General relations for quantum gases in two and three dimensions. II. Bosons and mixtures

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(Received 5 October 2012; published 30 November 2012)

We derive exact general relations between various observables for N bosons with zero-range interactions, in two or three dimensions, in an arbitrary external potential. Some of our results are analogous to relations derived previously for two-component fermions and involve derivatives of the energy with respect to the two-body s-wave scattering length a. Moreover, in the three-dimensional case, where the Efimov effect takes place, the interactions are characterized not only by a, but also by a three-body parameter R_t. We then find additional relations which involve the derivative of the energy with respect to R_t. In short, this derivative gives the probability of finding three particles close to each other. Although it is evaluated for a totally lossless model, it also gives the three-body loss rate always present in experiments (due to three-body recombination to deeply bound diatomic molecules), at least in the limit where the so-called inelasticity parameter η is small enough. As an application, we obtain, within the zero-range model and to first order in η, an analytic expression for the three-body loss rate constant for a nondegenerate Bose gas at thermal equilibrium with infinite scattering length. We also discuss the generalization to arbitrary mixtures of bosons and/or fermions.

DOI: 10.1103/PhysRevA.86.053633 PACS number(s): 67.85.−d

I. INTRODUCTION

Ultracold atomic gases with resonant interactions, that is having a s-wave scattering length much larger in absolute value than the interaction range, can now be studied experimentally thanks to the broad magnetic Feshbach resonances, not only with two-component fermions [1,2] but also with bosons [3–7] or mixtures [8,9]. In this resonant regime, one can neglect the range of the interaction, which is equivalent to replacing the interaction with contact conditions on the N-body wave function: In three dimensions (3D), this constitutes the so-called zero-range model [10–16], that can also be defined in 2D (see, e.g., [17–20]), and of course in 1D [21,22]. In each dimension, these models include a length, the so-called d-dimensional scattering length a. In three dimensions, when the Efimov effect occurs [10], an additional length has to be introduced, the so-called three-body parameter [23].

For the zero-range models, it was gradually realized that several observables, such as the short-distance behavior of the pair distribution function $g^{(2)}(\mathbf{r})$ or the tail of the momentum distribution $n(\mathbf{k})$, can be related to derivatives of the energy with respect to the d-dimensional scattering length a. In 1D, the value of $g^{(2)}(0)$ was directly related to such a derivative by the Hellmann-Feynman theorem [21]; the coefficient of the leading $1/k^4$ term in $n(k)$ at large k was then related to the singular behavior of the wave function for two close particles, and ultimately to $g^{(2)}(0)$, by general properties of the Fourier transform [24]. In 3D, for spin-1/2 fermions (where the Efimov effect does not occur), an extension of the 1D relations was obtained by a variety of techniques [25–30], including the original 1D techniques. Generalizations were then obtained for 2D systems, for fermions or bosons [31–34].

This is the second of a series of two articles on such general relations. The first one covered two-component fermions (Ref. [34], hereafter referred to as Article I). Here, we consider single-component bosons, as well as mixtures. In the 3D case, remarkably, the Efimov effect leads to modifications or even breakdown of some relations, and to the appearance of additional relations involving the derivative of the energy with respect to the three-body parameter R_t. Several of the results presented here were already contained in Ref. [35] and rederived in Ref. [36] with a different technique, which allowed the authors of Ref. [36] to obtain still other Efimovian relations for N bosons.[1]

The article is organized as follows. Section II introduces the zero-range model and associated notations for the single-component bosons. Section III presents relations which are analogous to the fermionic ones. Additional relations resulting from the Efimov effect are derived in Sec. IV. As an application, the three-body loss rate of a nondegenerate Bose gas for an infinite scattering length is calculated in Sec. V. Finally the case of an arbitrary mixture is addressed in Sec. VI. We conclude in Sec. VII. Note that, for convenience, the main relations are displayed in Tables I–III.

II. MODEL AND NOTATIONS

In 3D, the zero-range model imposes the Wigner-Bethe-Peierls contact condition on the N-body wave function: For any pair of particles i,j, when one takes the limit of a vanishing distance $r_{ij} \equiv |\mathbf{r}_i - \mathbf{r}_j|$ with a fixed value of the center of mass $\mathbf{c}_{ij} = (\mathbf{r}_i + \mathbf{r}_j)/2$ different from the positions $\mathbf{r}_k$ of the other $N-2$ particles, the wave function has to behave as

$$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \left(\frac{1}{r_{ij}} - \frac{1}{a}\right) A_{ij}(\mathbf{c}_{ij},(\mathbf{r}_k)_{k\neq i,j}) + O(r_{ij}), \qquad (1)$$

where a is the 3D scattering length. The *a priori* unknown functions A_{ij} are determined from the fact that ψ solves the free Schrödinger equation over the domain where the positions

[1]The "three-body contact" parameter C_3 of Ref. [36] is equal to $(\partial_{\ln R_t} E)_a m/(2\hbar^2)$ in our notations.

TABLE I. For single-component bosons, relations which are analogous to the fermionic case. In three dimensions, the derivatives are taken for a fixed three-body parameter R_t. As discussed in the text, in three dimensions, the relation between energy and momentum distribution is valid if the large cutoff limit $\Lambda \to +\infty$ exists, which is not the case for Efimovian states (i.e., eigenstates whose energy depends on R_t). The notation (A,A) is defined in Eq. (8) in the text. $\gamma = 0.577\,215\ldots$ is Euler's constant.

Three dimensions		Two dimensions	
	$C \equiv \lim_{k\to+\infty} k^4 n(\mathbf{k})$		(1)
$C = 32\pi^2 (A,A)$	(2a)	$C = 8\pi^2 (A,A)$	(2b)
$\int d^3c\, g^{(2)}\left(\mathbf{c}+\frac{\mathbf{r}}{2},\mathbf{c}-\frac{\mathbf{r}}{2}\right) \underset{r\to 0}{\sim} \frac{C}{(4\pi)^2}\frac{1}{r^2}$	(3a)	$\int d^2c\, g^{(2)}\left(\mathbf{c}+\frac{\mathbf{r}}{2},\mathbf{c}-\frac{\mathbf{r}}{2}\right) \underset{r\to 0}{\sim} \frac{C}{(2\pi)^2}\ln^2 r$	(3b)
$\left(\frac{\partial E}{\partial(-1/a)}\right)_{R_t} = \frac{\hbar^2 C}{8\pi m}$	(4a)	$\frac{dE}{d(\ln a)} = \frac{\hbar^2 C}{4\pi m}$	(4b)
$E - E_{\rm trap} \overset{\text{if}\,\exists\,\lim}{=} \frac{\hbar^2 C}{8\pi m a} + \lim_{\Lambda\to\infty}\int_{k<\Lambda}\frac{d^3k}{(2\pi)^3}\frac{\hbar^2k^2}{2m}\left[n(\mathbf{k})-\frac{C}{k^4}\right]$	(5a)	$E - E_{\rm trap} = \lim_{\Lambda\to\infty}\left[-\frac{\hbar^2 C}{4\pi m}\ln\left(\frac{a\Lambda e^\gamma}{2}\right) + \int_{k<\Lambda}\frac{d^2k}{(2\pi)^2}\frac{\hbar^2k^2}{2m}n(\mathbf{k})\right]$	(5b)
$\frac{1}{2}\left(\frac{\partial^2 E_n}{\partial(-1/a)^2}\right)_{R_t} = \left(\frac{4\pi\hbar^2}{m}\right)^2 \sum_{n',E_{n'}\neq E_n}\frac{\lvert(A^{(n')},A^{(n)})\rvert^2}{E_n-E_{n'}}$	(6a)	$\frac{1}{2}\frac{d^2E_n}{d(\ln a)^2} = \left(\frac{2\pi\hbar^2}{m}\right)^2\sum_{n',E_{n'}\neq E_n}\frac{\lvert(A^{(n')},A^{(n)})\rvert^2}{E_n-E_{n'}}$	(6b)

of the particles are two by two distinct: $E\psi = H\psi$ with

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

and U is the external potential. Also ψ is normalized to unity.

If there are three bosons or more, the Efimov effect occurs [10], and the zero-range model has to be supplemented by a three-body contact condition that involves a positive length, the three-body parameter R_t: In the limit where *three* particles approach each other (which one can take to be particles 1, 2, and 3 due to the bosonic symmetry), there exists a function B, hereafter called the three-body regular part, such that

$$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) \underset{R\to 0}{\sim} \Phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\, B(\mathbf{c}_{123},\mathbf{r}_4,\ldots,\mathbf{r}_N), \tag{3}$$

where $\mathbf{c}_{123} = (\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3)/3$ is the center of mass of particles 1, 2, and 3, Φ is the zero-energy three-body scattering state

$$\Phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = \frac{1}{R^2}\sin\left[|s_0|\ln\frac{R}{R_t}\right]\phi_{s_0}(\mathbf{\Omega}), \tag{4}$$

and R and $\mathbf{\Omega}$ are the hyperradius and the hyperangles associated with particles 1, 2, and 3. We take the limit $R\to 0$ in Eq. (3) for fixed $\mathbf{\Omega}$ and $\mathbf{c}_{123}$ (in analogy with the two-body contact condition).

