Unitary gas in an isotropic harmonic trap: Symmetry properties and applications

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We consider N atoms trapped in an isotropic harmonic potential, with s-wave interactions of infinite scattering length. In the zero-range limit, we obtain several exact analytical results: mapping between the trapped problem and the free-space zero-energy problem, separability in hyperspherical coordinates, SO(2,1) hidden symmetry, existence of a decoupled bosonic degree of freedom, and relations between the moments of the trapping potential energy and the moments of the total energy.

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I. INTRODUCTION

Strongly interacting degenerate Fermi gases with two spin components are studied in present experiments with ultracold atoms [1]: by tuning the interaction strength between the atoms of different spin states *via* a Feshbach resonance, one can even reach the so-called unitary limit [2] where the interaction strength in the s-wave channel reaches the maximal amplitude allowed by quantum mechanics in a gas. More precisely, this means that the s-wave scattering amplitude between two particles reaches the value

$$f_k = -\frac{1}{ik} \tag{1}$$

for the relative momenta k that are relevant in the gas, in particular for k of the order of the Fermi momentum k_F of the particles. This implies that the s-wave scattering length a is set to infinity (which is done in practice by tuning an external magnetic field). This also implies that $k|r_e| \ll 1$, where r_e is the effective range of the interaction potential, a condition well satisfied in present experiments on broad Feshbach resonances.

The maximally interacting gas defined by these conditions is called the unitary gas [2]. It has universal properties since all the details of the interaction have dropped out of the problem. Theoretically, for spin-1/2 fermions with equal populations in the two spin states, equilibrium properties have been calculated in the thermodynamical limit in the spatially homogeneous case using Monte Carlo methods; at finite temperature [3–5], and at zero temperature with a fixed node approximation [6,7] or with a quantum Monte Carlo technique [8]. In practice, the unitary gases produced experimentally are stored in essentially harmonic traps, which raises the question of the effect of such an external potential. In this paper, we consider a specific aspect of this question: restricting to perfectly isotropic harmonic traps, but with no constraint on the relative spin populations, we show that the unitary quantum gas admits interesting symmetry properties that have measurable consequences on its spectrum and on the many-body wave functions. These properties imply that there is a mapping between the N-body eigenfunctions in a trap and the zero-energy N-body eigenfunctions in free space; the N-body problem is separable in hyperspherical coordinates; and there exist relations between the moments of the trapping potential energy and those of the total energy at thermal equilibrium.

A unitary Bose gas was not produced yet. This is related to the Efimov effect [9]: when three bosons interact with a short-range potential of infinite scattering length, an effective three-body attraction takes place, leading in free space to the existence of weakly bound trimers. This effective attraction generates high values of k so that the unitarity condition Eq. (1) is violated. It also gives a short lifetime to the gas by activating three-body losses due to the formation of deeply bound molecules [10–12]. In an isotropic harmonic trap, for three bosons, there exist Efimovian states [13,14], but there also exist eigenstates not experiencing the Efimov effect [13,15]. These last states are universal (in the sense that they depend only on $\hbar$, the mass m, and the oscillation frequency ω of an atom in the trap) and they are predicted to be long-lived [15]. The results of the present paper apply to all universal states, fermionic or bosonic, but do not apply to the Efimovian states. For spin-1/2 fermions, all states are expected to be universal [1–8,15,16].

II. OUR MODEL FOR THE UNITARY GAS

The physical system considered in this paper is a set of N particles of equal mass m (an extension to different masses is given in Appendix A). The particles are of arbitrary spin and follow arbitrary statistics; the Hamiltonian is supposed to be spin-independent so that the N-body wave function ψ that we shall consider corresponds to a given spin configuration [17]. The particles are trapped by the same isotropic harmonic potential and have a common oscillation frequency ω. We collect all the positions $\vec{r}_i$ of the particles in a single $3N$ component vector:

$$\vec{X} \equiv (\vec{r}_1, \ldots, \vec{r}_N). \tag{2}$$

Its norm

$$X = \|\vec{X}\| = \sqrt{\sum_{i=1}^{N} r_i^2} \tag{3}$$

is called the hyperradius. We will also use the unit vector

$$\vec{n} \equiv \vec{X}/X \tag{4}$$

(which may be parametrized by $3N-1$ hyperangles). The coordinates $(X, \vec{n})$ are called hyperspherical coordinates [18].

The total trapping potential energy simply writes

$$H_{\text{trap}} = \frac{1}{2} m\omega^2 X^2. \tag{5}$$

The interaction between the particles is assumed to be at the unitary limit defined in Eq. (1); one can then replace the interaction by contact conditions on the N-body wave function (this is a well established procedure, see, e.g., [16,19,20] and references therein): when the distance $r_{ij} = \|\vec{r}_j - \vec{r}_i\|$ between particles i and j tends to zero, there exists a function A such that

$$\psi(\vec{X}) \underset{r_{ij}\to 0}{=} \frac{\mathcal{A}(\vec{R}_{ij}, \{\vec{r}_k : k \neq i, j\})}{r_{ij}} + O(r_{ij}), \tag{6}$$

where $\vec{R}_{ij} = (\vec{r}_i + \vec{r}_j)/2$ is the fixed center-of-mass position of particles i and j, and $\{\vec{r}_k : k \neq i, j\}$ are the positions of the other particles. In these contact conditions it is assumed that $\vec{R}_{ij}$ differs from all the $\vec{r}_k$'s, $k \neq i, j$, and that none of these $\vec{r}_k$'s coincide.

When none of the particle positions coincide, the stationary wave function ψ solves Schrödinger's equation, $H\psi = E\psi$, with the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\Delta_{\vec{X}} + \frac{1}{2} m\omega^2 X^2. \tag{7}$$

At first sight, the eigenvalue problem $H\psi = E\psi$ is straightforward, since H takes the same expression as the Hamiltonian of a noninteracting gas. However, the mathematical difficulty and the physical effect of the interactions are contained in the contact conditions Eq. (6). Technically, this means that the domain of our Hamiltonian differs from the one of the ideal gas problem.

