Rotons in interacting ultracold Bose gases

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In three dimensions, non-interacting bosons undergo Bose-Einstein condensation at a critical temperature, $T_c$, which is slightly shifted by $\Delta T_c$, if the particles interact. We calculate the excitation spectrum of interacting Bose-systems, $^4$He and $^{87}$Rb, and show that a roton minimum emerges in the spectrum above a threshold value of the gas parameter. We provide a general theoretical argument for why the roton minimum and the maximal upward critical temperature shift are related. We also suggest two experimental avenues to observe rotons in condensates. These results, based upon a Path-Integral Monte-Carlo approach, provide a microscopic explanation of the shift in the critical temperature and also show that a roton minimum does emerge in the excitation spectrum of particles with a structureless, short-range, two-body interaction.

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The importance of interactions on the macroscopic scale is characterised by the gas parameter, $\gamma = na^3$, which is proportional to the ratio of the volume occupied by the particles compared to that available to them. Bose-Einstein condensates in ultra-cold gases are usually in the weakly interacting limit [3]; and away from the Feshbach resonance experiments could only explore the dilute limit, $\gamma \sim 10^{-6}$ [3]. However the use of Feshbach resonances in $^{85}$Rb has facilitated the creation of condensates with tunable values of $\gamma$ up to approximately $8 \times 10^{-3}$ [6]. In condensates of $^7$Li, values of $\gamma$ up to $\sim 50$ have been achieved [4], although with non-uniform density distribution due to trapping. We note here that $\gamma$ is not at all small, $\sim 0.2$, in the case of liquid $^4$He [7,8].

Interactions also induce a shift in the condensation critical temperature, $T_c$, which was first reported for the $^4$He-Vycor system [9] confirming earlier theoretical predictions [4,13]

$$\Delta T_c \equiv \frac{T_c - T_c^{(0)}}{T_c^{(0)}} \approx C \gamma^{1/3}$$

where $T_c^{(0)}$ is the critical temperature of an ideal Bose-gas with the same density and $C$ is a positive dimensionless constant. Different theoretical approaches aimed at determining this dimensionless constant resulted in significant discrepancy for some time, with consensus finally provided by Monte Carlo simulations [14].

For small $\gamma$, the Bogoliubov spectrum [11] accurately describes the excitation spectrum, while for larger $\gamma$, such as in liquid $^4$He, it deteriorates and a roton minimum is observed [15]. Path integral Monte Carlo calculations [11,16] and an experiment [7] have shown that equation (2) becomes invalid for $\gamma \gtrsim 10^{-3}$. For even higher $\gamma$, the system freezes and the roton minimum goes soft.

In fact, $\Delta T_c$ has a maximum when $\gamma \approx 10^{-2}$ as can be seen in Fig. 1. Since the onset of condensation is associated with the energies of available states, we might postulate the peak in $\Delta T_c$ to be accompanied by the transition to the roton regime as $\gamma$ increases. Below we substantiate this claim.

Contrary to earlier studies in which the condensate was

![FIG. 1. The critical temperature shift $\Delta T_c$, is plotted as a function of $\gamma$ as derived by Grüter et al. [11]. Note the different scales on the ordinate. Reproduced through the courtesy of the authors of Ref. [11]. The shaded area covers the range where the maximum shift is located.](image-url)
rotating fast [17] or particles had laser-induced dipole moments [18], we show that the roton minimum may also occur in a homogeneous system where the two-body interaction is short-range and structureless. This fact may give hope for indirectly observe rotons in Bose-Einstein condensates utilising already existing experimental apparatus. Moreover, our simulations imply that the excitation of rotons is also connected to the shift of the critical temperature of condensation scrutinized in earlier studies.

**Theoretical model:** We assume that our system can be described using only two-body interaction potentials between the constituents and can be modelled by the hard-sphere potential with diameter \(a\). We have varied \(a\), while keeping \(n\) constant, to sample different values of \(\gamma\). The systems were homogeneous and periodic boundary condition have been applied.

**Numerical details:** We have carried out path integral Monte Carlo (PIMC) simulations [19] for both \(^4\)He and \(^{87}\)Rb in order to determine the energy spectrum, \(\varepsilon(k)\). The configurations of the system are sampled via the density matrix. Although the exact density matrix is not continuous step in \(g\), however, this approach introduces a non-continuous step in \(g\), and leads to unacceptable error in \(S(k)\) below \(r_c^{-1}\). The truncation error can be suppressed by varying the cut-off, \(r_c\), and taking the average of the values of \(S(k)\) obtained this way.

