$ is a C^∞ rotationally invariant function, equal to 1 in $\mathbf{x} = \mathbf{0}$, and of compact support included inside $B \equiv [-1/2,1/2]^3$ (which allows us to replace the set D by $\mathbb{R}^3$ in the integration and in the summation). After the change of variable $\mathbf{k} = 2\pi\mathbf{x}/L$, we decompose $\mathbb{R}^3$ as a collection of cubes of size unity (as in Ref. [149]) to obtain

$$\frac{h^2L}{m} R_1^\phi = \sum_{\mathbf{n}\in\mathbb{Z}^{3*}} \int_B d^3x \left[\frac{\phi(\varepsilon\mathbf{n} + \varepsilon\mathbf{x})}{(\mathbf{n}+\mathbf{x})^2} - \frac{\phi(\varepsilon\mathbf{n})}{n^2} \right] + \int_B d^3x \frac{\phi(\varepsilon\mathbf{x})}{x^2}, \tag{F4}$$

with $h = 2\pi\hbar$ is Planck's constant and $\varepsilon \equiv b/L$ is the small parameter. As shown in Ref. [149], the right-hand side of Eq. (F4) has a finite limit when $\varepsilon \to 0$, here called $\mathcal{C} \simeq 8.913\,63$, that one can obtain by taking ε to zero inside the sum and the integral, which amounts to replacing ϕ by unity. The deviation of Eq. (F4) from its $\varepsilon \to 0$ limit can thus be exactly written as $\{S[f] + \varepsilon^3 f(\mathbf{0})\}/\varepsilon$, with $S[f] = \varepsilon^3 \sum_{\mathbf{n}\in\mathbb{Z}^3} \int_B d^3x [f(\varepsilon\mathbf{n} + \varepsilon\mathbf{x}) - f(\varepsilon\mathbf{n})]$, that we treat as we did for Eq. (F2). Here, $f(\mathbf{x}) = [\phi(\mathbf{x}) - 1]/x^2$ (extended by continuity to $\mathbf{x} = \mathbf{0}$) is a C^∞ function since ϕ is rotationally invariant. In the fourth-order Taylor-Lagrange formula, $O(\varepsilon^4)$ is replaced with the more accurate $O[\varepsilon^4/(1+\varepsilon^2 n^2)^3]$, due to the fact that the fourth order derivatives of $f(\mathbf{x})$ are uniformly bounded and decrease as $1/x^6$ at infinity. The integral of the Laplacian of f appears as in Eq. (F1), except that is in integrated over the whole $\mathbb{R}^3$ space, which gives zero. We finally obtain

$$\frac{h^2L}{m} R_1^\phi \underset{b\to 0}{=} \mathcal{C} + \left(\frac{b}{L}\right)^2 \lim_{\mathbf{x}\to\mathbf{0}} \frac{\phi(\mathbf{x}) - 1}{x^2} + O(b/L)^3. \tag{F5}$$

Turning back to the lattice model, we now evaluate how R_1 deviates from its $b \to 0$ limit for the uncut parabolic dispersion relation $\mathbf{k} \to \hbar^2k^2/(2m)$. The difference between the smoothly cut R_1^ϕ and the uncut R_1^{parab} (times h^2L/m) is now of the form $\varepsilon^2 f(\mathbf{0})$ plus $1/\varepsilon$ times the difference $S[f]$ between an integral and a Riemann sum, with $f(\mathbf{x}) = [\phi(\mathbf{x}) - 1]/x^2$ as before is C^∞. We then use the result (F1); the key point being that the integration domain is B (rather than the whole space), so that the integral of the Laplacian of f over B gives a nonzero surface contribution and equals the flux of the gradient of f through the surface of B. This leads to Eq. (133) for the particular case of the parabolic dispersion relation. The surface term can be evaluated explicitly, as in Sec. VII B, from the integral evaluated in polar coordinates:

$$\int_{[-1,1]^2} \frac{dxdy}{(1+x^2+y^2)^2} = \sqrt{8} \arcsin\frac{1}{\sqrt{3}}. \tag{F6}$$