This model is expected to be exact for universal states in the limit of a zero range of the interaction potential [19]. To be more explicit, let us consider equal mass fermions of spin $1/2$, interacting *via* a separable potential, in continuous space [14] or in a Hubbard-type lattice model [3–5,21], with an infinite scattering length. It is then believed that in the limit of a vanishing range of the interaction all the eigenenergies and eigenvectors converge to a well-defined limit, independent of the specific details of the model (hence the concept of universality), and that the values of the limits are given by the solutions of the above zero-range model. In this frame, it is natural to assume that the zero-range model defines a Hermitian Hamiltonian problem [22], a fact that may be checked explicitly for $N=3$ from the analytical solution [15].

III. SCALING PROPERTIES OF THE TRAPPED UNITARY GAS

A. What is scale invariance?

A fundamental property of the contact conditions Eq. (6) is their invariance by a rescaling of the spatial coordinates. More precisely, we define a rescaled wave function ψ_λ by

$$\psi_\lambda(\vec{X}) \equiv \psi(\vec{X}/\lambda), \tag{8}$$

where $\lambda > 0$ is the scaling factor. Then, if ψ obeys the contact conditions, so does ψ_λ for any λ. Note that this property holds only because the scattering length is infinite (for a finite value of a, $1/r_{ij}$ in Eq. (6) would be replaced by $1/r_{ij} - 1/a$, which breaks scale invariance). Since we are interested in universal states only, we assume that the domain of the Hamiltonian is also invariant by a spatial rescaling.

In free space (that is for $\omega=0$), this scale invariance implies the following property: if ψ is an eigenstate of energy E, then ψ_λ is an eigenstate of energy E/λ^2 for any λ [23]. This implies the absence of bound states in free space: otherwise the scaling transform would generate a continuum of states which are square integrable (after elimination of the center-of-mass variables), and this is forbidden for a Hermitian problem [24].

When $E=0$, one finds (see Appendix B) that the free space eigenstates can be assumed to be scale-invariant, i.e., there exists an exponent ν such that

$$\psi_\lambda(\vec{X}) = \lambda^{-\nu}\psi(\vec{X}). \tag{9}$$

Taking the derivative of this relation with respect to λ in $\lambda = 1$, this shows that ψ is an eigenstate of the dilatation operator,

$$\hat{D} \equiv \vec{X} \cdot \partial_{\vec{X}}, \tag{10}$$

with the eigenvalue ν. This result is interesting for Sec. IV.

The presence of a harmonic trap introduces the harmonic oscillator length scale $a_{\text{ho}} = \sqrt{\hbar/m\omega}$, so that the eigenstates cannot be scale-invariant as in Eq. (9). However, if ψ obeys the contact condition, so do the ψ_λ's: as we shall see, this allows us to identify general properties of the eigenstates in the trap.

B. Scaling solution in a time dependent trap

We now assume that the curvature of the isotropic trap, while keeping a fixed value for all times $t \leq 0$, has an arbitrary time dependence at positive times. We call $\omega(t)$ the resulting time-dependent oscillation frequency of an atom in the trap.

Let us assume that, at $t \leq 0$, the system is in a stationary state of energy E. Then at positive times the wave function of the system will be deduced from the $t=0$ wave function by the combination of gauge and scaling transform [25]:

$$\psi(\vec{X}, t) = \frac{e^{-iE\tau(t)/\hbar}}{\lambda(t)^{3N/2}} e^{imX^2\dot{\lambda}(t)/2\hbar\lambda(t)} \psi(\vec{X}/\lambda(t), 0), \tag{11}$$

where the time-dependent scaling parameter obeys the Newton-like equation

$$\ddot{\lambda} = \frac{\omega^2(0)}{\lambda^3} - \omega^2(t)\lambda \tag{12}$$

with the initial conditions $\lambda(0)=1$, $\dot{\lambda}(0)=0$. We also introduced an effective time τ given by

$$\tau(t) = \int_0^t \frac{dt'}{\lambda^2(t')}. \tag{13}$$

This result may be extended to an arbitrary initial state as follows:

$$\psi(\vec{X},t) = \frac{1}{\lambda(t)^{3N/2}} e^{imX^2\dot{\lambda}(t)/2\hbar\lambda(t)} \tilde{\psi}(\vec{X}/\lambda(t), \tau(t)), \tag{14}$$

where $\tilde{\psi}$ evolves with the $t<0$ Hamiltonian [i.e., in the unperturbed trap with an oscillation frequency $\omega(0)$].

As shown by Rosch and Pitaevskii [26], the existence of such a scaling and gauge time-dependent solution is related to a SO(2,1) hidden symmetry of the problem. This we rederive in the two next subsections.

C. Existence of an undamped breathing mode

We consider the following gedanken experiment: one perturbs the gas in an infinitesimal way by modifying the trap frequency in a time interval $0<t<t_f$. After the excitation period ($t>t_f$), the trap frequency assumes its initial value $\omega(0)$. The scaling parameter then slightly deviates from unity, $\lambda(t)=1+\delta\lambda(t)$ with $|\delta\lambda| \ll 1$. Linearizing the equation of motion Eq. (12) in $\delta\lambda$, one finds that $\delta\lambda$ oscillates as

$$\delta\lambda(t) = \epsilon e^{-2i\omega t} + \epsilon^* e^{2i\omega t} + O(\epsilon^2), \tag{15}$$

where we set $\omega=\omega(0)$ to simplify the notation. The gedanken experiment has therefore excited an undamped breathing mode of frequency 2ω [26].