We recall the definition of R and $\mathbf{\Omega}$: From the Jacobi coordinates $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$ and $\boldsymbol{\rho} = (2\mathbf{r}_3 - \mathbf{r}_1 - \mathbf{r}_2)/\sqrt{3}$, one forms the six-component vector $\mathbf{R} = (\mathbf{r},\boldsymbol{\rho})/\sqrt{2}$; then, the hyperradius $R = \sqrt{(r^2+\rho^2)/2}$ is the norm of $\mathbf{R}$, and $\mathbf{\Omega} = \mathbf{R}/R$ is its direction which can be parametrized by five hyperangles, so that $d^6R = R^5 dR d^5\Omega$. In Eq. (4), $s_0 = i\times 1.006\,237\,825\,10\ldots$ is Efimov's transcendental number, it is the imaginary solution (with positive imaginary part) of $s\cos(s\pi/2) = (8/\sqrt{3})\sin(s\pi/6)$; $\phi_{s_0}(\mathbf{\Omega})$ is the hyperangular part of the Efimov trimers' wave functions [10], which, in the present case (single-component bosons), is given by $\phi_{s_0}(\mathbf{\Omega}) \equiv \mathcal{N}(1+Q)\sinh[|s_0|(\frac{\pi}{2}-\alpha)]/\sin(2\alpha)$ where $Q = P_{13}+P_{23}$ and P_{ij} exchanges particles i and j, and where $\alpha \equiv \arctan(r/\rho)$. Here we introduced, for later convenience, a normalization factor such that $\int d^5\Omega\, |\phi_{s_0}(\mathbf{\Omega})|^2 = 1$. Using $\int d^5\Omega = \int_0^{\pi/2} d\alpha \sin^2\alpha\cos^2\alpha \int d^2\hat{r}\int d^2\hat{\rho}$, where $d^2\hat{r}$ and $d^2\hat{\rho}$ are the differential solid angles in 3D, we obtain [37,38]

$$\mathcal{N}^{-2} = \frac{6\pi^2}{|s_0|}\sinh(|s_0|\pi/2)\Big[\cosh(|s_0|\pi/2) + |s_0|\frac{\pi}{2}\sinh(|s_0|\pi/2) - \frac{4\pi}{3\sqrt{3}}\cosh(|s_0|\pi/6)\Big]. \tag{5}$$

For $N=3$ particles, it is well established that this model Hamiltonian is self-adjoint and that it is the zero-range limit of finite-range models; see, e.g., [16] and references therein. The fact that the zero-range (i.e., low-energy) regime can be described using the scattering length and a three-body parameter only is known as universality [15]. For $N=4$, an accurate numerical study [39] has shown, as was suggested by earlier numerical work [40–42] and as supported by experimental evidence [43], that there is no need to introduce a four-body parameter in the zero-range limit, implying that the zero-range model Hamiltonian considered here is self-adjoint for $N=4$. Physically, this is related to the fact that the introduction of R_t, imposed by the three-body Efimov effect, necessarily breaks the separability of the four-body problem at infinite scattering length; this precludes the simplest scenario imposing the introduction of a four-body parameter, namely, a four-body Efimov effect such as the one found for $3+1$ fermions in Ref. [44]. Here we consider an arbitrary value of N such that the model Hamiltonian is self-adjoint.

In 2D, the zero-range model is a direct generalization of the 3D one, since one simply replaces the 3D zero-energy two-body scattering wave function $r_{ij}^{-1} - a^{-1}$ by the 2D one $\ln(r_{ij}/a)$, where a is now the 2D scattering length. Accordingly, for any pair of particles i and j, in the limit $r_{ij} \equiv |\mathbf{r}_i - \mathbf{r}_j| \to 0$ with $\mathbf{c}_{ij} = (\mathbf{r}_i+\mathbf{r}_j)/2$ fixed, the N-body wave function satisfies in 2D

$$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \ln(r_{ij}/a)A_{ij}(\mathbf{c}_{ij},(\mathbf{r}_k)_{k\neq i,j}) + O(r_{ij}). \tag{6}$$

There is no Efimov effect in 2D so that no additional parameter is required [45–47]. The Hamiltonian is the corresponding 2D version of Eq. (2).

III. RELATIONS WHICH ARE ANALOGOUS TO THE FERMIONIC CASE

A first set of relations is given in Table I. These relations and derivations are largely analogous to the fermionic case (which was treated in Article I). An obvious difference with the fermionic case is that there are no longer spin indices in the pair distribution function $g^{(2)}$ and in the momentum distribution $n(\mathbf{k})$. Accordingly we now have $g^{(2)}(\mathbf{r},\mathbf{r}') = \langle \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})\rangle = \int d^d r_1 \cdots d^d r_N$ $|\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)|^2 \sum_{i\neq j} \delta(\mathbf{r}-\mathbf{r}_i)\delta(\mathbf{r}'-\mathbf{r}_j)$, where $\hat{\psi}$ is the bosonic field operator, and the momentum distribution is normalized as $\int n(\mathbf{k}) d^d k/(2\pi)^d = N$. Apart from numerical prefactors, there are two more important differences which appear in the 3D case due to the Efimov effect.

The first important difference is that the derivatives with respect to $1/a$ in Table I, Eqs. (4a) and (6a) have to be taken for a fixed three-body parameter R_t. This comes from the relation

$$\left(\frac{\partial E}{\partial(-1/a)}\right)_{R_t} = \frac{4\pi\hbar^2}{m}(A,A) \tag{7}$$

with the notation (given for generality in dimension d)

$$(A,A) \equiv \sum_{i<j} \int \left(\prod_{k\neq i,j} d^d r_k\right) \int d^d c_{ij} |A_{ij}(\mathbf{c}_{ij},(\mathbf{r}_k)_{k\neq i,j})|^2. \tag{8}$$

Equation (7) was already obtained in Ref. [16] in the case $N = 3$. A simple way to derive it for any N is to use a cubic lattice model, of lattice spacing b, with purely on-site interactions characterized by a coupling constant g_0 [see the Hamiltonian in Eq. (14) below, with $h_0 = 0$], adjusted to reproduce the correct scattering length [48]:

$$\frac{1}{g_0} = \frac{m}{4\pi\hbar^2 a} - \int_D \frac{d^3k}{(2\pi)^3}\frac{m}{\hbar^2 k^2}, \tag{9}$$

where the wave vector $\mathbf{k}$ of a single-particle plane wave on the lattice is restricted as usual to the first Brillouin zone $D = (-\frac{\pi}{b},\frac{\pi}{b})^3$. One then follows the same reasoning as in (Article I, Secs. V C–E). The key point here is that, in the limit of $b \ll |a|$, the three-body parameter corresponding to the lattice model is equal to a numerical constant times b.[2] Thus, varying the coupling constant g_0 while keeping b fixed is equivalent to varying a while keeping R_t fixed, so that

$$\frac{dE}{dg_0} = \left(\frac{dE}{d(-1/a)}\right)_{R_t} \frac{d(-1/a)}{dg_0}. \tag{10}$$

The left-hand side of Eq. (10) is given by the Hellmann-Feynman theorem:

$$\begin{aligned}\frac{dE}{dg_0} &= \frac{1}{2}\sum_{\mathbf{r}} b^3 \langle(\hat{\psi}^\dagger\hat{\psi}^\dagger\hat{\psi}\hat{\psi})(\mathbf{r})\rangle \\ &= \frac{N(N-1)}{2} \sum_{\mathbf{r},\mathbf{r}_3,\ldots,\mathbf{r}_N} b^{3(N-1)} |\psi(\mathbf{r},\mathbf{r},\mathbf{r}_3,\ldots,\mathbf{r}_N)|^2,\end{aligned} \tag{11}$$

where ψ is the eigenstate wave function on the lattice. In the zero-range limit $b \ll |a|$, ψ has to match the contact condition (1): Its two-body regular part A_{12}, defined as

$$\psi(\mathbf{r},\mathbf{r},\mathbf{r}_3,\ldots,\mathbf{r}_N) \equiv \phi(\mathbf{0})A_{12}(\mathbf{r},\mathbf{r}_3,\ldots,\mathbf{r}_N), \tag{12}$$

with the correctly normalized zero-energy two-body lattice scattering wave function $\phi(\mathbf{r})$ [$\phi(\mathbf{r}) = r^{-1} - a^{-1} + o(1)$ at $r \gg b$], has to converge to the zero-range model regular part. Similarly, in the right-hand side of Eq. (10), the lattice model's $[dE/d(-1/a)]_{R_t}$ tends to that of the zero-range model if one takes the zero-range limit while keeping R_t fixed.[3] Finally, the last factor of Eq. (10) can be evaluated from Eq. (9). Using the relation $\phi(\mathbf{0}) = -4\pi\hbar^2/(mg_0)$ established in Ref. [34], we obtain Eq. (7). The same lattice model reasoning explains why the second-order derivative in Table I, Eq. (6a) also has to be taken for a fixed R_t.

The second important difference with respect to the fermionic case is that the relation Table I, Eq. (5a) breaks down in general, and holds only for special states for which the infinite-cutoff limit $\Lambda \to \infty$ exists (such as the universal states for three trapped bosons of Refs. [49,50]). This was overlooked in Ref. [32], and was shown for an Efimov trimer in Ref. [38]. The correct relation valid for any N-body state in the presence of the Efimov effect was obtained in Ref. [36].

IV. ADDITIONAL RELATIONS COMING FROM THE EFIMOV EFFECT

In addition to modifying relations which already existed for fermions, the Efimov effect gives rise to additional relations, involving the derivative of the energy with respect to the logarithm of the three-body parameter. These relations are displayed in Table II.