Finally, we consider a general dispersion relation (132), with $\eta_{\mathbf{x}} = \frac{1}{2}x^2 + O(x^4)$ for $\mathbf{x} \to \mathbf{0}$. One can consider the difference between the corresponding R_1 and R_1^{parab}. The corresponding function $f(\mathbf{x}) = 1/(2\eta_{\mathbf{x}}) - 1/x^2$ is then not C^∞ in $\mathbf{x} = \mathbf{0}$. For example, for the Hubbard model, $\eta_{\mathbf{x}} = [3 - \sum_i \cos 2\pi x_i]/(2\pi)^2$ is not rotationally invariant and $f(\mathbf{x})$ behaves as $\sum_i x_i^4/x^4$ at low x, its $\mathbf{x} \to \mathbf{0}$ limit depends on the direction of $\mathbf{x}$. This limiting behavior, however, is scaling invariant, a feature that holds for a general dispersion relation. The nth order derivatives of f are then $O(1/x^n)$ for $\mathbf{x} \to \mathbf{0}$. For this class of functions, we introduce $S^*[f]$ defined as $S[f]$ in Eq. (F1) except that one excludes the term $\mathbf{n} = \mathbf{0}$ in the sum. This implies that in the equivalent of Eq. (F2), there is an isolated contribution, the integral of f over εB, which is $O(\varepsilon^3)$ and negligible. Then reproducing the analysis with the fourth-order Taylor-Lagrange formula, we obtain

$$S^*[f] = \frac{\varepsilon^2}{24} \int_B d^3x \Delta f(\mathbf{x}) + O(\varepsilon^3). \tag{F7}$$

Since $(h^2L/m)(R_1 - R_1^{\text{parab}}) = S^*[f]/\varepsilon$, we obtain Eq. (133).

APPENDIX G: ISENTROPIC DERIVATIVES OF MEAN ENERGY IN CANONICAL ENSEMBLE

One considers a system with a Hamiltonian $H(\lambda)$ depending on some parameter λ, and at thermal equilibrium in the canonical ensemble at temperature T, with a density operator $\rho = \exp(-\beta H)/Z$. In terms of the partition function $Z(T,\lambda) = \text{Tr}e^{-\beta H(\lambda)}$, with $\beta = 1/(k_B T)$, one has the usual relations for the free energy F, the mean energy $\bar{E} = \text{Tr}(\rho H)$, and the entropy $S = -k_B \text{Tr}(\rho \ln \rho)$:

$$F(T,\lambda) = -k_B T \ln Z(T,\lambda), \tag{G1}$$

$$F(T,\lambda) = \bar{E}(T,\lambda) - TS(T,\lambda), \tag{G2}$$

$$\partial_T F(T,\lambda) = -S(T,\lambda). \tag{G3}$$

One now varies λ for a fixed entropy S. The temperature is thus a function $T(\lambda)$ of λ such that $S(T(\lambda),\lambda) =$ constant. The derivatives of the mean energy for fixed entropy are $(d\bar{E}/d\lambda)_S \equiv \frac{d}{d\lambda}[\bar{E}(T(\lambda),\lambda)]$ and $(d^2\bar{E}/d\lambda^2)_S \equiv \frac{d^2}{d\lambda^2}[\bar{E}(T(\lambda),\lambda)]$. Writing (G2) for $T = T(\lambda)$ and taking the first-order and the second-order derivatives of the resulting

equation with respect to λ, one finds

$$\left(\frac{d\bar{E}}{d\lambda}\right)_S = \partial_\lambda F\left(T\left(\lambda\right),\lambda\right) \tag{G4}$$

$$\left(\frac{d^2\bar{E}}{d\lambda^2}\right)_S = \partial_\lambda^2 F\left(T(\lambda),\lambda\right) - \frac{\left[\partial_T\partial_\lambda F\left(T(\lambda),\lambda\right)\right]^2}{\partial_T^2 F\left(T(\lambda),\lambda\right)}. \tag{G5}$$