D. Raising and lowering operators, and SO(2,1) hidden symmetry

We now interpret the above undamped oscillation in terms of a property of the N-body spectrum of the system. Expanding Eq. (11) to first order in $\delta\lambda(t)$ leads to

$$\psi(\vec{X},t) = e^{i\alpha}[e^{-iEt/\hbar} - \epsilon e^{-i(E+2\hbar\omega)t/\hbar} L_+ + \epsilon^* e^{-i(E-2\hbar\omega)t/\hbar} L_-]\psi(\vec{X},0) + O(\epsilon^2) \tag{16}$$

(the phase α depends on the details of the excitation procedure). This reveals that the initial stationary state E was coupled by the excitation procedure to other stationary states of energies $E\pm 2\hbar\omega$. Remarkably, the wave function of these other states can be obtained from the initial one by the action of raising and lowering operators:

$$L_+ = +\frac{3N}{2} + \hat{D} + \frac{H}{\hbar\omega} - m\omega X^2/\hbar, \tag{17}$$

$$L_- = -\frac{3N}{2} - \hat{D} + \frac{H}{\hbar\omega} - m\omega X^2/\hbar. \tag{18}$$

Repeated action of L_+ and L_- will thus generate a ladder of eigenstates with regular energy spacing $2\hbar\omega$.

The hidden SO(2,1) symmetry of the problem then results from the fact that H, L_+, and L_- have commutation relations equal (up to numerical factors) to the ones of the Lie algebra of the SO(2,1) group, as was checked in [26]:

$$[H,L_+] = 2\hbar\omega L_+, \tag{19}$$

$$[H,L_-] = -2\hbar\omega L_-, \tag{20}$$

$$[L_+,L_-] = -4\frac{H}{\hbar\omega}. \tag{21}$$

Note that these commutation relations by themselves do not imply the existence of the hidden SO(2,1) symmetry. One has also to check that the operators L_+ and L_- preserve the domain of the Hamiltonian, that is, here the contact conditions Eq. (6) defining the unitary gas. The contact conditions are indeed preserved here [27].

From the general theory of Lie algebras, one may form the so-called Casimir operator which commutes with all the elements of the algebra, that is, with H and $L_\pm$; it is given by [26]

$$\hat{\mathcal{C}} = H^2 - \frac{1}{2}(\hbar\omega)^2(L_+L_- + L_-L_+). \tag{22}$$

Consider a ladder of eigenstates; as we will show later, the Hermiticity of H implies that the energy of a universal state is bounded from below, see Eq. (31), so that this ladder has a ground energy step, of value E_g. Within this ladder, the Casimir invariant assumes a constant value,

$$\mathcal{C} = E_g(E_g - 2\hbar\omega). \tag{23}$$

This allows us to express in an elegant way the operator H_g giving the ground-state energy of each ladder [28]:

$$H_g = \hbar\omega + [\hat{\mathcal{C}} + (\hbar\omega)^2]^{1/2}. \tag{24}$$

E. Existence of a bosonic degree of freedom

A physical interpretation of the SO(2,1) hidden symmetry is the following. Using the notations of the previous subsection, we define the operators b and $b^\dagger$ by

$$b = \left[\frac{\hbar\omega}{2(H+H_g)}\right]^{1/2} L_-, \tag{25}$$

$$b^\dagger = L_+\left[\frac{\hbar\omega}{2(H+H_g)}\right]^{1/2}. \tag{26}$$

Using the commutation relations of the SO(2,1) algebra and the expression of the Casimir operator, one may check that b and $b^\dagger$ obey a bosonic commutation relation:

$$[b,b^\dagger] = 1 \tag{27}$$

so that they may be interpreted as annihilation and creation operators for a bosonic degree of freedom of the unitary gas. Furthermore, the N-body Hamiltonian may be split as a sum of two commuting terms:

$$H = H_g + 2\hbar\omega b^\dagger b. \tag{28}$$

Excitation of this bosonic degree of freedom corresponds to an excitation of the breathing mode identified in Sec. III C.

In practice, this excitation may be due to an external change of the curvature of the trap (as in Sec. III C), but may also have a more intrinsic, thermal origin, as considered in Sec. V.

F. Virial theorem

Another application of the existence of raising and lowering operators is the virial theorem for the unitary gas. For a given eigenstate of H of energy E and real wave function ψ, $L_-|\psi\rangle$ is either zero (if ψ is the ground step of a ladder) or an eigenstate of H with a different energy. Assuming that H is Hermitian, this implies $\langle\psi|L_-|\psi\rangle=0$, and leads to [29,30]

$$\langle\psi|H|\psi\rangle = 2\langle\psi|H_{\text{trap}}|\psi\rangle. \tag{29}$$

At thermodynamical equilibrium, one thus has

$$\langle H\rangle = 2\langle H_{\text{trap}}\rangle, \tag{30}$$

that is, the total energy is twice the mean trapping potential energy. A direct consequence of this virial theorem is that the eigenenergy of a universal state is positive:

$$E \geqslant 0 \tag{31}$$

since the trapping potential energy is positive. Slightly better lower bounds are derived in Appendix C, see Eqs. (C7) and (C16) for $N>2$.

This virial theorem is actually also valid for an anisotropic harmonic trap (this result is due to Frédéric Chevy). One uses the Ritz theorem, stating that an eigenstate of a Hermitian Hamiltonian is a stationary point of the mean energy. As a consequence, the function of λ

$$E(\lambda) \equiv \frac{\langle\psi_\lambda|H|\psi_\lambda\rangle}{\langle\psi_\lambda|\psi_\lambda\rangle} = \lambda^{-2}\langle\psi|H-H_{\text{trap}}|\psi\rangle + \lambda^2\langle\psi|H_{\text{trap}}|\psi\rangle \tag{32}$$

satisfies $(dE/d\lambda)(\lambda=1)=0$, which leads to the virial theorem. This relies simply on the scaling properties of the harmonic potential, irrespective of its isotropy.

The proportionality between $\langle H\rangle$ and $\langle H_{\text{trap}}\rangle$ resulting from the virial theorem was checked experimentally [31].

IV. MAPPING TO ZERO-ENERGY FREE-SPACE EIGENSTATES

Usually, the presence of a harmonic trap in the experiment makes the theoretical analysis more difficult than in homogeneous systems. Here we show that, remarkably, the case of an isotropic trap for the unitary gas can be mapped exactly to the zero-energy free-space problem (which remains, of course, an unsolved many-body problem) [32].