A. Derivative of the energy with respect to the three-body parameter

Our first additional relation [Table II, Eq. (1)] expresses the derivative of the energy with respect to the three-body parameter R_t in terms of the three-body regular part defined in Eq. (3). This is similar to the relation (7) between the derivative with respect to the scattering length and the (two-body) regular

[2] The value of this constant is irrelevant for what follows. It could be calculated, e.g., by equating the energies of the weakly bound Efimov trimers of the lattice model with those of the zero-range model. This was done, e.g., in Refs. [16,49], not for the lattice model, but for a Gaussian separable potential model.

[3] The zero-range limit for a fixed R_t can be taken by repeatedly dividing b by the discrete scaling factor $\exp(\pi/|s_0|)$ and by adjusting g_0 so that a remains fixed. In this limit the ground-state energy tends to $-\infty$ as follows from the Thomas effect, but the restriction of the spectrum to any fixed energy window converges (see, e.g., Ref. [16]).

TABLE II. For single-component bosons in 3D, additional relations coming from the Efimov effect. B is the three-body regular part of the N-body wave function, $g^{(3)}$ is the triplet distribution function, Γ is the decay rate due to three-body losses, and η is the corresponding inelasticity parameter (see text). The integral in Eq. (2) in the table is taken for fixed relative coordinates.

$\left(\frac{\partial E}{\partial(\ln R_t)}\right)_a = \frac{\hbar^2}{m}\frac{\sqrt{3}\,\lvert s_0\rvert^2}{4} N(N-1)(N-2)\int d^3c_{123}\, d^3r_4\cdots d^3r_N\,\lvert B(\mathbf{c}_{123},\mathbf{r}_4,\ldots,\mathbf{r}_N)\rvert^2$	(1)
$\int d^3c_{123}\, g^{(3)}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) \underset{R\to 0}{\sim} \lvert\Phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\rvert^2 \left(\frac{\partial E}{\partial(\ln R_t)}\right)_a \frac{4}{\sqrt{3}\,\lvert s_0\rvert^2}\frac{m}{\hbar^2}$	(2)
$\hbar\Gamma \underset{\eta\to 0}{\sim} \left(\frac{\partial E}{\partial(\ln R_t)}\right)_a \frac{2\eta}{\lvert s_0\rvert}$	(3)

part.[4] We will first derive this relation using the zero-range model in the case $N=3$, and then using a lattice model for any N.

1. Derivation using the zero-range model for three particles

We consider two wave functions ψ_1,ψ_2, satisfying the two-body boundary condition (1) with the same scattering length a, and the three-body boundary conditions (3),(4) with different three-body parameters R_{t1},R_{t2}. The corresponding three-body regular parts are denoted by B_1,B_2. We show in Appendix A that

$$\langle\psi_1,H\psi_2\rangle-\langle H\psi_1,\psi_2\rangle=\frac{\hbar^2}{m}\frac{3\sqrt{3}|s_0|}{2}\sin\left[|s_0|\ln\frac{R_{t2}}{R_{t1}}\right]\times\int d^3c_{123}B_1^*(\mathbf{c}_{123})B_2(\mathbf{c}_{123}),\tag{13}$$

which yields Eq. (1) in Table II, by choosing ψ_i as an eigenstate of energy E_i and taking the limit $R_{t2}\to R_{t1}$.[5]

2. Derivation using a lattice model

We now derive Table II, Eq. (1) for all N using as in Sec. III a cubic lattice model, except that the Hamiltonian now contains a three-body interaction term (of coupling constant h_0) allowing one to adjust the three-body parameter R_t without changing the lattice spacing:

$$\begin{aligned}H_{\rm latt}=&\int_D\frac{d^3k}{(2\pi)^3}\frac{\hbar^2k^2}{2m}\hat{c}^\dagger(\mathbf{k})\hat{c}(\mathbf{k})+\sum_{\mathbf{r}}b^3U(\mathbf{r})(\hat{\psi}^\dagger\hat{\psi})(\mathbf{r})\\&+\frac{g_0}{2}\sum_{\mathbf{r}}b^3(\hat{\psi}^\dagger\hat{\psi}^\dagger\hat{\psi}\hat{\psi})(\mathbf{r})\\&+h_0\sum_{\mathbf{r}}b^3(\hat{\psi}^\dagger\hat{\psi}^\dagger\hat{\psi}^\dagger\hat{\psi}\hat{\psi}\hat{\psi})(\mathbf{r}).\end{aligned}\tag{14}$$

Here the bosonic field operator obeys discrete commutation relations $[\hat{\psi}(\mathbf{r}),\hat{\psi}^\dagger(\mathbf{r}')]=\delta_{\mathbf{r}\mathbf{r}'}/b^3$ and the plane-wave annihilation operators obey as usual $[\hat{c}_{\mathbf{k}},\hat{c}^\dagger_{\mathbf{k}'}]=(2\pi)^3\delta(\mathbf{k}-\mathbf{k}')$ provided that $\mathbf{k}$ and $\mathbf{k}'$ are restricted to the first Brillouin zone D.

We then define the zero-energy three-body scattering state $\phi_0(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ as the solution of $H_{\rm latt}|\phi_0\rangle=0$ for $a=\infty$, with the boundary condition

$$\phi_0(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\sim\Phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\tag{15}$$

in the limit where all interparticle distances tend to infinity. Here Φ is the zero-range model's zero-energy scattering state, given in Eq. (4). This defines the three-body parameter $R_t(b,h_0)$ for the lattice model (since Φ depends on R_t). The Hellmann-Feynman theorem gives

$$\begin{aligned}\frac{\partial E}{\partial h_0}&=\sum_{\mathbf{r}}b^3\,\langle(\psi^\dagger\psi^\dagger\psi^\dagger\psi\psi\psi)(\mathbf{r})\rangle\\&=N(N-1)(N-2)\sum_{\mathbf{r},\mathbf{r}_4,\ldots,\mathbf{r}_N}b^{3(N-2)}\\&\quad\times|\psi(\mathbf{r},\mathbf{r},\mathbf{r},\mathbf{r}_4,\ldots,\mathbf{r}_N)|^2.\end{aligned}\tag{16}$$

For the lattice model we define the three-body regular part B through

$$\psi(\mathbf{r},\mathbf{r},\mathbf{r},\mathbf{r}_4,\ldots,\mathbf{r}_N)=\phi_0(\mathbf{0},\mathbf{0},\mathbf{0})\,B(\mathbf{r},\mathbf{r}_4,\ldots,\mathbf{r}_N);\tag{17}$$

in the zero-range limit, we expect that this lattice model's regular part tends to the regular part of the zero-range model defined in Eqs. (3) and (4). Thus, in the zero-range limit,

$$\left(\frac{\partial E}{\partial(\ln R_t)}\right)_a=N(N-1)(N-2)|\phi_0(\mathbf{0},\mathbf{0},\mathbf{0})|^2\left(\frac{\partial h_0}{\partial(\ln R_t)}\right)_b\times\int d^3r\,d^3r_4\cdots\,d^3r_N\,|B(\mathbf{r},\mathbf{r}_4,\ldots,\mathbf{r}_N)|^2.\tag{18}$$

It remains to evaluate the derivative of h_0 with respect to R_t: This is achieved by applying (18) to the case of an Efimov trimer in free space, where the regular part can be deduced from the known expression [38] for the normalized wave function. This yields Eq. (1) in Table II.

B. Short-distance triplet distribution function

Similarly to the pair distribution function $g^{(2)}$, one defines the triplet distribution function $g^{(3)}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=\langle\hat{\psi}^\dagger(\mathbf{r}_1)\hat{\psi}^\dagger(\mathbf{r}_2)\hat{\psi}^\dagger(\mathbf{r}_3)\hat{\psi}(\mathbf{r}_3)\hat{\psi}(\mathbf{r}_2)\hat{\psi}(\mathbf{r}_1)\rangle$, which is given in first quantization by $N(N-1)(N-2)\int d^3r_4\cdots\,d^3r_N\,|\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)|^2$. In the limit $R\to0$ where the three positions $\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3$ approach each other, the many-body wave function behaves according to Eq. (3). The result Table II, Eq. (2), where the integral over $\mathbf{c}_{123}$ is taken for fixed $\mathbf{R}$ and $\mathbf{\Omega}$, then directly follows, using Table II, Eq. (1).

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[4]We note that it was already speculated in Ref. [27] that, in the presence of the Efimov effect, "a three-body analog of the contact" may "play an important role."

[5]We note that ψ_1 and ψ_2 do not satisfy the lemma of Article I, Eq. (33) because they are too singular for $R\to0$. If this lemma was applicable, the right-hand side of Eq. (13) would be zero and the two-body contact condition (1) would define a self-adjoint Hamiltonian without need of the extra, three-body contact condition (3), which is not the case.

As a consequence, in a measurement of the positions of all the particles, the mean number of triplets of particles having a small hyperradius R is given by

$$N_{\text{triplets}}(R<\epsilon) = \frac{1}{3!}\int_{R<\epsilon} d^3r_1 d^3r_3 d^3r_3 g^{(3)}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) \underset{\epsilon\to 0}{\sim} \frac{m}{2\hbar^2|s_0|^2}\left(\frac{\partial E}{\partial(\ln R_t)}\right)_a \times \epsilon^2\left[1-\text{Re}\,\frac{(\epsilon/R_t)^{2i|s_0|}}{1+i|s_0|}\right], \quad (19)$$

where we used the Jacobian $\frac{D(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)}{D(\mathbf{c}_{123},\mathbf{R})}=3\sqrt{3}$ and the division by 3! takes into account the indistinguishability of the particles within a triplet.

