Impurity Expulsion From a Bose-Einstein Condensate

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Abstract

When a sizable, hard-sphere-like impurity is placed in a trapped Bose-Einstein condensate, it will create a hole in the condensate wave function. Since it costs more energy to drill a hole at the wave function’s maximum (near the trap center) than at its minimum (near the trap edge), the impurity will be expelled from the condensate. This suggests that C_{60} molecules freely falling through a condensate of atomic hydrogen may be deflected by a radial acceleration comparable to g. The scattered fullerenes would then form a characteristic banded density pattern outside of the trap. The detection of these deflected molecules can be used to identify the onset of Bose-Einstein condensation.
The Bose-Einstein condensation (BEC) of particles is the macroscopic occupation of a single quantum state. When the effect of interaction is weak, this occupation magnifies the ground state energy by a factor \( N \) equal to the number of condensed particles. For macroscopic \( N \approx 10^{24} \), this extraordinarily large factor can be exploited to magnify minute changes in the ground state. Thus to the extent that the environment affects the condensate’s ground state, BEC is potentially an exceedingly sensitive probe of its environment.

In this work, we consider the effect of placing a hard sphere impurity into the condensate, which forces a hole in the condensate wave function. For translationally invariant systems, such as bulk liquid helium, it is immaterial where this hole is located. However, for atomic trap experiments \([1-4]\), because the condensate wave function is inhomogeneous, there is a position-dependent energy penalty. This energy penalty is ordinarily too small to be detected. We show here that such a minute energy difference can be magnified by BEC into a macroscopic observable phenomenon.

This effect is generic, depending only on the inhomogeneity of the ground state wave function and its macroscopic occupation. It is sufficient to examine the problem in its simplest conceptual context. Consider a non-interacting Bose gas of mass \( m \) confined to a spherical cavity (an infinite square well) of radius \( b \). An impurity, regarded as a hard sphere of radius \( a \), is placed at a distance \( d \) from the cavity center. The situation is illustrated in Fig.1. The cavity traps the Bose gas, but it may or may not also confine the impurity. The impurity can, but need not be microscopic. The effect is actually most pronounced when \( a \) is comparable to \( b \). Classically, there is no interaction between the hard sphere and the cavity. However, when the cavity is filled with a Bose gas, the ground state energy is altered by the presence of the impurity and there is a quantum mechanically induced interaction between the two.

We will assume that the impurity is sufficiently massive that the Born-Oppenheimer approximation is adequate. Unless noted, distances are measured in units of \( b \) and energies in units of \( \frac{\hbar^2}{2m_b^2} \). The effective impurity potential is then \( V(d) = NE_0 \), where \( E_0 \) is the ground state energy of a single particle confined in a unit spherical cavity with an off-center hole:

\[
-\nabla^2 \psi(r) = E\psi(r),
\]
\[
\psi(r) = 0 \text{ at } |r| = 1 \text{ and } |r - d| = a.
\]

When \( d = 0 \), the ground state energy and wave function are known analytically: \( E_0 = \frac{\pi^2}{(1-a)^2}, \psi_0(r) = \frac{1}{r} \sin[\pi(r-a)/(1-a)] \). When \( d > 0 \), spherical symmetry is broken and the problem is non-trivial. While this can still be solved by some brute-force numerical method, the recent suggested use of a conformal transformation \([5]\) is more elegant. Since cylindrical symmetry remains intact, the wave function can be written as \( \psi(r) = \rho^{-1/2}e^{im\theta}R(\rho, z) \), with

\[
\left[ -\frac{\partial^2}{\partial z^2} - \frac{\partial^2}{\partial \rho^2} + \frac{m^2}{\rho^2} - \frac{1}{4} \right] R(\rho, z) = ER(\rho, z).
\]

Let \( Z = z + i\rho, \tilde{Z} = \tilde{z} + i\tilde{\rho} \), the transformation \([6]\)

\[
\tilde{Z} = \frac{Z - c}{1 - cZ}
\]
with \( c \) real, will map the unit circle \( z^2 + \rho^2 = 1 \) to the unit circle \( \tilde{z}^2 + \tilde{\rho}^2 = 1 \) and the off-center circle \((z-d)^2 + \rho^2 = a^2\) to the on-center circle \( \tilde{z}^2 + \tilde{\rho}^2 = \tilde{a}^2 \) with \( \tilde{a} = (d + a - c)/(1 - cd - ca) \), provided that \( c = (1 + d^2 - a^2 - \sqrt{(1 + d^2 - a^2)^2 - 4d^2})/(2d) \). Under this transformation, both the two dimensional Laplacian and the \( 1/\rho^2 \) term in (2) are transformed with the same multiplicative factor \( J(\tilde{r}) = \left[ (1 + \tilde{z}c)^2 + (\tilde{\rho}c)^2 \right]^2 / (1 - c^2)^2 \),

\[
- \frac{\partial^2}{\partial z^2} - \frac{\partial^2}{\partial \rho^2} + \frac{m^2 - \frac{1}{4}}{\rho^2} \longrightarrow J(\tilde{r}) \left[ - \frac{\partial^2}{\partial \tilde{z}^2} - \frac{\partial^2}{\partial \tilde{\rho}^2} + \frac{m^2 - \frac{1}{4}}{\tilde{\rho}^2} \right].
\]

Thus in terms of the transformed coordinates, \( \psi(\tilde{r}) \) satisfies

\[
J(\tilde{r}) \left( - \tilde{\nabla}^2 \right) \psi(\tilde{r}) = E \psi(\tilde{r}),
\]

\( \psi(\tilde{r}) = 0 \) at \(|\tilde{r}| = 1\) and \(|\tilde{r}| = \tilde{a} \).