More precisely, all the universal N-body eigenstates can be put in the unnormalized form:

$$|\psi_{\nu,q}\rangle = (L_+)^q e^{-\hat{X}^2/2a_{\text{ho}}^2}|\psi_\nu^0\rangle \tag{33}$$

and have an energy

$$E_{\nu,q} = (\nu+2q+3N/2)\hbar\omega, \tag{34}$$

where q is a non-negative integer, L_+ is the raising operator defined in Eq. (17), and ψ_ν^0 is a zero-energy eigenstate of the free-space problem which is scale-invariant:

$$\psi_\nu^0(\vec{X}/\lambda) = \psi_\nu^0(\vec{X})/\lambda^\nu \tag{35}$$

for all real scaling parameter λ, ν being the real scaling exponent [33].

We also show that the reciprocal is true, that is each zero-energy free-space eigenstate which is scale-invariant with a real exponent ν generates a semi-infinite ladder of eigenstates in the trap, according to Eqs. (33) and (34).

We note that Eq. (34) generalizes to excited states a relation obtained in [34] for the many-body ground state.

A. From a trap eigenstate to a free-space eigenstate

We start with an arbitrary eigenstate in the trap. By repeated action of L_- on this eigenstate, we produce a sequence of eigenstates of decreasing energies. According to the virial theorem Eq. (29), the total energy of a universal state is positive, see Eq. (31). This means that the sequence produced above terminates. We call ψ the last nonzero wave function of the sequence, an eigenstate of H with energy E that satisfies $L_-|\psi\rangle=0$. To integrate this equation, we use the hyperspherical coordinates $(X,\vec{n})$ defined in Eqs. (3) and (4). Noting that the dilatation operator is simply $\hat{D}=X\partial_X$ in hyperspherical coordinates, we obtain

$$\psi(\vec{X}) = e^{-X^2/2a_{\text{ho}}^2}X^{E/(\hbar\omega)-3N/2}f(\vec{n}). \tag{36}$$

Then one defines

$$\psi^0(\vec{X}) \equiv e^{X^2/2a_{\text{ho}}^2}\psi(\vec{X}). \tag{37}$$

One checks that this wave function obeys the contact conditions Eq. (6), since X^2 varies quadratically with r_{ij} at fixed R_{ij} and $\{\vec{r}_k, k\neq i,j\}$. ψ^0 is then found to be a zero-energy eigenstate in free space, by direct insertion into Schrödinger's equation. But one has also from Eqs. (36) and (37)

$$\psi^0(\vec{X}) = X^{E/(\hbar\omega)-3N/2}f(\vec{n}), \tag{38}$$

so that ψ^0 is scale-invariant, with a real exponent ν related to the energy E by Eq. (34). This demonstrates Eqs. (33) and (34) for $q=0$, that is, for the ground step of each ladder.

One just has to apply a repeated action of the raising operator L_+ on the ground step wave function to generate a semi-infinite ladder of eigenstates: this corresponds to $q>0$ in Eqs. (33) and (34). Note that the repeated action of L_+ cannot terminate since $L_+|\psi\rangle=0$ for a nonzero ψ implies that ψ is not square-integrable.

B. From a free-space eigenstate to a trap eigenstate

The reciprocal of the previous subsection is also true: starting from an arbitrary zero-energy free-space eigenstate that is scale-invariant, one multiplies it by the Gaussian factor $\exp(-X^2/2a_{\text{ho}}^2)$, and one checks that the resulting wave function is an eigenstate of the Hamiltonian of the trapped system, obeying the contact conditions [35]. Applying L_+ then generates the other trap eigenstates of a ladder.

C. Separability in hyperspherical coordinates

Let us reformulate the previous mapping using the hyperspherical coordinates $(X,\vec{n})$ defined in Eqs. (3) and (4). A free-space scale-invariant zero-energy eigenstate takes the form $\psi^0(\vec{X})=X^\nu f_\nu(\vec{n})$, and the universal eigenstates in the trap have an unnormalized wave function

$$\psi_{\nu,q}(\vec{X}) = X^\nu e^{-X^2/2a_{\rm ho}^2} L_q^{(\nu-1+3N/2)}(X^2/a_{\rm ho}^2) f_\nu(\vec{n}), \qquad (39)$$

where $L_q^{(\cdot)}$ is the generalized Laguerre polynomial of degree q. This is obtained from the repeated action of L_+ in Eq. (33) and from the recurrence relation obeyed by the Laguerre polynomials:

$$(q+1)L_{q+1}^{(s)}(u) - (2q+s+1-u)L_q^{(s)}(u) + (q+s)L_{q-1}^{(s)}(u) = 0. \qquad (40)$$

We have thus separated out the hyperradius X and the hyperangles $\vec{n}$. The hyperangular wave functions $f_\nu(\vec{n})$ and the exponents ν are not known for $N\geqslant 4$. However, we have obtained the hyperradial wave functions, i.e., the X dependent part of the many-body wave function. A more refined version of these separability results can be obtained by first separating out the center of mass (see Appendix C), but this is not useful for the next section.

V. MOMENTS OF THE TRAPPING POTENTIAL ENERGY

A. Exact relations

As an application of the above results, we now obtain the following exact relations on the statistical properties of the trapping potential energy, relating its moments to the moments of the full energy, when the gas is at thermal equilibrium [36]. For the definition of the trapping potential energy, see Eq. (5).

At zero temperature, its moments as a function of the ground-state energy E_0 are given by

$$\langle (H_{\rm trap})^n\rangle = E_0(E_0+\hbar\omega)\cdots(E_0+(n-1)\hbar\omega)/2^n. \qquad (41)$$

At finite temperature T, the first moment is given by the virial theorem

$$\langle H_{\rm trap}\rangle = \langle H\rangle/2 \qquad (42)$$

and the second moment by

$$\langle (H_{\rm trap})^2\rangle = \left[\langle H^2\rangle + \langle H\rangle \hbar\omega \,\mathrm{cotanh}\left(\frac{\hbar\omega}{k_B T}\right)\right]/4. \qquad (43)$$

B. Derivation from the separability

The zero temperature result Eq. (41) follows directly from Eq. (39): for $q=0$, the Laguerre polynomial is constant so that the probability distribution of X is a power law times a Gaussian; the moments are then given by integrals that can be expressed in terms of the Γ function.