An alternative is to fit a trial function to \(g(r)\). The trial function used below has been derived from the Ornstein-Zernike equation with the Percus-Yevick (PY) closure [24] providing the analytical, but implicit solution \(g_{PY}(r) = \mathcal{L}^{-1}\{G_{PY}(z)\}\), where \(\mathcal{L}^{-1}\) stands for the inverse Laplace-transform and \(G_{PY}(z)\) is known explicitly [23, 26]. The function, \(G_{PY}(z)\), has a pole at the origin, \(z_0 = 0\), and infinitely many distinct conjugate pairs of poles, \(z_\ell = \kappa_\ell + i k_\ell (\ell = 1, 2, \ldots)\). The distribution of these zeros completely determines \(g_{PY}(r)\), and thus all thermodynamical quantities of the system, for a fixed value of \(\gamma\). Figure 2 depicts the real part of the three lowest lying zeros, while the inset shows all the zeros over the complex plane for different \(\gamma\). The leftmost curve belongs to \(\gamma = 0.095\), while the rightmost to \(\gamma = 1.91\). As \(\gamma\) increases the zeros move towards the imaginary axis and all zeros become purely imaginary for \(\gamma = 1.91\).

In order to check our PIMC results and also to smooth the simulation data of \(g(r)\) we determine the fitting parameters \(C_1, k_1, \delta_1\), and \(\kappa_1\) for each value of \(\gamma\). Although

\[
S(k) = \frac{\hbar^2 k^2}{2m \varepsilon(k)} \coth \left( \frac{\varepsilon(k)}{2kT} \right) \xrightarrow{T\to0} \frac{\hbar^2 k^2}{2m \varepsilon(k)}
\]

providing an upper bound on \(\varepsilon(k)\).

Due to the finite size of the system, \(g(r)\) can only be calculated over a limited range (repeated use of the periodic boundary condition would lead to unphysical spatial correlation). One may assume that \(g(r > r_c) = 1\) for some cut-off \(r_c\), however, this approach introduces a non-continuous step in \(g(r)\) at \(r_c\) and leads to unacceptable error in \(S(k)\) below \(r_c^{-1}\). The truncation error can

\[
g_{PY}(r) \equiv 1 + \frac{C_1}{r} \cos (k_1 r + \delta_1 e^{-\kappa_1 r}).
\]

In Fig. 2 the real parts of the first three lowest lying poles are shown. One may notice that \(k_1\) approaches zero rapidly, and therefore the corresponding oscillatory contribution to \(g(r)\) is only weakly damped. The imaginary part, \(k_1\), falls between \(\pi\) and \(3\pi\) providing a characteristic wavenumber, i.e. a broad qualitative estimate on where the roton minimum may occur, i.e. between \(\pi/a\) and \(3\pi/a\).

In order to check our PIMC results and also to smooth the simulation data of \(g(r)\) we determine the fitting parameters \(C_1, k_1, \delta_1,\) and \(\kappa_1\) for each value of \(\gamma\). Although
κ₁ and k₁ could be determined from GPY(ζ), we treat them as free parameters, and compare their fitted values to those the pole-structure suggests. The comparison provides a test of the accuracy of our PIMC calculation. Satisfactory agreement between the fitted function and raw data can be seen in Fig. 3. The advantage of using the fitted gPY(r) is that it can be extrapolated to larger system sizes and its derivative may be easily calculated.

The key result of our work, the excitation spectra of ⁴He and ⁸⁷Rb can be seen in Fig. 4. The maximum in ΔT_c occurs at γ ≈ 0.01, while we find that the roton minimum appears at γ ≈ 0.2. Although the onset of the roton minimum does not appear to directly coincide with the maximum of ΔT_c, the minimum is preceded by another qualitative change, namely the development of a point of inflection in ε(k). By taking the second derivative of ε(k), as shown in the inset of Fig. 4(a), we can determine the approximate value of γ for which the spectrum develops this inflection point. The data indicate that this occurs approximately at γ ≈ 0.014 which falls exactly into the region where the critical temperature reaches its maximum.