This equation can be solved by expanding \( \psi(\tilde{r}) \)

\[
\psi(\tilde{r}) = \sum_i C_i k_i^{-1} \phi_i(\tilde{r}),
\]

and diagonalizing the resulting matrix

\[
M_{ij} = k_i \langle \phi_i | J | \phi_j \rangle k_j,
\]

where \( \phi_i(\tilde{r}) \) and \( k_i^2 \) are the complete set of eigenfunctions and eigenvalues of (2) with \( J = 1 \).

The resulting ground state energies from this transformed Hamiltonian are shown as black dots in Fig. 2. \( e_0 = \pi^2 \) is the ground state energy of the cavity without the impurity. The matrix (2) is diagonalized using 100 basis states. For all impurity sizes, the energy is lowered as the impurity moves off-center. The intuitive reason for this is stated in the abstract. When the impurity approaches the cavity surface, \( d \rightarrow 1 - a, \tilde{a} \rightarrow 1 \), the basis states \( \phi_i \) are tightly squeezed and the method converges slowly. This poor convergence shows up in Fig. 2 as an unphysical up-turn in energy near \( d \approx 1 - a \) for \( a = 1/3 \) and \( a = 1/5 \). At the point of contact, the basis states are squeezed out of existence and the method fails. Thus if the impurity is not confined by the cavity, this method cannot be used for \( d > 1 - a \).

For the latter situation, the following variational trial function gives an excellent account of the off-center energy:

\[
\psi_{\text{var}}(r) = (1 - \frac{a}{|r - d|})(1 - r)e^{-\alpha \hat{r} \cdot \hat{d}}.
\]

The variational parameter \( \alpha \) jumps quickly from zero to some \( a \)-dependent value for \( d > 0.1 \).

The resulting energies for \( a = 1/3 \) and \( a = 1/5 \), as computed by the Monte Carlo method, are shown as dash lines in Fig.2. The energy is continuous and smooth across the contact point and is only slightly above the diagonalization results.

When the impurity is microscopic, \( a \ll 0.1 \), both of the above methods are inefficient and the energy shift cannot be accurately computed. In this case, we follow the original suggestion of Huang and Yang [8] and replace the impurity boundary condition by a pseudopotential. Thus instead of (2), we solve,
\[
\left(-\nabla^2 + 4\pi a \delta^3 (r-d) \frac{\partial}{\partial |r-d|} |r-d| \right) \psi(r) = E \psi(r),
\]

\[
\psi(r) = 0 \quad \text{at} \quad |r| = 1,
\]

perturbatively in powers of \(a\). The result,

\[
\frac{E_0}{e_0} = 1 + 2aj_0^2(\pi d) + (2a)^2 j_0^3(\pi d) \left[ \cos(\pi d) - \frac{1}{4} j_0(\pi d) \right],
\]

is shown as indicated in Fig.2. The first order term is proportional to the cavity ground state density, which makes precise the notion that the energy penalty is greatest at the maximum of the ground state wave function. Note however that, for \(a \geq 1/5\), the actual energy is much steeper than the first or second order results. The second order term above is from summing over only the s-wave intermediate states. As pointed out by Huang and Yang [8], such a second order energy shift can be positive because the pseudopotential is not hermitian and a singular negative term is removed by the derivative operation on the wave function. Since we have summed only over the s-wave intermediate states, the negative singular term in \(\psi_0^{(1)}\), which should be proportional to \(1/|r-d|\), started out as proportional to \(1/r\). Accordingly, we removed this contribution to the second order energy. This s-wave-only second order energy, while in principle incomplete, is exactly correct in the limit of \(d \to 0\). As shown in Fig. 2, its inclusion yielded excellent agreement with numerical results at all values of \(d\) for \(a \leq 1/10\). In comparison, the first order result is good only for \(a < 1/20\). The effect of interaction among the condensed atoms can be incorporated via the Gross-Pitaevskii mean-field. The result is a slight energy shift [9] in accordance with the sign of the scattering length. For a condensate of atomic hydrogen, this effect is particularly negligible because of hydrogen’s anomalously small s-wave scattering length [4].