For finite T, the idea of our derivation is the following: the hyperradial part of the N-body wave function $\psi_{\nu,q}$ is known from Eq. (39); and thus the probability distribution of X in the state $|\psi_{\nu,q}\rangle$ is known, in terms of ν,q. While the thermal distribution of q is simple, the one of ν is not, but ν is related to the total energy by Eq. (34).

We will need the intermediate quantities

$$B_{n,p}(q,s) \equiv \frac{\displaystyle\int_0^\infty du\, e^{-u} u^{s+n} L_{q+p}^{(s)}(u) L_q^{(s)}(u)}{\displaystyle\int_0^\infty du\, e^{-u} u^s [L_q^{(s)}(u)]^2}, \qquad (44)$$

where $s\geqslant 0$; n, q are non-negative integers; and p is an integer of arbitrary sign. These quantities can be calculated with the $n=0$ "initial" condition $B_{0,p}=\delta_{0,p}$ and the recurrence relation

$$B_{n+1,p} = -(q+p+1)B_{n,p+1} + [2(q+p)+s+1]B_{n,p} - (q+p+s)B_{n,p-1} \qquad (45)$$

which follows from the recurrence relation Eq. (40) on Laguerre polynomials.

This allows us to calculate the moments of the trapping energy in the step q of a ladder of exponent ν, using Eq. (39):

$$\frac{\langle \psi_{\nu,q}|X^{2n}|\psi_{\nu,q}\rangle}{\langle \psi_{\nu,q}|\psi_{\nu,q}\rangle} = B_{n,0}(q,s)a_{\rm ho}^{2n}. \qquad (46)$$

Here we have set

$$s = \nu - 1 + 3N/2 \qquad (47)$$

in accordance with Eq. (39). We shall need the values of $B_{n,0}$ for $n\leqslant 2$:

$$B_{1,0}(q,s) = s + 2q + 1, \qquad (48)$$

$$B_{2,0}(q,s) = s^2 + s(6q+3) + 6q^2 + 6q + 2. \qquad (49)$$

Assuming thermal equilibrium in the canonical ensemble, the thermal average can be performed over the statistically independent variables q and s. The moments of q are easy to calculate, because of the ladder structure with equidistant steps:

$$\langle q^n\rangle = \frac{\displaystyle\sum_{q=0}^{+\infty} q^n e^{-2q\hbar\omega/k_B T}}{\displaystyle\sum_{q=0}^{+\infty} e^{-2q\hbar\omega/k_B T}}. \qquad (50)$$

The moments of s are not known exactly but they can be eliminated in terms of the moments of the total energy E and of the moments of q using the relation $E=(s+1+2q)\hbar\omega$. This leads to the exact relations (42) and (43). This method in principle allows us to calculate relations for moments of arbitrary given order, but the algebra becomes cumbersome.

C. Derivation from the existence of a bosonic degree of freedom

The relations Eqs. (42) and (43) may also be derived in a purely algebraic way by using the bosonic creation and annihilation operators of Sec. III E. Taking the sum of Eqs. (17) and (18) one expresses $H_{\rm trap}$ in terms of $L_\pm$ and H:

$$H_{\text{trap}} = \frac{1}{2}H - \frac{\hbar\omega}{4}(L_+ + L_-). \quad (51)$$

Then from Eqs. (25) and (26) and Eq. (28) one can express $L_\pm$ and H as functions of the ladder ground energy operator H_g and $b, b^\dagger$. We finally obtain

$$H_{\text{trap}} = \frac{1}{2}\hbar\omega A^\dagger A \quad \text{with} \quad A = \sqrt{\frac{H_g}{\hbar\omega} + b^\dagger b} - b. \quad (52)$$

In the calculation of the thermal averages $\langle H_{\text{trap}}\rangle$ and $\langle (H_{\text{trap}})^2\rangle$ it remains to take the expectation value over H_g and the bosonic degree of freedom, that may be considered as independent variables in the sense that, e.g.,

$$\langle H_g b^\dagger b\rangle = \langle H_g\rangle\langle b^\dagger b\rangle. \quad (53)$$

The calculation is simplified by the observation that the expectation value of the obtained terms with odd powers of b or $b^\dagger$ is exactly zero. One can use Wick's theorem to calculate the expectation value of $(b^\dagger b)^2$. One also eliminates the expectation value of H_g using Eq. (28). One obtains Eq. (42) for the first moment. For the second moment

$$4\langle (H_{\text{trap}})^2\rangle = \langle H^2\rangle + \langle H\rangle\hbar\omega[2\langle b^\dagger b\rangle + 1]. \quad (54)$$

The Bose formula giving $\langle b^\dagger b\rangle$ finally leads to Eq. (43). This nicely shows how the last term of Eq. (43) originates from the thermal fluctuations of the bosonic degree of freedom, that is, of the breathing mode of the unitary gas.

VI. CONCLUSION

In this paper we have derived several exact properties of the unitary gas in an isotropic harmonic trap. The spectrum is formed of ladders; the steps of a ladder are spaced by an energy $2\hbar\omega$, and linked by raising and lowering operators. This property may be interpreted in terms of a hidden SO(2,1) symmetry [26] or in terms of the existence of a bosonic degree of freedom. This allows us to map the trapped problem to the free-space one. A lower bound on the energy of the universal states was derived, showing that the ladders are actually semi-infinite ladders. A related property is that the problem is separable in hyperspherical coordinates. The hyperradial part of the stationary state wave functions is thus known. This allows us to derive exact relations between the moments of the trapping potential energy and the moments of the total energy. The relation between the first moments is the virial theorem; the relation between the second moments may be useful for thermometry, as will be studied elsewhere.

