Physics/Statistical physics, thermodynamics

Exact scaling transform for a unitary quantum gas in a time dependent harmonic potential

Yvan Castin

Laboratoire Kastler Brossel, École normale supérieure, 24, rue Lhomond, 75231 Paris, France

Presented by Jean Dalibard

Abstract

A unitary quantum gas is a gas of quantum particles with a binary interaction of infinite scattering length and negligible range. It has been produced in recent experiments with gases of fermionic atoms by means of a Feshbach resonance. Using the Fermi pseudo-potential model for the atomic interaction, we show that the time evolution of such a gas in an isotropic three-dimensional time dependent harmonic trap is exactly given by a gauge and scaling transform. *To cite this article: Y. Castin, C. R. Physique 5 (2004).*

Résumé

Évolution d'un gaz quantique unitaire dans un potentiel harmonique variable : solution par changement d'échelle. Nous entendons par « gaz quantique unitaire » une assemblée de particules dont le mouvement est décrit quantiquement et qui interagissent par un potentiel de longueur de diffusion infinie et de portée négligeable devant leur distance moyenne et leur longueur d'onde thermique. Un tel gaz a été produit récemment à l'aide d'une résonance de Feshbach dans un gaz d'atomes fermioniques. En modélisant les interactions entre particules par le pseudo-potentiel de Fermi, nous montrons que l'évolution d'un gaz unitaire dans un potentiel de piégeage harmonique isotrope tridimensionnel de dépendance temporelle quelconque est décrite exactement par la composition d'un changement d'échelle et d'une transformation de jauge. *Pour citer cet article : Y. Castin, C. R. Physique 5 (2004).*

1. Introduction

Experiments with quantum gases of spin 1/2 fermionic atoms are currently making rapid progresses. One of the most fascinating properties of these fermionic gases is the possibility to freely tune the sign and the strength of the atomic interactions without reducing the lifetime of the sample: the value of the *s*-wave scattering length a of two particles with opposite spin components can virtually be adjusted from $-\infty$ to $+\infty$ with a Feshbach resonance technique [1], without inducing any instability of the gas even in the unitary limit $a = \pm\infty$ [2]. These systems are still gases, in the sense that the effective range of the interaction potential is negligible as compared to the mean interparticle separation and to the thermal de Broglie

wavelength. We shall take advantage of this crucial property and model the true interaction potential by the so-called Fermi pseudo-potential [3].

Such stability of the strongly interacting Fermi gases opens up fascinating possibilities, e.g. the study of the crossover between a Bose–Einstein condensate of dimers (already observed, see [4–7]) and a BCS condensate of pairs, by passing through the strongly interacting regime $k_F|a| \gg 1$, where k_F is the Fermi momentum [8,9]. In the unitary limit $k_F|a| \to +\infty$, the thermodynamic properties of the spatially homogeneous gas are universal: they depend only on the Fermi energy and on the temperature. At zero temperature, the chemical potential of the homogeneous gas is then $\mu = \eta\mu_0$ where η is a pure number and μ_0 is the chemical potential of the ideal Fermi gas [2,10]. An accurate measurement of η would provide a crucial test of many-body theories [2,5,7].

The standard imaging technique used with quantum gases is to switch off the trapping potential, to let the gas expand and to perform a light absorption imaging of the atomic cloud. Such a ballistic expansion acts as a magnifying lens: it was used to reveal the vortex lattice in a rotating Bose–Einstein condensate [11], and very recently to obtain the value of the universal number η for the unitary Fermi gas [7]. Clearly the interpretation of the time of flight images strongly relies on a theoretical understanding of the time evolution of the gas in a time dependent harmonic potential. In the case of a pure Bose–Einstein condensate in the regime $k_F|a| \ll 1$, this was achieved starting from the Gross–Pitaevskii equation by a gauge plus scaling transform [12,13]. When the Bose or Fermi gas enters the strongly interacting regime $k_F|a| > 1$, no solution starting from first principles is available[1] and one relies on the hydrodynamic approximation [14].

Here we consider the idealized case of an isotropic and harmonic three-dimensional trapping potential. In the limit of an infinite scattering length, we show that the Fermi pseudo-potential has a scaling invariance that rigorously allows the use of a gauge plus scaling transform similar to the one of [15] to describe the time evolution of the gas due to an arbitrary variation of the trapping frequency.