It remains to use (G1) to obtain a microscopic expression of the above partial derivatives of F, from the partition function expressed as a sum $Z=\sum_n e^{-\beta E_n}$ over the eigenstates n of the Hamiltonian:

$$\partial_\lambda F\left(T,\lambda\right) = \overline{\frac{dE}{d\lambda}}, \tag{G6}$$

$$\partial_\lambda^2 F\left(T,\lambda\right) = \overline{\frac{d^2E}{d\lambda^2}} - \beta\mathrm{Var}\left(\frac{dE}{d\lambda}\right), \tag{G7}$$

$$\partial_T^2 F\left(T,\lambda\right) = -\frac{\mathrm{Var}E}{k_B T^3}, \tag{G8}$$

$$\partial_T\partial_\lambda F\left(T,\lambda\right) = \frac{\mathrm{Cov}\left(E,dE/d\lambda\right)}{k_B T^2}. \tag{G9}$$

Here the expectation value $\overline{(\cdots)}$ stands for a sum over the eigenenergies with the canonical probability weights, and Var and Cov are the corresponding variance and covariance; for example,

$$\mathrm{Cov}(E,dE/d\lambda) \equiv \sum_n E_n \frac{dE_n}{d\lambda}\frac{e^{-\beta E_n}}{Z} - \overline{E}\,\overline{\frac{dE}{d\lambda}}. \tag{G10}$$

Insertion of Eq. (G6) into Eq. (G4) gives Eq. (146). Insertion of Eqs. (G7)–(G9) into Eq. (G5) gives Eq. (150).

APPENDIX H: NONZERO $1/a$ AND r_e CORRECTIONS WITHIN A LADDER OF THE TRAPPED UNITARY GAS

For N spin-1/2 fermions at the unitary limit in an isotropic harmonic trap, there is separability of the wave function in internal hyperspherical coordinates [185]:

$$\psi\left(\mathbf{r}_1,\ldots,\mathbf{r}_N\right) = \psi_{\mathrm{c.m.}}\left(\mathbf{C}\right) R^{-(3N-5)/2} F(R)\Phi\left(\Omega\right), \tag{H1}$$

where $\mathbf{C}$ is the center-of-mass location of the N fermions, R is the hyperradius, and Ω is a set of $3N-4$ hyperangles constructed from the Jacobi coordinates (see, e.g., Ref. [122]). One has the general formulas $\mathbf{C}=\sum_{i=1}^N m_i\mathbf{r}_i/M$ and $R^2=\sum_{i=1}^N m_i(\mathbf{r}_i-\mathbf{C})^2/\bar{m}$, where $M=\sum_{i=1}^N m_i$ is the total mass, $\bar{m}$ an arbitrary mass unit, and m_i is the mass of particle i (here equal to m). We shall not need the expression of the hyperangles. Equation (H1) is due to the separability of the noninteracting Hamiltonian in a harmonic trap and to the fact that the Bethe-Peierls contact condition does not break this separability for $1/a=0$. One finds that $\Phi(\Omega)$ is an eigenstate of the Laplacian on the unit sphere of dimension $3N-4$, with contact conditions. Corresponding eigenvalues are conveniently written as

$$\left(\frac{3N-5}{2}\right)^2 - s^2, \quad s>0.$$

In the N-body case, s is not known analytically. On the contrary, $F(R)$ solves a simple 2D Schrödinger-like equation

$$\left(E-E_{\mathrm{c.m.}}\right)F(R) = -\frac{\hbar^2}{2\bar{m}}\left[F''(R)+\frac{1}{R}F'(R)\right] + \left(\frac{\hbar^2 s^2}{2\bar{m}R^2}+\frac{1}{2}\bar{m}\omega^2R^2\right)F(R). \tag{H2}$$

This leads to a spectrum of the form (165), with eigenfunctions expressed in terms of generalized Laguerre polynomials multiplied by a Gaussian [185].