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APPENDIX A: EXTENSION TO PARTICLES WITH DIFFERENT MASSES

All our results remain valid if the particles have different masses $m_1, \ldots, m_N$; provided that the oscillation frequency ω remains the same for all the particles. We define a mean mass:

$$m \equiv \frac{m_1 + \cdots + m_N}{N}. \quad (A1)$$

The definition of $\vec{X}$ and X, given by Eqs. (2) and (3) for equal masses, has to be generalized to

$$\vec{X} \equiv \left(\sqrt{\frac{m_1}{m}}\vec{r}_1, \ldots, \sqrt{\frac{m_N}{m}}\vec{r}_N\right), \quad (A2)$$

$$X \equiv \|\vec{X}\| = \sqrt{\sum_{i=1}^{N}\frac{m_i}{m}r_i^2}. \quad (A3)$$

With this new definition of X, the trapping potential energy is still given by Eq. (5).

In the definition of the zero-range model, the contact conditions Eq. (6) remain unchanged, except that the fixed center-of-mass position of particles i and j is now $\vec{R}_{ij} \equiv (m_i\vec{r}_i + m_j\vec{r}_j)/(m_i + m_j)$.

In Appendix C, the center-of-mass position has to be redefined as

$$\vec{C} = \frac{(m_1\vec{r}_1 + \cdots + m_N\vec{r_N})}{(m_1 + \cdots + m_N)} \quad (A4)$$

and the internal hyperangular coordinates become

$$R = \sqrt{\sum_{i=1}^{N}\frac{m_i}{m}(\vec{r}_i - \vec{C})^2}, \quad (A5)$$

$$\vec{\Omega} = \left(\sqrt{\frac{m_1}{m}}\frac{\vec{r}_1 - \vec{C}}{R}, \ldots, \sqrt{\frac{m_N}{m}}\frac{\vec{r}_N - \vec{C}}{R}\right). \quad (A6)$$

With these modified definitions, all the results of this paper remain valid.

APPENDIX B: SCALE INVARIANCE OF THE ZERO-ENERGY FREE-SPACE EIGENSTATES

In this Appendix, we show that the zero-energy free-space eigenstates of the Hamiltonian may be chosen as being scale-invariant, that is as, eigenstates of the dilatation operator $\hat{D}$, under conditions ensuring the Hermiticity of the Hamiltonian.

Consider the zero-energy eigensubspace of the free-space Hamiltonian. This subspace is stable under the action of $\hat{D}$. If one assumes that $\hat{D}$ is diagonalizable within this subspace, the corresponding eigenvectors form a complete family of scale invariant zero-energy states. If $\hat{D}$ is not diagonalizable, we introduce the Jordan normal form of $\hat{D}$.

Let us start with the case of a Jordan normal form of dimension 2, written as

$$\mathrm{Mat}(\hat{D}) = \begin{pmatrix} \nu & 1 \\ 0 & \nu \end{pmatrix}, \tag{B1}$$

in the sub-basis $|e_1\rangle, |e_2\rangle$. The ket $|e_1\rangle$ is an eigenstate of $\hat{D}$ with the eigenvalue ν. We assume that the center-of-mass motion is at rest, with no loss of generality since it is separable in free space. Using the internal hyperspherical coordinates $(R, \vec{\Omega})$ defined in Appendix C, we find that $\hat{D}$ reduces to the operator $R\partial_R$. Integrating $R\partial_R e_1 = \nu e_1$ leads to

$$e_1(\vec{X}) = R^\nu \phi_1(\vec{\Omega}). \tag{B2}$$

The ket $|e_2\rangle$ is not an eigenstate of $\hat{D}$ but obeys $R\partial_R e_2 = \nu e_2 + e_1$, which, after integration, gives

$$e_2(\vec{X}) = R^\nu \ln R \phi_1(\vec{\Omega}) + R^\nu \phi_2(\vec{\Omega}). \tag{B3}$$

One can assume that ϕ_1 and ϕ_2 are orthogonal on the unit sphere (by redefining e_2 and ϕ_2). It remains to use the fact that both e_1 and e_2 are zero-energy free-space eigenstates. From the form of the Laplacian in hyperspherical coordinates in $d=3N-3$ dimensions, see Eq. (C5), the condition $\Delta_{\vec{X}} e_1 = 0$ leads to

$$T_{\vec{\Omega}} \phi_1 = -\nu(\nu + d - 2)\phi_1. \tag{B4}$$

The condition $\Delta_{\vec{X}} e_2 = 0$ then gives $T_{\vec{\Omega}}\phi_2 = -\nu(\nu+d-2)\phi_2 - (2\nu+d-2)\phi_1$, which leads to the constraint [37]

$$\nu = 1 - d/2. \tag{B5}$$

At this stage, for this "magic" value of ν, it seems that there may exist non-scale-invariant zero-energy eigenstates.

To proceed further, one has to check for the Hermiticity of the free-space Hamiltonian. This requires a reasoning at arbitrary, nonzero energy. We use the fact that the following wave function obeys the contact conditions:

$$\psi(\vec{X}) = u(R) R^\nu \phi_1(\vec{n}), \tag{B6}$$

where $u(R)$ is a function with no singularity, except maybe in $R=0$ [38]. Using again the expression of the Laplacian in internal hyperspherical coordinates, one finds that ψ is an eigenstate of the free-space Hamiltonian if $u(R)$ is an eigenstate of

$$\hat{h} = -\frac{\hbar^2}{2m}(\partial_R^2 + R^{-1}\partial_R). \tag{B7}$$

One checks that Hermiticity of the free-space Hamiltonian for the wave function ψ implies Hermiticity of $\hat{h}$ for the wave function $u(R)$. Note that $\hat{h}$ is simply the free-space Hamiltonian for 2D isotropic wave functions. It is Hermitian over the domain of wave functions $u(R)$ with a noninfinite limit in $R=0$. Including the ket $|e_2\rangle$ in the domain of the N-body free-space Hamiltonian amounts to allowing for wave functions $u(R)$ that diverge as $\ln R$ for $R\to 0$: this breaks the Hermiticity of $\hat{h}$, since this leads to a (negative energy) continuum of square integrable eigenstates of $\hat{h}$,

$$u_\kappa(R) = K_0(\kappa R) \tag{B8}$$

with eigenenergy $-\hbar^2\kappa^2/2m$, for all $\kappa > 0$. Here $K_0(x)$ is a modified Bessel function of the second kind. Hermiticity may be restored by a filtering of this continuum [40], adding the extra contact condition $u(R) = \ln(R/l) + o(1)$ for $R \to 0$, but the introduction of the fixed length l breaks the universality of the problem and is beyond the scope of this paper (see [43] for a more detailed discussion). We thus exclude e_2 from the domain of the Hamiltonian.