C. Decay rate due to three-body losses

In experiments, the cold atomic gases are only metastable: There exist deeply bound dimer states, that is, with a binding energy of order $\hbar^2/(mb^2)$, where b is the van der Waals length of the real atomic interaction. These deeply bound states can be populated by three-body collisions, which are strongly exothermic (with respect to the trapping potential depth) and thus lead to a net loss of atoms. Usually, one expects that these deeply bound dimer states have a vanishingly small effect on the metastable many-body states for $b\to 0$; the metastable states then converge to stationary states described by the zero-range model.

In the presence of the Efimov effect, however, the probability p_{close} to find three particles within a distance b (e.g., with a hyperradius $R<b$) vanishes only as b^2 according to Eqs. (3), (4), and (19). As the three-body loss rate scales as $p_{\text{close}}\hbar/mb^2$, it does not vanish in the zero-range limit [13,51]. Fortunately, one can still in that limit simply include the losses by modifying the three-body boundary conditions [52,53]: One keeps Eq. (3) with a modified Φ deduced from Eq. (4) by the substitution

$$\sin\left[|s_0|\ln\frac{R}{R_t}\right] \to \frac{1}{2i}[e^{-\eta}e^{i|s_0|\ln(R/R_t)} - e^{\eta}e^{-i|s_0|\ln(R/R_t)}]. \quad (20)$$

The so-called inelasticity parameter $\eta\geqslant 0$ determines the extent to which the reflection of the incoming hyperradial wave $\exp[-i|s_0|\ln(R/R_t)]$ on the point $R=0$ (where the nonuniversal short-range three-body physics takes place) is elastic.

In this work, we have considered so far the ideal case where η is strictly zero. We now show that this allows us to access the decay rate due to three-body losses to first order in η by taking simply a derivative of the lossless eigenenergies E. In a first approach, generalizing to three-body losses the procedure used for two-body losses in Ref. [27], we simply assume that $E(\ln R_t)$ is an analytic function of $\ln R_t$. As the substitution (20) simply amounts to performing the change

$$\ln R_t \to \ln R_t - \frac{i\eta}{|s_0|}, \quad (21)$$

we conclude that the resulting eigenenergy for nonzero η acquires an imaginary part $-i\hbar\Gamma/2$ given to first order in η by Eq. (3) in Table II. Furthermore, we have developed an alternative approach, that relates for arbitrary η the decay rate Γ to the integral of $|B|^2$, where B is defined by Eq. (3); see Appendix B. Combining this with Table II, Eq. (1) in the limit $\eta\to 0$ reproduces the relation Table II, Eq. (3).

V. APPLICATION: THREE-BODY LOSS RATE FOR A BOSE GAS AT THERMAL EQUILIBRIUM

We consider a 3D Bose gas, in a cubic quantization box of volume V, at thermal equilibrium in the grand-canonical ensemble and in the thermodynamic limit. Within the zero-range model, with a truncation of the three-body energy spectrum (that is, introducing a lower energy cutoff, as discussed below), Eq. (3) of Table II can be used to obtain, to first order in the inelasticity parameter η, the three-body loss constant L_3 customarily defined by

$$\frac{d}{dt}N = -L_3 n^2 N, \quad (22)$$

where N is the mean particle number and $n=N/V$ the mean density. Applying Table II, Eq. (3) to each many-body eigenstate, taking a truncated thermal average,[6] and keeping in mind that each loss event eliminates three particles from the system,[7] we obtain

$$\frac{dL_3}{d\eta}(\eta=0) = \frac{6}{\hbar|s_0|n^2N}\left(\frac{\partial\Omega}{\partial(\ln R_t)}\right)_{\mu,T}, \quad (23)$$

where the derivative of the grand potential Ω is taken for fixed chemical potential μ and temperature T.

To obtain analytical results, we restrict consideration to the nondegenerate limit $\mu\to-\infty$, where the density vanishes, $n\lambda^3\to 0$, with $\lambda=[2\pi\hbar^2/(mk_BT)]^{1/2}$ the thermal de Broglie wavelength. One then can use the virial expansion [54–58]:

$$\Omega(\mu,T) = -\frac{V}{\lambda^3}k_BT\sum_{q\geqslant 1} b_q e^{q\beta\mu}, \quad (24)$$

with $\beta=1/(k_BT)$, and b_q depending only on the q-body physics and temperature. The leading-order contribution that involves $\ln R_t$ is thus for $q=3$, so that

$$\frac{dL_3}{d\eta}(\eta=0) \underset{n\lambda^3\to 0}{\to} -\frac{12\pi}{|s_0|}\frac{\hbar\lambda^4}{m}\left(\frac{\partial b_3}{\partial(\ln R_t)}\right)_T, \quad (25)$$

where we used $n\lambda^3\sim\exp(\beta\mu)$.

The coefficient b_q can be deduced from the solution of the q-body problem. We thus restrict our consideration to the resonant case $1/a=0$, where the analytical solution for $q=3$ is known in free space [10]. Due to the separability in hyperspherical coordinates [59] the solution is also known for

[6] To give a meaning to an N-body thermal average within the zero-range model requires, for $N\geqslant 4$, a procedure whose identification is beyond the scope of this paper. This is here a formal issue, as we will consider the nondegenerate limit, allowing us to restrict our attention to the three-body sector.

[7] If one normalizes to unity the eigenstate ψ at time 0, the norm squared $\|\psi(t)\|^2$ is the probability that no loss event occurred during t. For the complex eigenenergy $E-i\hbar\Gamma/2$, this leads to a loss event rate equal to Γ, and to a particle loss rate $dN/dt=-3\Gamma$.

the case of an isotropic harmonic trap [49,50], which allows us to use the technique developed in [58,60] to write b_3 as

$$b_3 = 3^{3/2} \lim_{\omega\to 0} \left[\frac{Z_3}{Z_1} - Z_2 + \frac{1}{3}Z_1^2\right], \quad (26)$$

where $Z_q(\omega)$ is the canonical partition function at temperature T for the system of q interacting bosons in the harmonic trapping potential $U(\mathbf{r}) = \frac{1}{2}m\omega^2 r^2$. Since the center of mass is separable, Z_3/Z_1 simply equals the partition function Z_3^{int} of the internal variables. The internal three-body eigenspectrum in the trap involves fully universal states (not depending on R_t), and a single Efimovian channel with R_t-dependent eigenenergies $E_n(\omega)$, $n \in \mathbb{Z}$, solving a transcendental equation. Within the boundary conditions (3),(4), the sequence $E_n(\omega)$ is unbounded below. To give a mathematical existence to thermal equilibrium, we thus truncate the sequence, labeling the ground three-body state with the quantum number $n = 0$ and then keeping only $n \geqslant 0$ in the thermal average.[8] In the free-space limit $\omega \to 0$, this corresponds to a purely geometric spectrum of trimer states with a ratio $\exp(-2\pi/|s_0|)$ and a ground-state Efimov trimer energy

$$E_0(\omega) \underset{\omega\to 0}{\to} -\frac{2\hbar^2}{mR_t^2} e^{(2/|s_0|)\text{Im}\ln\Gamma(1+s_0)} \equiv -E_t. \quad (27)$$

Given E_t, this uniquely determines the three-body parameter R_t.[9] This finally leads to

$$\left(\frac{\partial b_3}{\partial(\ln R_t)}\right)_T = -\frac{3^{3/2}}{k_B T} \lim_{\omega\to 0} \sum_{n\geqslant 0} e^{-\beta E_n(\omega)} \frac{\partial E_n(\omega)}{\partial(\ln R_t)}. \quad (28)$$

Details of the calculation of that limit are exposed in Appendix C. The resulting expression for the three-body loss rate constant can be split into contributions of the three-body bound free-space spectrum and the continuous free-space spectrum:

$$\frac{dL_3}{d\eta}(\eta = 0) \underset{n\lambda^3\to 0}{\to} 72\sqrt{3}\,\frac{\hbar\lambda^4}{m}(S_{\text{bound}} + S_{\text{cont}}). \quad (29)$$

The bound-state contribution naturally appears as a (rapidly converging) discrete sum over the trimer states:

$$S_{\text{bound}} = \frac{\pi}{|s_0|} \sum_{n\geqslant 0} \beta E_t e^{-2\pi n/|s_0|} \exp(\beta E_t e^{-2\pi n/|s_0|}). \quad (30)$$

This allows prediction of the mean number N_{trim} of trimers with energy $E_{\text{trim}} = -E_t e^{-2\pi n/|s_0|}$ in the lossless system at thermal equilibrium: Since the contribution to dN/dt (to first order in η) of the term of index n in Eq. (30) is intuitively $-3\Gamma_{\text{trim}} N_{\text{trim}}$, where the decay rate of the trimer is $\Gamma_{\text{trim}} \simeq (2\eta/\hbar|s_0|)\partial_{\ln R_t} E_{\text{trim}}$, we obtain

$$\frac{N_{\text{trim}}}{N} \underset{n\lambda^3\to 0}{\sim} 3^{3/2}(n\lambda^3)^2 e^{-\beta E_{\text{trim}}}. \quad (31)$$

This agrees with Eq. (188) of Ref. [55] obtained from a chemical equilibrium reasoning.