2. The model based on the Fermi pseudo-potential

Consider an assembly of N non-relativistic particles, with an arbitrary spin. These particles may be indistinguishable bosons or fermions, or even be distinguishable. All the particles have the same mass m and interact *via* the same binary interaction potential independent of the spin degrees of freedom. The interaction potential is the Fermi pseudo-potential with coupling constant g related to the s-wave scattering length a by $g = 4\pi\hbar^2 a/m$. At this stage, $0 < |a| < +\infty$, we shall take the unitary limit $|a| \to +\infty$ later.

Let $\psi(\mathbf{r_1}, \ldots, \mathbf{r_N})$ be the wavefunction of the gas corresponding to a given (but arbitrary) spin configuration. The wavefunction ψ then evolves according to the Schrödinger equation:

$$i\hbar\partial_t\psi = \sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}_i} + U(\mathbf{r}_i)\right]\psi + \sum_{1\leqslant i<j\leqslant N}g\delta(\mathbf{r}_i - \mathbf{r}_j)\psi_{ij}^{\mathrm{reg}}. \tag{1}$$

Here $\Delta_{\mathbf{r}_i}$ is the three-dimensional Laplacian with respect to the spatial coordinates $\mathbf{r}_i$ of particle number i, U is the trapping potential seen by each particle and each ψ_{ij}^{reg}, the so-called regular part of ψ in $\mathbf{r}_i = \mathbf{r}_j$, is the following function of $N-1$ vectors of coordinates:

$$\psi_{ij}^{\mathrm{reg}}\big(\{\mathbf{r}_k, k \neq i, j\}, \mathbf{R_{ij}}\big) = \lim_{r_{ij}\to 0}\frac{\partial}{\partial r_{ij}}(r_{ij}\psi), \tag{2}$$

where r_{ij} is the norm of $\mathbf{r_{ij}} \equiv \mathbf{r}_i - \mathbf{r}_j$ and where the limit and the partial derivative are taken for fixed positions $\mathbf{r}_k$ of the $N-2$ particles other than particles i and j, and for a fixed position of the center of mass of the particles i and j, $\mathbf{R_{ij}} \equiv (\mathbf{r}_i + \mathbf{r}_j)/2$.

The domain of the Hamiltonian corresponding to the Fermi pseudo-potential is therefore not the Hilbert space of the non-interacting gas, but a functional space with specific boundary conditions for the wavefunction ψ. More precisely, as we now see, the model amounts to replacing the true interaction potential by *contact* conditions, i.e. by boundary conditions on ψ when the distance r_{ij} between two particles tends to zero, the wavefunction ψ otherwise evolving with the interaction free Schrödinger equation [16]. As the wavefunction ψ does not contain any delta singularity, each delta singularity in the interaction term of Eq. (1) has indeed to be compensated by a delta singularity in the kinetic energy term. In 3D this implies that ψ can diverge as $1/r_{ij}$ when $r_{ij} \to 0$, a divergence which is still square integrable. Two cases can occur:

---

[1] It was expected that a gauge plus scaling transform would provide an exact solution to the N-body problem in a strictly two-dimensional Bose gas in an isotropic harmonic trap [15], for an interaction potential modeled by a delta distribution. Actually a delta interaction potential in 2D does not lead to a mathematically well defined problem and the required regularisation [17] breaks the scaling invariance.

– case (i): $\lim_{r_{ij}\to 0} \psi = 0$: no delta singularity occurs from the kinetic energy operator, and there is no delta singularity from the interaction term as ψ_{ij}^{reg} vanishes. For instance, this is the case when particles i and j are indistinguishable fermions in the same spin state.

– case (ii): ψ has a $1/r_{ij}$ singularity:

$$\psi = \frac{A}{r_{ij}} + B + \text{O}(r_{ij}), \tag{3}$$

where A and B are still functions of the $\mathbf{r}_k$'s with $k \neq i, j$, and of $\mathbf{R}_{ij}$. The regular part of ψ is then $\psi_{ij}^{\text{reg}} = B$. Writing the kinetic energy operator for the pair of particles i, j as $\Delta_{\mathbf{r}_i} + \Delta_{\mathbf{r}_j} = \frac{1}{2}\Delta_{\mathbf{R}_{ij}} + 2\Delta_{\mathbf{r}_{ij}}$ and using $\Delta(1/r) = -4\pi\delta(\mathbf{r})$, we find that the total coefficient of $\delta(\mathbf{r}_i - \mathbf{r}_j)$ in the right-hand side of Eq. (1) vanishes provided that $A + aB = 0$.