This discussion may be extended to Jordan forms of higher order. For example, a Jordan form of dimension 3 generates a ket $|e_3\rangle$ such that $(\hat{D}-\nu)e_3 = e_2$. But e_2 must be excluded from the domain of the Hamiltonian by the above reasoning. Since we want the domain to be stable under $\hat{D}$, e_3 must be excluded as well.

As a conclusion, to have a free-space N-body Hamiltonian that is both Hermitian and universal (i.e., with a scale-invariant domain) forces us to reject the non-scale-invariant zero-energy eigenstates, of the form Eq. (B3).

APPENDIX C: SEPARABILITY IN INTERNAL HYPERSPHERICAL COORDINATES

We develop here a refined version of the separability introduced in Sec. IV C. First, we separate out the center-of-mass coordinates. Then we obtain the separability in hyperspherical coordinates relative to the internal variables of the gas, which allows us to derive an effective repulsive $N-1$ force and to get a lower bound on the energy slightly better than the one $E \geq 0$ ensuing from the virial theorem.

Let us introduce the following set of coordinates:

$$\vec{C} = \sum_{i=1}^{N} \vec{r}_i / N \tag{C1}$$

is the position of the center of mass (CM);

$$R = \sqrt{\sum_{i=1}^{N} (\vec{r}_i - \vec{C})^2} \tag{C2}$$

is the internal hyperradius; and

$$\vec{\Omega} = \left(\frac{\vec{r}_1 - \vec{C}}{R}, \ldots, \frac{\vec{r}_N - \vec{C}}{R} \right) \tag{C3}$$

is a set of dimensionless internal coordinates that can be parametrized by $3N-4$ internal hyperangles. In these coordinates, the Hamiltonian decouples as $H = H_{CM} + H_{\mathrm{int}}$ with

$$H_{CM} = -\frac{\hbar^2}{2Nm}\Delta_{\vec{C}} + \frac{1}{2}Nm\omega^2 C^2, \tag{C4}$$

$$H_{\mathrm{int}} = -\frac{\hbar^2}{2m}\left[\partial_R^2 + \frac{3N-4}{R}\partial_R + \frac{1}{R^2}T_{\vec{\Omega}}\right] + \frac{1}{2}m\omega^2 R^2, \tag{C5}$$

where $T_{\vec{\Omega}}$ is the Laplacian on the unit sphere of dimension $3N-4$. The contact conditions do not break the separability of the center of mass valid in a harmonic trap, so that the stationary state wave function may be taken of the form

$$\psi(\vec{X}) = \psi_{CM}(\vec{C})\psi_{\rm int}(R,\vec{\Omega}). \tag{C6}$$

At this point, this separability of the center of mass, combined with the virial theorem of Eq. (29), already gives an improved lower bound on the energy of a universal state [41]:

$$E \geqslant \frac{3}{2}\hbar\omega. \tag{C7}$$

To proceed further, one can show [42] that there is separability in internal hyperspherical coordinates:

$$\psi_{\rm int}(R,\vec{\Omega}) = \Phi(R)\phi(\vec{\Omega}). \tag{C8}$$

This form may be injected into the internal Schrödinger equation

$$H_{\rm int}\psi_{\rm int} = E_{\rm int}\psi_{\rm int}. \tag{C9}$$

One finds that $\phi(\vec{\Omega})$ is an eigenstate of $T_{\vec{\Omega}}$ with an eigenvalue that we call $-\Lambda$. Note that the contact conditions Eq. (6) put a constraint on $\phi(\vec{\Omega})$ only [38]. The equation for $\Phi(R)$ reads

$$-\frac{\hbar^2}{2m}\left(\partial_R^2 + \frac{3N-4}{R}\partial_R\right)\Phi + \left(\frac{\hbar^2\Lambda}{2mR^2} + \frac{1}{2}m\omega^2R^2\right)\Phi = E_{\rm int}\Phi. \tag{C10}$$

A useful transformation of this equation is obtained by the change of variable

$$\Phi(R) \equiv R^{(5-3N)/2}F(R), \tag{C11}$$

resulting in

$$-\frac{\hbar^2}{2m}\left(\partial_R^2 + \frac{1}{R}\partial_R\right)F + \left(\frac{\hbar^2 s_R^2}{2mR^2} + \frac{1}{2}m\omega^2R^2\right)F = E_{\rm int}F(R), \tag{C12}$$

where s_R is such that

$$s_R^2 = \Lambda + \left(\frac{3N-5}{2}\right)^2. \tag{C13}$$

Formally, the equation for F is Schrödinger's equation for a particle of zero angular momentum moving in two dimensions in a harmonic potential plus a potential $\propto s_R^2/R^2$.

For $s_R^2 \geqslant 0$, one can choose $s_R \geqslant 0$. Assuming that there is no N-body resonance, $F(R)$ is bounded for $R \to 0$ [43]. The eigenfunctions of Eq. (C12) can then be expressed in terms of the generalized Laguerre polynomials:

$$F(R) = R^{s_R}L_q^{s_R}[R^2/a_{\rm ho}^2]e^{-R^2/2a_{\rm ho}^2} \tag{C14}$$

with the spectrum

$$E_{\rm int} = (s_R + 1 + 2q)\hbar\omega. \tag{C15}$$

This gives a lower bound on the energy of any universal N-body eigenstate:

$$E \geqslant \frac{5}{2}\hbar\omega \tag{C16}$$

for $N>2$ and in the absence of a N-body resonance.