The continuous-spectrum contribution to Eq. (29) naturally appears as an integral over positive energies E; see Appendix C. Mathematically, it can also be turned into a (rapidly converging) discrete sum that is easier to evaluate:[10]

$$S_{\text{cont}} = \frac{1}{2} + \sum_{n\geqslant 1} e^{-n\pi|s_0|} \text{Re}[\Gamma(1 - in|s_0|)(\beta E_t)^{in|s_0|}]. \quad (32)$$

As expected, S_{cont} is a log-periodic function of E_t. In practice, because $|s_0| > 1$, it has weak amplitude oscillations, between the extreme values $\simeq 0.478$ and $\simeq 0.522$. Our continuous-spectrum contribution to L_3 is equivalent, to first order in η, to the result of a direct three-body loss rate calculation for the thermal ensemble of free-space three-boson scattering states [64].

In experiments, the interaction potential has a finite range b, and the actual L_3 will deviate from the above results. For clarity, we now denote with an asterisk the quantities corresponding to a finite b. Due to the three-body losses, the so-called weakly bound trimer states are actually not bound states; they are resonances with complex energies $E_n^* - i\hbar\Gamma_n^*/2$. Assuming that $\Gamma_n^* \ll |E_n^*|$, we can name these resonances quasibound states or quasitrimers. Their contribution to the decay rate of the Bose gas, from the reasoning below Eq. (30), can be estimated as

$$\Gamma^*_{\text{quasibound}} \simeq 3^{3/2}(n\lambda^3)^2 N \sum_{n\geqslant 0} \Gamma_n^* e^{-\beta E_n^*}. \quad (33)$$

This is meaningful provided that the thermal-equilibrium trimer population formula Eq. (188) of Ref. [55] makes sense in the presence of losses, that is, the formation rate of quasitrimers of quantum number n has to remain much larger than Γ_n^* (in the zero-range framework, this is ensured by first taking the limit $\eta \to 0$ and then the limit of vanishing density $n\lambda^3 \to 0$). Evaluation of the finite-b positive-energy continuous-spectrum contribution $L^*_{3,\text{cont}>0}$ to the three-body loss rate constant is beyond the scope of this work. We can simply point out that taking the limit $b \to 0$ (with a fixed, infinite scattering length) makes $L^*_{3,\text{cont}>0}$ converge to the value obtained in the zero-range finite-η model; further, taking the zero-η limit gives

$$\lim_{\eta\to 0} \frac{1}{\eta}\Big(\lim_{b\to 0} L^*_{3,\text{cont}>0}\Big) = \frac{dL_{3,\text{cont}}}{d\eta}(\eta = 0). \quad (34)$$

In practice, as soon as $b \ll \lambda$ and $\eta \ll 1$, we expect that $L^*_{3,\text{cont}>0} \simeq \eta \frac{dL_{3,\text{cont}}}{d\eta}(\eta = 0)$.

VI. ARBITRARY MIXTURE

In this section we consider a mixture of bosonic and/or fermionic atoms with an arbitrary number of spin components.

[8] Physically, our $n = 0$ trimer state corresponds to the lowest weakly bound trimer. As usual in cold-atom physics, the deeply bound (here trimer) states are excluded from the thermal ensemble since their (very exothermic) collisional formation simply leads to particle losses.

[9] In reality, for an interaction with finite range or effective range b, the Efimovian trimer spectrum is only asymptotically geometric ($n \to +\infty$); there exist various models [61,62], however, where E_t is of order $\exp(-2\pi/|s_0|)\hbar^2/(mb^2)$ so that $R_t \gg b$, the ground-state Efimovian trimer is close to the zero-range limit, and the spectrum is almost entirely geometric.

[10] This is rapidly converging since $|\Gamma(1 - in|s_0|)|^2 = \pi n|s_0|/\sinh(\pi n|s_0|)$ [63].

TABLE III. Main results for an arbitrary mixture. In three dimensions, if the Efimov effect occurs, the derivatives must be taken for fixed three-body parameter(s), the expression for E in line 4 breaks down, and the last two lines, with derivatives of the free energy F and of the mean energy E respectively taken at fixed temperature T and entropy S, are meaningless in the absence of spectral selection (see Sec. V). $\gamma = 0.577\,215\ldots$ is Euler's constant.

Three dimensions		Two dimensions	
$\frac{\partial E}{\partial(-1/a_{\sigma\sigma'})} = \frac{2\pi\hbar^2}{\mu_{\sigma\sigma'}}(A,A)_{\sigma\sigma'}$	(1a)	$\frac{\partial E}{\partial(\ln a_{\sigma\sigma'})} = \frac{\pi\hbar^2}{\mu_{\sigma\sigma'}}(A,A)_{\sigma\sigma'}$	(1b)
$C_\sigma \equiv \lim_{k\to+\infty} k^4 n_\sigma(\mathbf{k}) = \sum_{\sigma'}(1+\delta_{\sigma\sigma'})\frac{8\pi\mu_{\sigma\sigma'}}{\hbar^2}\frac{\partial E}{\partial(-1/a_{\sigma\sigma'})}$	(2a)	$C_\sigma \equiv \lim_{k\to+\infty} k^4 n_\sigma(\mathbf{k}) = \sum_{\sigma'}(1+\delta_{\sigma\sigma'})\frac{4\pi\mu_{\sigma\sigma'}}{\hbar^2}\frac{\partial E}{\partial(\ln a_{\sigma\sigma'})}$	(2b)
$\int d^3c\, g^{(2)}_{\sigma\sigma'}\left(\mathbf{c}+\frac{m_{\sigma'}}{m_\sigma+m_{\sigma'}}\mathbf{r},\mathbf{c}-\frac{m_\sigma}{m_\sigma+m_{\sigma'}}\mathbf{r}\right)$		$\int d^2c\, g^{(2)}_{\sigma\sigma'}\left(\mathbf{c}+\frac{m_{\sigma'}}{m_\sigma+m_{\sigma'}}\mathbf{r},\mathbf{c}-\frac{m_\sigma}{m_\sigma+m_{\sigma'}}\mathbf{r}\right)$	
$\underset{r\to0}{\sim}(1+\delta_{\sigma\sigma'})\frac{\mu_{\sigma\sigma'}}{2\pi\hbar^2}\frac{\partial E}{\partial(-1/a_{\sigma\sigma'})}\frac{1}{r^2}$	(3a)	$\underset{r\to0}{\sim}(1+\delta_{\sigma\sigma'})\frac{\mu_{\sigma\sigma'}}{\pi\hbar^2}\frac{\partial E}{\partial(\ln a_{\sigma\sigma'})}\ln^2 r$	(3b)
$E - E_{\rm trap} = \sum_{\sigma\leqslant\sigma'}\frac{1}{a_{\sigma\sigma'}}\frac{\partial E}{\partial(-1/a_{\sigma\sigma'})}$		$E - E_{\rm trap} = \lim_{\Lambda\to\infty}\Big[-\sum_{\sigma\leqslant\sigma'}\frac{\partial E}{\partial(\ln a_{\sigma\sigma'})}\ln\left(\frac{a_{\sigma\sigma'}\Lambda e^\gamma}{2}\right)$	
$+\sum_\sigma\int\frac{d^3k}{(2\pi)^3}\frac{\hbar^2k^2}{2m_\sigma}\left[n_\sigma(\mathbf{k})-\frac{C_\sigma}{k^4}\right]$	(4a)	$+\sum_\sigma\int_{k<\Lambda}\frac{d^2k}{(2\pi)^2}\frac{\hbar^2k^2}{2m_\sigma}n_\sigma(\mathbf{k})\Big]$	(4b)
$\frac{1}{2}\frac{\partial^2E_n}{\partial(-1/a_{\sigma\sigma'})^2} = \left(\frac{2\pi\hbar^2}{\mu_{\sigma\sigma'}}\right)^2\sum_{n',E_{n'}\neq E_n}\frac{\lvert(A^{(n')},A^{(n)})_{\sigma\sigma'}\rvert^2}{E_n-E_{n'}}$	(5a)	$\frac{1}{2}\frac{\partial^2E_n}{\partial(\ln a_{\sigma\sigma'})^2} = \left(\frac{\pi\hbar^2}{\mu_{\sigma\sigma'}}\right)^2\sum_{n',E_{n'}\neq E_n}\frac{\lvert(A^{(n')},A^{(n)})_{\sigma\sigma'}\rvert^2}{E_n-E_{n'}}$	(5b)
$\left(\frac{\partial^2F}{\partial(-1/a_{\sigma\sigma'})^2}\right)_T < 0$	(6a)	$\left(\frac{\partial^2F}{\partial(\ln a_{\sigma\sigma'})^2}\right)_T < 0$	(6b)
$\left(\frac{\partial^2E}{\partial(-1/a_{\sigma\sigma'})^2}\right)_S < 0$	(7a)	$\left(\frac{\partial^2E}{\partial(\ln a_{\sigma\sigma'})^2}\right)_S < 0$	(7b)