An impurity of radius \(a\) and mass \(M\) will therefore be expelled from the condensate with radial acceleration

\[
a_r = \frac{N}{M} \frac{\hbar^2}{2m b^2} \left( \frac{1}{b} \frac{\partial E_0}{\partial d} \right).
\]

Since the fall-off in energy is increasingly steep as \(a\) approaches 1, the expulsion force is greater for larger impurities. If the impurity is microscopic, with \(a \ll 0.1\), the perturbative result [8] can be used. For an order-of-magnitude estimate we can keep only the first order term and replace the derivative by its average value,

\[
a_r \approx \frac{\pi^2 \hbar^2 N}{M m b^3} \left( \frac{a}{b} \right).
\]

We have restored all factors of \(\hbar/m\) and \(b\) so that the overall dependence on \(b\) is clear. Note that this radial acceleration is proportional to the condensate density \(\approx N/b^3\). Currently, all experimental traps are highly cylindrical. For these cases, we can make an equal volume replacement: \(b^3 \to \frac{2}{3} b^2 L\), where \(L\) is the length of the cylinder,
This corresponds to an impurity expelled radially from the middle of the cylinder. The numerical value $\frac{4}{3}\pi^2 = 13.16$ is in good agreement with the exact cylindrical value of $4/J_1^2(z_1) = 14.84$, where $z_1$ is the first zero of $J_0(z)$.

If the impurity is microscopic, the expulsion will be most pronounced for an impurity with a large radius-to-mass ratio, i.e., a hollow molecule. For $C_{60}$, we have $M \approx 10^{-24}$ kg and $a \approx 4 \times 10^{-10}$ m. The latest reported Bose condensate in atomic hydrogen by Fried et al [4] is ideal with optimal $\hbar/m = 6.65 \times 10^{-42}$ J-m$^2$ and the largest reported $N \approx 10^9$. This condensate is highly elongated with cylindrical radius $b = 7.5 \mu$m and length $L = 5$ mm. If $C_{60}$ molecules were sprinkled over this condensate, they would be deflected by an average radial acceleration of

$$a_r \approx 17 \text{ m/s}^2 \approx 2 g.$$  (13)

For Na and Rb condensates, the effect would be reduced by a factor of 1/23 and 1/87 respectively, modulo differences in condensate density. Since the Li condensate will collapse beyond a critical $N_c \approx 10^3$, it will not be a favored condensate to observe this effect. To model the fullerene’s additional surface attraction for hydrogen one should properly interpret $a$ as the exact scattering length. Thus even if the surface attraction were to reduce the equivalent hard sphere radius by a factor of 2, the radial acceleration would still be comparable to $g$.

The actual radial acceleration can be computed from the cylindrical energy shift

$$E_0 - e_0 = \frac{\hbar^2}{m} \frac{4a}{b^2L} \frac{J_0^2(z_1d/b)}{J_1^2(z_1)}.$$  (14)

Fig.3 shows the trajectories of $C_{60}$ molecules released uniformly at a height of $6b = 45 \mu$m above the cylindrical center and freely falling through the hydrogen condensate. They are narrowly focused near the trap’s edge at $\approx 15 \mu$m below the trap center. Below this point the beam diverges but is still bounded by two caustics. The density distribution at $6b = 45 \mu$m below the cylindrical center is shown in Fig.4. Most of the fullerenes are expelled out of the trap forming a sharply defined band just outside of the trap. The surprise is that the distribution is not diffuse, but is bounded by two high density caustics. This characteristic distribution is also generic. A similar band is also found using harmonic oscillator wave functions. For weaker repulsions (such as that exerted by the Na condensate), the focal plane and the caustics would form further down from the trap, but the banded density distribution would remain unchanged.

We emphasize that this deflection is a purely quantum mechanical phenomenon. Classically, if $C_{60}$ molecules were raining down on such a low density hydrogen vapor, only one out of 100 would encounter a single hydrogen atom.

Since this repulsion is effective only when the atoms are condensed in the ground state, the detection of these deflected fullerenes can be used to identify the onset of Bose-Einstein condensation. Finally, if the impurity has a negative scattering length with respect to the condensed atoms, the impurity will be attracted and centrally focused by the condensate. In either case, a uniform distribution of impurities will become patterned after passing through a condensate.
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FIG. 1. A Bose gas confined in a spherical cavity of radius $b$ and excluded from an off-center impurity, which is a hard-sphere of radius $a$. 
FIG. 2. The ground state energy of a spherical cavity with an off-center hard-sphere. $a$ and $d$ are measured in units of $b$. $e_0$ is the ground state energy without the hard-sphere.
FIG. 3. Classical trajectories of $C_{60}$ molecules falling through a cylindrical condensate of atomic hydrogen. The circular cross-section of the cylinder is distorted by unequal x and y scales into an ellipse. See text for details.
FIG. 4. The density distribution of C₆₀ molecules falling through a cylindrical condensate of atomic hydrogen at 45 μm below the cylindrical center. The fullerenes are released at 45 μm above the trap center with initial uniform density n₀. The condensate’s cylindrical radius is 7.5 μm.