For a complex s_R^2, the effective two-dimensional (2D) Hamiltonian is not Hermitian and this case has to be discarded. For $s_R^2<0$, Whittaker functions are square integrable solutions of the effective 2D problem for all values $E_{\rm int}$ so that, again, the problem is not Hermitian. One may add extra boundary conditions to filter out an orthonormal discrete subset (as was done for $N=3$ bosons [9,13,15,45]) but this breaks the scaling invariance of the domain and generates nonuniversal states beyond the scope of the present paper.

To make the link with the approach of Sec. IV, we note that

$$F(R) = R^{s_R} \tag{C17}$$

is a solution of the effective 2D problem (C12) for $\omega=0$, $E_{\rm int}=0$. Thus a solution of the internal problem Eq. (C9) at zero energy in free space is given by

$$\psi_{\rm int}(R,\Omega) = R^{(5-3N)/2+s_R}\phi(\vec{\Omega}). \tag{C18}$$

Multiplying this expression by $C^lY_l^m(\vec{C}/C)$, one recovers the ψ_ν^0's of Sec. IV, with

$$\nu = \frac{5-3N}{2} + s_R + l. \tag{C19}$$

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[24] This can be seen using the Hellmann-Feynman theorem, valid for Hermitian Hamiltonians: taking the derivative with respect to λ of $\langle\psi_\lambda|H|\psi_\lambda\rangle=E/\lambda^2$, one gets $-2E/\lambda^3=\langle\psi_\lambda|(dH/d\lambda)|\psi_\lambda\rangle=0$, in contradiction with $E<0$.

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[28] Note that E_g is larger than $\hbar\omega$, according to a lower bound on the energy derived in Appendix C: as a consequence, E_g is a univocal function of $\mathcal{C}$.

[29] Here the scalar product is the usual $3N$-uple integral restricted to the manifold of positions $\vec{r}_i\neq\vec{r}_j$ for all $i\neq j$. As a consequence, one does not have to introduce the Dirac distributions originating from the action of the Laplacian on the $1/r_{ij}$ divergencies imposed by the contact conditions.

[30] For a real ψ normalized to unity, one finds $\langle\psi|\hat{D}|\psi\rangle=-3N/2$, from the identity $\psi\vec{X}\cdot\partial_{\vec{X}}\psi=\mathrm{div}\left(\frac{1}{2}\vec{X}\psi^2\right)-\frac{3N}{2}\psi^2$ and Ostrogradsky's theorem.

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[36] Strictly speaking, the system cannot thermalize, as can be realized in several ways: the breathing mode is undamped (see Sec. III C), the Casimir operator is a constant of motion (see Sec. III D), the bosonic degree of freedom is decoupled [see Eq. (28) in Sec. III E]. However, in practice the trapping potential is not perfectly isotropic, and the range of the interaction is not stricly zero. This leads to a weak coupling between the bosonic degree of freedom associated with the breathing mode and the other degrees of freedom. Therefore the system can thermalize.

[37] To obtain Eq. (B5), consider $\psi_2\equiv R^\nu u(R)\phi_2(\vec{\Omega})$. This wave

function satisfies the contact conditions [38]. It thus belongs to the domain of H [for an appropriate $u(R)$]. Since $He_1=0$, Hermiticity of H implies $\langle e_1, H\psi_2\rangle=0$; which leads to the result.

[38] To establish this fact, one needs the following lemma: if $\psi(\vec{X})$ obeys the contact conditions, so does $u(R)\psi(\vec{X})$, where $u(R)$ is a function with no singularity, except maybe in $R=0$. This lemma results from the fact that $R^2=R_0^2+O(r_{ij}^2)$, where R_0^2 is a nonzero constant in the $r_{ij}\to 0$ limit [39], so that $u(R)=u(R_0)+O(r_{ij}^2)$.

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[41] Indeed, one has $\langle H\rangle=2\langle H_{\rm trap}\rangle\geq\langle NmC^2\rangle=\langle H_{CM}\rangle\geq 3/2\hbar\omega$.

[42] The whole algebra of Sec. IV may be reproduced for the internal problem, with the modified raising and lowering operators: $\mathcal{L}_\pm\equiv\pm\left(\frac{3N-3}{2}+R\partial_R\right)+\frac{H_{\rm int}}{\hbar\omega}-\frac{m\omega}{\hbar}R^2$.

[43] The absence of N-body resonance corresponds to the simple boundary condition: (i) $F(R)$ bounded for $R\to 0$. For $0<s_R<1$, N-body resonances can be taken into account by the modified boundary condition: (ii) $F(R)=AR^{s_R}[R^{-2s_R}-\epsilon l^{-2s_R}]+O(R^{-s_R+2})$, where $l\in]0,+\infty]$ and $\epsilon=\pm 1$ are fixed. If one is not exactly on the N-body resonance, one has $l<\infty$, which breaks scale invariance, thus invalidating the results of this paper. Exactly on the N-body resonance (e.g., when the energy of the N-body bound state in free space vanishes), one has $l=\infty$, which preserves scale invariance: all the results of this paper remain valid; one must only replace s_R by $-s_R$ in Eqs. (C14), (C15), and (C17)–(C19), and Eq. (C16) becomes $E\geq 3/2\hbar\omega$. For $s_R=0$, N-body resonances can be taken into account by the modified boundary condition (iii) $F(R)=A\ln(R/l)+o(1)$, where $l\in]0,+\infty[$ is fixed. If one is not exactly on the N-body resonance, one has $l<\infty$, which breaks scale invariance, thus invalidating the results of this paper. Being exactly on the N-body resonance corresponds to taking the limit $l\to\infty$ in (iii), which is equivalent to (i): the results of this paper then remain valid. For $s_R\geq 1$, the wave function $F(R)=R^{-s_R}$ is not square integrable near $R=0$ in two dimensions, so that the description of N-body resonances becomes more complicated (see [44] for the case $N=2$).

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