The N particles are thus divided into groups, each group corresponding to a given chemical species and to a given spin state. We label these groups by an integer $\sigma \in \{1,\ldots,n\}$. Assuming that there are no spin-changing collisions, the number N_σ of atoms in each group is fixed, and one can consider that particle i belongs to the group σ if $i \in I_\sigma$, where the I_σ's are a fixed partition of $\{1,\ldots,N\}$ which can be chosen arbitrarily. For example, a possible choice is $I_1 = \{1,\ldots,N_1\}$; $I_2 = \{N_1+1,\ldots,N_1+N_2\}$; etc. The wave function $\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is then symmetric (respectively antisymmetric) with respect to the exchange of two particles belonging to the same group I_σ of bosonic (respectively fermionic) particles. Each atom has a mass m_i and is subject to a trapping potential $U_i(\mathbf{r}_i)$, and the scattering length between atoms i and j is a_{ij}. We set $m_i = m_\sigma$ and $a_{ij} = a_{\sigma\sigma'}$ for $i \in I_\sigma$ and $j \in I_{\sigma'}$. The reduced masses are $\mu_{\sigma\sigma'} = m_\sigma m_{\sigma'}/(m_\sigma + m_{\sigma'})$. We shall denote by $\mathcal{P}_{\sigma\sigma'}$ the set of all pairs of particles with one particle in group σ and the other one in group σ', each pair being counted only once:

$$\mathcal{P}_{\sigma\sigma'} \equiv \{(i,j) \in (I_\sigma \times I_{\sigma'}) \cup (I_{\sigma'} \times I_\sigma)\ /\ i < j\}. \tag{35}$$

The definition of the zero-range model is modified as follows: In the contact conditions (1),(6), the scattering length a is replaced by a_{ij}, and the limit $r_{ij} \to 0$ is taken for a fixed center-of-mass position $\mathbf{c}_{ij} = (m_i\mathbf{r}_i + m_j\mathbf{r}_j)/(m_i + m_j)$; moreover Schrödinger's equation becomes

$$\sum_{i=1}^N \left[-\frac{\hbar^2}{2m_i}\Delta_{\mathbf{r}_i} + U_i(\mathbf{r}_i)\right]\psi = E\,\psi. \tag{36}$$

Our results are summarized in Table III, where we introduced the notation in dimension d

$$(A^{(1)},A^{(2)})_{\sigma\sigma'} \equiv \sum_{(i,j)\in\mathcal{P}_{\sigma\sigma'}} \int \left(\prod_{k\neq i,j} d^dr_k\right) \int d^dc_{ij} \times A^{(1)*}_{ij}(\mathbf{c}_{ij},(\mathbf{r}_k)_{k\neq i,j}) A^{(2)}_{ij}(\mathbf{c}_{ij},(\mathbf{r}_k)_{k\neq i,j}). \tag{37}$$

Since $a_{\sigma\sigma'} = a_{\sigma'\sigma}$ there are only $n(n+1)/2$ independent scattering lengths, and the partial derivatives with respect to one of these independent scattering lengths are taken while keeping fixed the other independent scattering lengths. We note that, in Ref. [32], Eqs. (4a) and (4b) of Table III were already partially obtained.[11]

In 3D the three-body Efimov effect occurs, except for a mixture of only two fermionic groups with a heavy-to-light mass ratio $m_\sigma/m_{\sigma'} < 13.6069\cdots$ [65–67]. When the three-body Efimov effect occurs, as for single-component bosons, the derivatives with respect to any scattering length have *a minimum* to be taken for fixed three-body parameter(s), and the relation between E and the momentum distribution [Table III, Eq. (4a)] breaks down, which was not realized in Ref. [32];[12] moreover, we expect new relations analogous to the ones given in Sec. IV for bosons. Furthermore, we assume here that there is no fermionic group σ with a mass ratio $m_\sigma/m_{\sigma'} > 13.384$ with respect to any other group σ', so as to avoid a four-body Efimov effect [44]. More generally, the zero-range model Hamiltonian is assumed to be self-adjoint without introducing interaction parameters other than scattering lengths and three-body parameters.

[11]Our expressions Table III, Eqs. (4a) and (4b) complete the ones in Ref. [32] in the following way. In Ref. [32],the coefficient of $1/a_{\sigma\sigma'}$ was not expressed as $\partial E/\partial(1/a_{\sigma\sigma'})$; only the case of a spatially homogeneous system was covered; finally, an arbitrary mixture was covered only in 3D, while in 2D only the case of a two-component Fermi-Fermi mixture was covered.

[12]Indeed, in the presence of the Efimov effect, the momentum distribution has a subleading contribution $\delta n_\sigma(k)$ scaling as $1/k^5$, evaluated in the bosonic case in Ref. [68], leading to a divergent integral in this relation. For two-component fermions with a mass ratio sufficiently close to 1, the integral converges, because $\delta n_\sigma(k) \propto 1/k^{5+2s}$ where $s > 0$ is the scaling exponent of the three-body wave function, $\psi(\lambda\mathbf{r}_1,\lambda\mathbf{r}_2,\lambda\mathbf{r}_3) \propto \lambda^{s-2}$ for $\lambda \to 0$; see a note in Ref. [26] and note 6 in Ref. [34].

The derivations of the relations of Table III are analogous to the ones already given for two-component fermions and single-component bosons. The lemmas of Article I, Eqs. (33) and (35), are replaced by

$$\langle\psi_1,H\psi_2\rangle-\langle H\psi_1,\psi_2\rangle = \begin{cases} \frac{2\pi\hbar^2}{\mu_{\sigma\sigma'}}\left(\frac{1}{a^{(1)}_{\sigma\sigma'}}-\frac{1}{a^{(2)}_{\sigma\sigma'}}\right)(A^{(1)},A^{(2)})_{\sigma\sigma'} & \text{in 3D,}\\ \frac{\pi\hbar^2}{\mu_{\sigma\sigma'}}\ln\left(a^{(2)}_{\sigma\sigma'}/a^{(1)}_{\sigma\sigma'}\right)(A^{(1)},A^{(2)})_{\sigma\sigma'} & \text{in 2D,}\end{cases} \tag{38}$$

where ψ_1 and ψ_2 obey the same contact conditions (including the three-body ones if there is an Efimov effect), *except* for the independent scattering length $a_{\sigma\sigma'}$, which is equal to $a^{(i)}_{\sigma\sigma'}$ for ψ_i, $i=1,2$. The momentum distribution for the group σ is normalized as $\int n_\sigma(\mathbf{k})d^dk/(2\pi)^d = N_\sigma$. The pair distribution function is now defined by

$$g^{(2)}_{\sigma\sigma'}(\mathbf{u},\mathbf{v}) = \int d^dr_1\cdots d^dr_N|\psi(\mathbf{r}_1,\dots,\mathbf{r}_N)|^2 \times \sum_{i\in I_\sigma, j\in I_{\sigma'}, i\neq j}\delta(\mathbf{u}-\mathbf{r}_i)\delta(\mathbf{v}-\mathbf{r}_j). \tag{39}$$

The Hamiltonian of the lattice model used in some of the derivations now reads

$$H_{\rm latt} = H_0 + \sum_{\sigma\leqslant\sigma'} g_{0,\sigma\sigma'}\,W_{\sigma\sigma'}, \tag{40}$$

where $H_0=\sum_{i=1}^N[-\frac{\hbar^2}{2m_i}\Delta_{\mathbf{r}_i}+U_i(\mathbf{r}_i)]$ with the discrete Laplacian defined by $\langle\mathbf{r}|\Delta_\mathbf{r}|\mathbf{k}\rangle\equiv -k^2\langle\mathbf{r}|\mathbf{k}\rangle$ (for $\mathbf{k}$ in the first Brillouin zone) and $W_{\sigma\sigma'}=\sum_{(i,j)\in\mathcal{P}_{\sigma\sigma'}}\delta_{\mathbf{r}_i,\mathbf{r}_j}b^{-d}$. In the formulas of Article I involving the two-body scattering problem, one has to replace g_0 by $g_{0,\sigma\sigma'}$, a by $a_{\sigma\sigma'}$, and m by $2\mu_{\sigma\sigma'}$. Denoting the corresponding zero-energy scattering wave function by $\phi_{\sigma\sigma'}(\mathbf{r})$, the lemma in Article I, Eq. (56), is replaced by $\langle\psi'|W_{\sigma\sigma'}|\psi\rangle = |\phi_{\sigma\sigma'}(\mathbf{0})|^2\,(A',A)_{\sigma\sigma'}$.

VII. CONCLUSION

In dimensions two and three, we obtained several relations valid for any eigenstate of the N-boson problem with zero-range interactions. The interactions are characterized by the 2D or 3D two-body s-wave scattering length a and, in 3D when the Efimov effect takes place, by a three-body parameter R_t. Our expressions relate various observables to derivatives of the energy with respect to these interaction parameters. Some of the expressions, initially obtained in Ref. [35], were derived in Ref. [36] with a different technique. For completeness, we have also generalized some of the relations to arbitrary mixtures of Bose and/or Fermi gases.

For the bosons in 3D, especially interesting are the relations involving the derivative of the energy with respect to the three-body parameter. Physically, one of then predicts (to first order in the inelasticity parameter η) the decay rate Γ of the system due to three-body losses, which occur in cold-atom experiments by recombination to deeply bound dimers. This means that one can extract Γ from the eigenenergies of a purely lossless ($\eta=0$) model. As an application, we analytically obtained (within the zero-range model, and to first order in η) the three-body loss rate constant L_3 for the 3D nondegenerate Bose gas at thermal equilibrium with infinite scattering length. Experimentally, this quantity is under current study with real atomic gases [64].

Mathematically, the 3D relations hold under the assumption that the two-body scattering length and the three-body parameter are sufficient to make the N-boson problem well defined, with a self-adjoint Hamiltonian. Therefore they may be used to numerically test this assumption, for example by checking the consistency between the values of the derivative of the energy with respect to the three-body parameter obtained in different ways. Three possible ways are by numerical differentiation of the energy, use of the present relation on the short-distance triplet distribution function, or use of the virial theorem which also involves this derivative [69].