A way of summarizing the two cases is then simply to impose the boundary conditions:

$$\psi(\mathbf{r_1}, \ldots, \mathbf{r_N}) = A\big(\{\mathbf{r}_k, k \neq i, j\}, \mathbf{R_{ij}}\big)\big[r_{ij}^{-1} - a^{-1}\big] + \text{O}(r_{ij}) \tag{4}$$

the first case corresponding to $A = 0$ and the second one to $A \neq 0$. Having ensured that all the delta singularities cancel in the Schrödinger equation, we can now restrict it to the manifold where the positions of the particles are two by two distinct:

$$i\hbar\partial_t \psi = \sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}_i} + U(\mathbf{r}_i)\right]\psi \quad \text{for } r_{ij} \neq 0, \ \forall i \neq j. \tag{5}$$

Eqs. (4) and (5) constitute the basis of our model.

3. Scaling transform in the unitary limit

We specialize the previous section to the case of the unitary quantum gases: the scattering length is now infinite, so that we set to zero the $1/a$ term in the boundary conditions (4), to obtain

$$\psi(\mathbf{r_1}, \ldots, \mathbf{r_N}) = \frac{A(\{\mathbf{r}_k, k \neq i, j\}, \mathbf{R_{ij}})}{r_{ij}} + \text{O}(r_{ij}). \tag{6}$$

Note that the unitary limit does not look in any way singular in our formulation of the model, as the scattering length only appears through its inverse in Eq. (4). Also we restrict to the case of an isotropic harmonic potential:

$$U(\mathbf{r}) = \frac{1}{2}m\omega^2(t)r^2, \tag{7}$$

where the oscillation frequency $\omega(t)$ of a particle in a trap is constant and equal to ω_0 for $t < 0$ and has an arbitrary time dependence for $t \geq 0$. The ballistic expansion of the gas mentioned in the introduction corresponds to setting ω to zero for $t \geq 0$.

We assume that the state vector of the gas for $t < 0$ is a steady state of Schrödinger's equation with the energy E. The corresponding wavefunction for the considered spin configuration is ψ_0, which in particular obeys the boundary condition equation (6). Our ansatz for the time-dependent wavefunction, inspired from [12,13,15], is then

$$\psi(\mathbf{r_1}, \ldots, \mathbf{r_N}, t) = \mathcal{N}(t)\, e^{i\sum_{j=1}^{N} mr_j^2 \dot{\lambda}(t)/2\hbar\lambda(t)} \psi_0\big(\mathbf{r_1}/\lambda(t), \ldots, \mathbf{r_N}/\lambda(t)\big), \tag{8}$$

where the time dependent normalisation factor $\mathcal{N}(t)$ and the time dependent scaling factor $\lambda(t)$ need to be determined. This ansatz is the combination of a gauge transformation (see the Gaussian phase factor) and a time dependent scaling transform (see the rescaling of the coordinates by $\lambda(t)$ in ψ_0).

The first step is to check that the ansatz equation (8) is in the right Hilbert space, i.e. that it satisfies the boundary conditions equation (6). The scaling transform indeed preserves the boundary conditions: it rescales and multiplies the function A by λ but does not lead to the appearance of a O(1) term in Eq. (6). Note that for a non-zero value of $1/a$ the conclusion would be different if $A \neq 0$. The gauge transform also preserves the boundary conditions: for fixed $\mathbf{r}_k$'s we write $r_i^2 + r_j^2 = 2R_{ij}^2 + r_{ij}^2/2$ so that for a fixed $\mathbf{R_{ij}}$, the gauge transform involves only as a non-constant factor

$$e^{imr_{ij}^2\dot{\lambda}/4\hbar\lambda} = 1 + imr_{ij}^2\dot{\lambda}/4\hbar\lambda + \text{O}(r_{ij}^4). \tag{9}$$

As $r_{ij}^2 \times A/r_{ij} = \text{O}(r_{ij})$, the boundary conditions are preserved by the gauge transform, a conclusion that extends to the non-zero $1/a$ case.