The connection between the development of the inflection point and the maximum of ΔT_c may be illuminated by the following argument. At temperature T the occupancy of a state with energy ε(k) is determined by the Bose-Einstein distribution, f(T, ε). Bose-Einstein condensation occurs if the ground state is macroscopically occupied, i.e. the number of particles in any excited states, N_{ex}(T), is saturated

\[ N_{ex}(T) = \int_0^\infty G(\varepsilon) f(T, \varepsilon) d\varepsilon < N_{total}. \quad (5) \]

It is tacitly assumed that the chemical potential has reached its maximum value. The critical temperature, T_c, is thus determined by the excitation spectrum via the density of states, G(ε). If G(ε) increases for thermally available states, then the temperature must be decreased to reduce f(T, ε) and preserve the validity of inequality (5). The critical temperature should therefore decrease as well. The density of states corresponds to \( |dk/d\varepsilon| \), which is the reciprocal of the slope of the excitation spectrum.

For weakly interacting bosons, Bogoliubov’s result indicates that increasing γ increases the slope of ε(k), thus G(ε) must decrease around k ≈ 0. We can therefore conclude that the critical temperature of a weakly interacting Bose-gas ΔT_c must be positive. As γ increases, ε(k) develops an inflection point and becomes convex in a certain region. The decrease of the slope in this region opens an abundance of excited states for the particles,
manifested as a peak in $G(\varepsilon)$. These excited states can be populated at lower temperature, thus reducing the population of the ground state. Therefore the system has to be further cooled for macroscopical occupation of the ground state. Consequently, the critical temperature must decrease, resulting in $\Delta T_c$ decreasing also. As $\gamma$ increases further, the inflection gives rise to the roton minimum in the spectrum for non-vanishing momenta. Although the magnitude of the derivative starts to increase along the sides of the minimum, the density of states continues to increase, as there are now three sets of $k$ states which contribute to the density of states for a given energy (See Fig. 5).

Recently, a similar conjecture has been made in the context of two-dimensional dipolar systems. The interaction parameter corresponding to our $\gamma$ is the dipole coupling $D$. As $D$ increases the critical temperature develops a maximum. The authors mentioned the apparent coincidence of this maximum and the onset of the roton minimum, although they have not investigated this in detail. We note that their system and ours are dissimilar in two important aspects: dimensionality and the nature of interaction. Dimensionality is significant in that it influences which phases appear in the system, e.g. Berezinskii-Kosterlitz-Thouless phase rather than BEC. However the nature of the interactions—we feel—is more fundamental. The two-body interaction in our analysis is spherically symmetric, structureless and short-range, while their dipole interaction has strong angular dependence and long range influence. It is far from obvious a priori that hard core bosons, therefore, should establish a roton structure in the excitation spectrum at all, let alone that its appearance should correspond to the shift of the critical temperature.

Experimental verification of the predicted onset of the roton minimum may be possible by utilising a Feshbach resonance to tune the interaction strength and then using Bragg spectroscopy to probe the excitation spectrum. The values of $\gamma$ achieved by Papp et. al. approach the lower end of values for which we predict the inflection point in $\varepsilon(k)$ to occur, while Bragg spectroscopy has previously been used to measure the excitation spectrum of a weakly interacting BEC.

As a second scenario, quantum evaporation could be adapted for pancake shaped Bose-Einstein condensates. This technique proved to be a successful experimental method in the case of liquid $^4$He. An excitation having enough energy is capable of ejecting an atom from the condensate. However, phonons and rotons carry different momenta at the same energy, therefore the ejected atoms have different angular distribution depending on which type of excitations they interacted with. Therefore detecting the angular distribution of ejected atoms after exciting the condensate in a controlled manner, could prove the existence of rotons in BECs.

In this Letter, we have shown that the maximum observed in $\Delta T_c$ of an interacting BEC is related to the appearance of an inflection point in $\varepsilon(k)$. As $\gamma$ increases the inflection point signals the appearance of a roton minimum, characteristic of the excitation spectrum of e.g. superfluid $^4$He. We have also provided a physical argument as to why this happens and how it could be observed experimentally.

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![FIG. 5. Qualitative picture of the excitation spectrum (right) and the density of states (left). As $\varepsilon(k)$ develops a maximum (maxon) and a minimum (roton) the density of states diverges.](image-url)
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