ACKNOWLEDGMENTS

We thank N. Navon, S. Tan and J. von Stecher for stimulating discussions. The work of F.W. at UMass was supported by NSF under Grants No. PHY-0653183 and No. PHY-1005543. Our group at ENS is a member of IFRAF. We acknowledge support from ERC Project FERLODIM No. 228177.

APPENDIX A: DERIVATION OF A LEMMA

Here we derive the lemma (13) for three bosons in the zero-range model. The first step is to express the Hamiltonian in hyperspherical coordinates [16,70]: Using the value of the Jacobian given below Eq. (19),

$$\begin{aligned}\langle\psi_1,H\psi_2\rangle-\langle H\psi_1,\psi_2\rangle &= -\frac{\hbar^2}{2m}3\sqrt{3}\int_0^\infty dR\,R^5\int d^5\Omega\int d^3c \\ &\quad\times\left\{\psi_1^*\left(\frac{\partial^2}{\partial R^2}+\frac{5}{R}\frac{\partial}{\partial R}+\frac{T_\mathbf{\Omega}}{R^2}+\frac{1}{3}\Delta_\mathbf{c}\right)\psi_2-[\psi_1^*\leftrightarrow\psi_2]\right\}\\ &= -\frac{\hbar^2}{2m}3\sqrt{3}\left\{\int_0^\infty dR\,R^5\int d^5\Omega\,\mathcal{A}_\mathbf{c}(R,\mathbf{\Omega})\right.\\ &\quad\left.+\int d^5\Omega\int d^3c\,\mathcal{A}_R(\mathbf{\Omega},\mathbf{c})+\int_0^\infty dR\,R^5\int d^3c\,\mathcal{A}_\mathbf{\Omega}(R,\mathbf{c})\right\},\end{aligned} \tag{A1}$$

where $\mathbf{c}=\mathbf{c}_{123}$ and

$$\mathcal{A}_\mathbf{c}(R,\mathbf{\Omega}) \equiv \int d^3c\,\left\{\psi_1^*\,\frac{1}{3}\Delta_\mathbf{c}\,\psi_2-[\psi_1^*\leftrightarrow\psi_2]\right\}, \tag{A2}$$

$$\mathcal{A}_R(\mathbf{\Omega},\mathbf{c}) \equiv \int_0^\infty dR\,R^5\left\{\psi_1^*\left(\frac{\partial^2}{\partial R^2}+\frac{5}{R}\frac{\partial}{\partial R}\right)\psi_2 -[\psi_1^*\leftrightarrow\psi_2]\right\}, \tag{A3}$$

$$\mathcal{A}_\mathbf{\Omega}(R,\mathbf{c}) \equiv \int d^5\Omega\,\left\{\psi_1^*\frac{T_\mathbf{\Omega}}{R^2}\psi_2-\psi_2\frac{T_\mathbf{\Omega}}{R^2}\psi_1^*\right\}, \tag{A4}$$

$T_\mathbf{\Omega}$ being a differential operator acting on the hyperangles and called the Laplacian on the hypersphere.

The quantity $\mathcal{A}_R$ can be computed using the following simple lemma: If $\Phi_1(R)$ and $\Phi_2(R)$ are functions which decay quickly at infinity and have no singularity except may be at

$R=0$, then

$$\int_0^\infty dR\, R^5 \left\{ \Phi_1^* \left(\frac{\partial^2}{\partial R^2} + \frac{5}{R}\frac{\partial}{\partial R} \right) \Phi_2 - [\Phi_1^* \leftrightarrow \Phi_2] \right\} = -\lim_{R\to 0} R \left(\mathcal{F}_1^* \frac{\partial \mathcal{F}_2}{\partial R} - \mathcal{F}_2 \frac{\partial \mathcal{F}_1^*}{\partial R} \right), \tag{A5}$$

where $\mathcal{F}_i(R) \equiv R^2\,\Phi_i(R)$. Expressing the right-hand side of Eq. (A5) thanks to the boundary condition (3) then yields the desired result (13), because the other two contributions $\mathcal{A}_{\mathbf{c}}$ and $\mathcal{A}_{\mathbf{\Omega}}$ both vanish, as we now show.

The quantity $\mathcal{A}_{\mathbf{c}}(R,\mathbf{\Omega})$, rewritten as $\frac{1}{3}\int d^3c\,\nabla_{\mathbf{c}}\cdot(\psi_1^*\nabla_{\mathbf{c}}\psi_2 - \psi_2\nabla_{\mathbf{c}}\psi_1^*)$ and transformed with the divergence theorem, is zero, since the ψ_i's are regular functions of $\mathbf{c}$ for every $(R,\mathbf{\Omega})$ except on a set of measure zero.

It remains to show that

$$\mathcal{A}_{\mathbf{\Omega}}(R,\mathbf{c}) = 0 \ \text{ for any } \mathbf{c} \quad \text{and} \quad R > 0. \tag{A6}$$

We will use the fact that ψ_1 and ψ_2 satisfy the two-body boundary condition (1) with the same a, and apply the lemma of Article I, Eq. (33). More precisely, we will show that for any smooth function $f(R,\mathbf{c})$ which vanishes in a neighborhood of $R=0$,

$$\int_0^\infty dR\,R^5 \int d^3c\, f(R,\mathbf{c})^2\,\mathcal{A}_{\mathbf{\Omega}}(R,\mathbf{c}) = 0; \tag{A7}$$

this clearly implies (A6). To show (A7) we note that

$$-\frac{\hbar^2}{2m}3\sqrt{3}\int_0^\infty dR\,R^5 \int d^3c\, f(R,\mathbf{c})^2\,\mathcal{A}_{\mathbf{\Omega}}(R,\mathbf{c}) = -\frac{\hbar^2}{2m}3\sqrt{3}\int_0^\infty dR\,R^5 \int d^5\Omega \int d^3c \left\{ (f\psi_1^*)\frac{T_{\mathbf{\Omega}}}{R^2}(f\psi_2) - [\psi_1^* \leftrightarrow \psi_2] \right\}, \tag{A8}$$

which can be rewritten as

$$\int d^3r_1 d^3r_2 d^3r_3 \{ (f\psi_1^*) H (f\psi_2) - [\psi_1^* \leftrightarrow \psi_2] \} + \frac{\hbar^2}{2m}3\sqrt{3}\int_0^\infty dR\,R^5 \int d^5\Omega \int d^3c \left\{ (f\psi_1^*) \times \left(\frac{\partial^2}{\partial R^2} + \frac{5}{R}\frac{\partial}{\partial R} + \frac{1}{3}\Delta_{\mathbf{c}} \right)(f\psi_2) - [\psi_1^* \leftrightarrow \psi_2] \right\}. \tag{A9}$$

The first integral in this expression vanishes, as a consequence of the lemma of Article I, Eq. (33). This lemma is indeed applicable to the wave functions $f\psi_i$: They vanish in a neighborhood of $R=0$ (see the discussion in Article I); moreover they satisfy the two-body boundary condition for the same value of the scattering length a (as follows from the fact that R varies quadratically with r for small r). The second integral in Eq. (A9) vanishes as well: The contribution of the partial derivatives with respect to R vanishes as a consequence of lemma (A5), and the contribution of $\Delta_{\mathbf{c}}$ vanishes because the $f\psi_i$'s are regular functions of $\mathbf{c}$.

APPENDIX B: RELATION BETWEEN Γ AND B FOR ANY η

In contrast to the remaining part of the paper, we assume here that the inelasticity parameter $\eta > 0$ and is not necessarily a small perturbation, so that the N-body wave function ψ obeys the contact conditions given by Eqs. (3) and (4) *modified* according to Eq. (20). As a consequence, ψ is in general an eigenstate of H with a complex energy $E - i\hbar\Gamma/2$, where Γ is the decay rate. If ψ is normalized to unity at time 0 then

$$\Gamma = -\frac{d}{dt}(\|\psi\|^2)(t=0). \tag{B1}$$

This can be transformed using the continuity equation

$$\partial_t|\psi(\mathbf{X},t)|^2 + \mathrm{div}_{\mathbf{X}}\mathbf{J} = 0, \tag{B2}$$

where we collected all the particles coordinates in a single vector $\mathbf{X} = (\mathbf{r}_1,\ldots,\mathbf{r}_N)$ with $3N$ components, and where we introduced the probability current in $\mathbb{R}^{3N}$:

$$\mathbf{J} = \frac{\hbar}{m}\mathrm{Im}\,(\psi^*\mathrm{grad}_{\mathbf{X}}\psi). \tag{B3}$$

Equation (B2) is valid for all $r_{ij} > 0$, and results as usual from Schrödinger's equation.