What is left is to check that the free particle Schrödinger equation (5) is satisfied by the ansatz for an appropriate choice of $\lambda(t)$ and $\mathcal{N}(t)$. One calculates the time derivative and the Laplacian of the ansatz. One uses the fact that ψ_0 is an eigenstate of energy E to express the action of the kinetic energy operator on ψ_0 in terms of $r_j^2 \psi_0$ terms and $E\psi_0$. Equating the terms $r_j^2 \psi_0$ on both sides of Eq. (5) leads to

$$\ddot{\lambda}(t) = \frac{\omega_0^2}{\lambda^3(t)} - \omega^2(t)\lambda(t) \tag{10}$$

to be solved with the initial conditions $\lambda(t < 0) = 1$, $\dot{\lambda}(t < 0) = 0$. For a ballistic expansion, one finds $\lambda(t) = (1 + \omega_0^2 t^2)^{1/2}$. Equating the terms proportional to ψ_0 gives $\dot{\mathcal{N}}/\mathcal{N} = -3N\dot{\lambda}/(2\lambda) - iE/(\hbar\lambda^2)$ which is readily integrated in $\mathcal{N}(t) = \lambda^{-3N/2}(t) \exp[-iE \int_0^t d\tau/\lambda^2(\tau)\hbar]$. The first factor in the right-hand side of this equation ensures the conservation of the norm of the wavefunction.

The ansatz equation (8) therefore gives, in the unitary limit, the exact time evolution of the initial state vector for an arbitrary time dependence of the isotropic harmonic potential. It rigorously confirms the scaling law that one would obtain from the zero temperature hydrodynamic approximation. It also allows to use the symmetry considerations developed in [15]: e.g. the limit of linear response to a sudden change in the frequency ω away from ω_0 gives rise to an undamped oscillation at frequency $2\omega_0$ which reveals the existence of N-body stationary states of energy $E \pm 2\hbar\omega_0$ coupled to ψ_0 by the excitation operator $\sum_{i=1}^{N} r_i^2$.

Acknowledgements

References

[1] J.M. Vogels, C.C. Tsai, R.S. Freeland, S. Kokkelmans, B.J. Verhaar, D.J. Heinzen, Phys. Rev. A 56 (1997) R1067.

[2] K.M. O'Hara, S.L. Hemmer, M.E. Gehm, S.R. Granade, J.E. Thomas, Science 298 (2002) 2179.

[3] Y. Castin, in: R. Kaiser, C. Westbrook, F. David (Eds.), Coherent Atomic Matter Waves, Lecture Notes of Les Houches Summer School, EDP Sciences and Springer-Verlag, 2001, pp. 1–136.

[4] M. Greiner, C.A. Regal, D.S. Jin, Nature 426 (2003) 537.

[5] S. Jochim, M. Bartenstein, A. Altmeyer, S. Riedl, C. Chin, J.H. Denschlag, R. Grimm, Science 302 (2003) 2101.

[6] M.W. Zwierlein, C.A. Stan, C.H. Schunck, S.M.F. Raupach, S. Gupta, Z. Hadzibabic, W. Ketterle, Phys. Rev. Lett. 91 (2003) 250401.

[7] T. Bourdel, L. Khaykovich, J. Cubizolles, J. Zhang, F. Chevy, M. Teichmann, L. Tarruell, S. Kokkelmans, C. Salomon, cond-mat/0403091.

[8] P. Nozières, S. Schmitt-Rink, J. Low Temp. Phys. 59 (1985) 195.

[9] M. Randeria, in: A. Griffin, D. Snoke, S. Stringari (Eds.), Bose–Einstein Condensation, Cambridge University Press, Cambridge, 1995.

[10] J. Carlson, S.-Y. Chang, V.R. Pandharipande, K.E. Schmidt, Phys. Rev. Lett. 91 (2003) 050401.

[11] K.W. Madison, F. Chevy, W. Wohlleben, J. Dalibard, Phys. Rev. Lett. 84 (2000) 806.

[12] Y. Castin, R. Dum, Phys. Rev. Lett. 77 (1996) 5315.

[13] Y. Kagan, E.L. Surkov, G. Shlyapnikov, Phys. Rev. A 54 (1996) R1753.

[14] C. Menotti, P. Pedri, S. Stringari, Phys. Rev. Lett. 89 (2002) 250402.

[15] L.P. Pitaevskii, A. Rosch, Phys. Rev. A 55 (1997) R853.

[16] D.S. Petrov, C. Salomon, G.V. Shlyapnikov, cond-mat/0309010.

[17] M. Olshanii, L. Pricoupenko, Phys. Rev. Lett. 88 (2002) 010402.