To derive Eqs. (169) and (170), one uses the fact that this separability extends to the functions $A_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j})$. One takes the limit $r_{ij}\to 0$ for a fixed $\mathbf{R}_{ij}$ in (H1): $\Phi(\Omega)$ diverges as R/r_{ij} (since it depends on the hyperangles only), $\mathbf{C}$ and R respectively tend to the center-of-mass position $\check{\mathbf{C}}$ and the hyperradius $\check{R}$ of a fictitious system of $N-1$ particles of total mass $M=Nm$, composed of a particle of position $\mathbf{R}_{ij}$ and mass $2m$, and $N-2$ fermions of positions $\mathbf{r}_k$, $k\neq i,j$ and mass m.[47] We thus obtain the form

$$A_{ij}(\mathbf{R}_{ij},(\mathbf{r}_k)_{k\neq i,j}) = \psi_{\mathrm{c.m.}}(\check{C})\check{R}^{-(3N-7)/2}F(\check{R})\check{\Phi}(\check{\Omega}). \tag{H3}$$

It remains to express the Hamiltonian [Table V, Eq. (2)] of the fictitious system in terms of its center-of-mass $\check{\mathbf{C}}$ and hyperspherical coordinates $(\check{R},\check{\Omega})$:

$$\mathcal{H}_{ij} = -\frac{\hbar^2}{2M}\Delta_{\check{C}} + \frac{1}{2}M\omega^2\check{C}^2 - \frac{\hbar^2}{2\bar{m}}\left[\partial_{\check{R}}^2 + \frac{3N-7}{\check{R}}\partial_{\check{R}} + \frac{1}{\check{R}^2}\Delta_{\check{\Omega}}\right] + \frac{1}{2}\bar{m}\omega^2\check{R}^2.$$

In the integral over $\check{R}$, we use the fact that F solves Eq. (H2) and we integrate by parts to obtain for $s>1/2$:[48]

$$(A,A) = \int_0^\infty d\check{R}F^2(\check{R})\int d\check{\Omega}\check{\Phi}^2(\check{\Omega}), \tag{H4}$$

$$(A,(\mathcal{H}-E)A) = \int_0^\infty d\check{R}\frac{\hbar^2F^2(\check{R})}{2\bar{m}R^2}\int d\check{\Omega}\check{\Phi}(\check{\Omega})[\Lambda-\Delta_{\check{\Omega}}]\check{\Phi}(\check{\Omega}), \tag{H5}$$

with

$$\Lambda = \left(\frac{3N-8}{2}\right)^2 + \frac{1}{4} - s^2.$$

Within a given SO(2,1) energy ladder, $\check{\Phi}$ is fixed, only F depends on the quantum number q. The normalization of ψ to unity imposes that $\int_0^{+\infty} dRRF^2(R)$ is also fixed within a ladder. From known integrals involving the Laguerre polynomials [see, e.g., Eq. (F7) in Ref. [214]), one gets Eqs. (169) and (170). Another by-product is for $N=3$, where $\check{\Phi}(\check{\Omega})$ is a spherical harmonic of spin l: This leads to

$$\partial_{r_e}E/\partial_{(-1/a)}E = \frac{m\omega}{4\hbar}\frac{\Gamma(s-1/2)}{\Gamma(s+1/2)}\left[s^2-\frac{1}{2}-l(l+1)\right].$$

[47] If the first Jacobi coordinates of the N particles are chosen to be $\propto\mathbf{r}_{ij}$, the other ones tend to the Jacobi coordinates of the fictitious system.

[48] Note that $F(R)$ scales as R^s for $R\to 0$. Also, each term of the sum over $i<j$ gives the same contribution, due to the fermionic antisymmetry, and we have dropped this sum and the ij indices for simplicity.

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