To avoid the singularities that appear in ψ for three coinciding particle positions, we introduce the exclusion volumes $B_{ijk}(\epsilon) = \{\mathbf{X} \in \mathbb{R}^{3N} / R_{ijk} < \epsilon\}$ for all triplets $\{i,j,k\}$ of particles (of hyperradius R_{ijk}) in the integral defining $\|\psi\|^2$, taking the limit $\epsilon \to 0$ at the end of the calculation. With the divergence theorem, this leads to

$$\Gamma = -\lim_{\epsilon\to 0}\int_{I_\epsilon} d^{3N}X\,\partial_t[|\psi(\mathbf{X},t=0)|^2] = -\lim_{\epsilon\to 0}\sum_{\{i,j,k\}}\int_{\partial B_{ijk}(\epsilon)} d^{3N-1}\mathbf{S}\cdot\mathbf{J} \tag{B4}$$

with the surface element $d^{3N-1}\mathbf{S}$ oriented towards the exterior of B_{ijk}. Here I_ϵ is $\mathbb{R}^{3N}$ minus the union of all $B_{ijk}(\epsilon)$; it is thus the set of all the $\mathbf{X}$ having all the $R_{ijk} > \epsilon$. Using the bosonic symmetry we single out the decay rate due to particles 1, 2, and 3:

$$\Gamma = -\frac{N(N-1)(N-2)}{3!}\lim_{\epsilon\to 0}\int_{\partial B_{123}(\epsilon)} d^{3N-1}\mathbf{S}\cdot\mathbf{J}. \tag{B5}$$

The integration domain in Eq. (B5), which is the boundary of $B_{123}(\epsilon)$, is actually a cylinder in $\mathbb{R}^{3N}$, and the coordinates numbers 10 to $3N$ of the surface element $d^{3N-1}\mathbf{S}$ are zero, so that one can keep the contribution to the probability current of the first three particles only: We can thus replace $d^{3N-1}\mathbf{S}\cdot\mathbf{J}$ with $d^8\mathbf{S}_t\cdot\mathbf{J}_t$, the nine-coordinate vectors $\mathbf{J}_t$ and $d^8\mathbf{S}_t$ coinciding with the first nine coordinates of $\mathbf{J}$ and $d^{3N-1}\mathbf{S}$. For fixed $\mathbf{r}_4,\ldots,\mathbf{r}_N$ we thus have to evaluate

$$\gamma(\epsilon) \equiv -\int_{R=\epsilon} d^8\mathbf{S}_t\cdot\mathbf{J}_t = \int_{R>\epsilon} d^3r_1 d^3r_2 d^3r_3\,\mathrm{div}_{\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3}\mathbf{J}_t, \tag{B6}$$

where we used the divergence theorem. We then change the integration variables from $\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3$ to $\mathbf{c}_{123},\mathbf{R}$, with the Jacobian given below Eq. (19). Further use of the identity

$$\sum_{i=1}^{3}\mathrm{div}_{\mathbf{r}_i}(\psi^*\mathrm{grad}_{\mathbf{r}_i}\psi - \text{c.c.}) = \mathrm{div}_{\mathbf{R}}(\psi^*\mathrm{grad}_{\mathbf{R}}\psi - \text{c.c.}) + \frac{1}{3}\mathrm{div}_{\mathbf{c}_{123}}(\psi^*\mathrm{grad}_{\mathbf{c}_{123}}\psi - \text{c.c.}), \tag{B7}$$

and backward application of the divergence theorem yields

$$\gamma(\epsilon) = -3\sqrt{3}\,\epsilon^5 \int d^3c_{123} \int d^5\Omega\, \frac{\hbar}{m} \mathrm{Im}[\psi^* \partial_R \psi]_{R=\epsilon}. \tag{B8}$$

The $R \to 0$ behavior of ψ being given by B times a known function [see Eqs. (3) and (4) modified according to Eq. (20)], we finally obtain

$$\Gamma = \frac{\hbar}{m} N(N-1)(N-2) \frac{\sqrt{3}}{4} |s_0| \sinh(2\eta) \|B\|^2 \tag{B9}$$

with $\|B\|^2 = \int d^3c_{123}\, d^3r_4 \cdots\, d^3r_N\, |B(\mathbf{c}_{123},\mathbf{r}_4,\ldots,\mathbf{r}_N)|^2$. In the limit $\eta \to 0$, $\|B\|^2$ tends to its value in the lossless model and we recover Table II, Eq. (3) using Table II, Eq. (1).

APPENDIX C: FREE-SPACE LIMIT OF A VIRIAL SUM

Here we derive the free-space limit (28) of a sum over the internal Efimovian eigenenergies $E_n(\omega)$ for three bosons in a harmonic trap with oscillation frequency ω, interacting in the zero-range limit with infinite scattering length. A rewriting of the implicit equation for E_n of Ref. [50] gives, for $n \in \mathbb{N}$,

$$\mathrm{Im} \ln \Gamma \left(\frac{1 + s_0 - \tilde{E}_n}{2} \right) + \frac{|s_0|}{2} \ln \left(\frac{2\hbar\omega}{E_t} \right) + n\pi = 0. \tag{C1}$$

We have introduced the notation $\tilde{E}_n = E_n/(\hbar\omega)$. Also, $\Gamma(z)$ is the Gamma function and its logarithm $\ln\Gamma(z)$ is the usual univalued function with a branch cut on the real negative axis. The left-hand side of Eq. (C1) can be shown to be a decreasing function of E_n, using relation 8.362(1) of Ref. [63], so that Eq. (C1) determines E_n in a unique way. The fact that E_t, as given by Eq. (27), is the free-space ground trimer binding energy can be checked from Eq. (C1) by a Stirling expansion for $\tilde{E}_n \to -\infty$.

To evaluate the sum in Eq. (28) for $\omega \to 0$, we collect the eigenenergies E_n into three groups. The (finite) *transition* group corresponds to $|E_n|$ not much larger than $\hbar\omega$, and gives a vanishing contribution to Eq. (28) for $\omega \to 0$. The *bound-state* group corresponds to negative eigenenergies with $|E_n| \gg \hbar\omega$; the corresponding free-space trimer sizes are much smaller than the harmonic oscillator length $[\hbar/(m\omega)]^{1/2}$, so that the trapping potential has a negligible effect and $E_n(\omega)$ is close to the free-space trimer energy of quantum number n:

$$E_n(\omega) \simeq -E_t e^{-2\pi n/|s_0|}. \tag{C2}$$

This directly leads to the contribution S_{bound} in Eq. (30).

Finally, the third group contains the positive eigenenergies with $E_n \gg \hbar\omega$, which will reconstruct the free-space continuous spectrum for $\omega \to 0$. As shown in Sec. 3.3.a of Ref. [16], these E_n are almost equally spaced by $2\hbar\omega$. We need here the leading-order deviation from equispacing, which we parametrize with a "quantum defect" Δ as

$$\tilde{E}_n \underset{n\to+\infty}{=} 2n + \Delta(E_n) + O(1/n). \tag{C3}$$

For $\tilde{E}_n \to +\infty$, Stirling's formula cannot be immediately applied to Eq. (C1) since the argument of the Gamma function remains at finite distance from the poles of Γ (on the real negative axis). Using $\Gamma(z)\Gamma(1-z) = \pi/\sin(\pi z)$ [63], we obtain the useful identity

$$-\mathrm{Im}\,\ln\Gamma\left(\frac{1+s_0-\tilde{E}}{2}\right) = \mathrm{Im}\,\ln\Gamma\left(\frac{1-s_0+\tilde{E}}{2}\right) + \frac{\pi}{2}\tilde{E} + \mathrm{Im}\,\ln[1 + e^{-\pi|s_0|}e^{-i\pi\tilde{E}}] \tag{C4}$$

for all real $\tilde{E}$. Note that the logarithm in the last term of that expression is unambiguously defined [by a series expansion of $\ln(1+u)$ with u] since $e^{-\pi|s_0|} < 1$. Stirling's expansion can now be used in the right-hand side of Eq. (C4), turning (C1) into an implicit equation for the quantum defect Δ:

$$\Delta(E) = \frac{|s_0|}{\pi} \ln\left(\frac{E}{E_t}\right) - \frac{2}{\pi}\mathrm{Im}\,\ln[1 + e^{-\pi|s_0|}e^{-i\pi\Delta(E)}]. \tag{C5}$$

Since $\exp(-\pi|s_0|) \ll 1$, we have a *small-deviation property*: $\Delta(E)$ only slightly deviates, by $O[\exp(-\pi|s_0|)]$, from the first term in the right-hand side of (C5). This deviation was not fully taken into account in Sec. 3.3.a of Ref. [16]. To remain exact, we multiply (C5) by $i\pi$ on both sides, and we exponentiate the resulting equation. Since $\exp[-2i\mathrm{Im}\,\ln(1+u)] = (1+u^*)/(1+u)$, we obtain a solvable equation for $\exp(i\pi\Delta)$ that determines Δ modulo 2. From the *small-deviation property* stated above, we can lift the modulo 2 uncertainty:

$$\Delta(E) = \frac{|s_0|}{\pi} \ln\left(\frac{E}{E_t}\right) + \frac{2}{\pi}\mathrm{Im}\,\ln\left[1 - e^{-\pi|s_0|}\left(\frac{E}{E_t}\right)^{-i|s_0|}\right]. \tag{C6}$$

Finally, it remains in Eq. (28) to replace the sum over n (for E_n in the third group) by an integral $\int_0^{+\infty} dE/(2\hbar\omega)$, where $2\hbar\omega$ is the leading-order level spacing, to obtain the continuous-spectrum contribution

$$\left(\frac{\partial b_3}{\partial(\ln R_t)}\right)_T^{\mathrm{cont}} = -\frac{3^{3/2}}{2k_BT}\int_0^{+\infty} dE\, e^{-\beta E}\frac{\partial\Delta(E)}{\partial(\ln R_t)}. \tag{C7}$$

After expansion of $\partial_{\ln R_t}\Delta(E)$ in powers of $e^{-\pi|s_0|}$, the integral over E can be expressed in terms of the Gamma function, which eventually leads to Eq. (32).

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