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LETTER TO THE EDITOR

The internal energy and condensate fraction of a trapped interacting Bose gas

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Abstract. We present a semiclassical two-fluid model for an interacting Bose gas confined in an anisotropic harmonic trap and solve it in the experimentally relevant region for a spin-polarized gas of ^{87}Rb atoms, obtaining the temperature dependence of the internal energy and of the condensate fraction. Our results are in agreement with recent experimental observations by Ensher *et al*.

Bose–Einstein condensation (BEC) has recently been realized in dilute vapours of spin-polarized alkali atoms, using advanced techniques for cooling and trapping [1–5]. These condensates consist of several thousands to several millions of atoms confined in a well which is generated from non-uniform magnetic fields. The confining potential is accurately harmonic along the three Cartesian directions and has cylindrical symmetry in most experimental set-ups.

The determination of thermodynamic properties such as the condensate fraction and the internal energy as functions of temperature is at present of primary interest in the study of these condensates [4, 5]. The nature of BEC is fundamentally affected by the presence of the confining potential [6] and finite-size corrections are appreciable, leading for instance to a reduction in the critical temperature [7–10]. Interaction effects are very small in the normal phase but become significant with the condensation-induced density increase. The correction to the transition temperature due to interactions has been recently computed by Giorgini *et al* [11].

The temperature dependence of the condensate fraction was recently measured [5] for a sample of around 40 000 ^{87}Rb atoms, the observed lowering in transition temperature being in agreement with theoretical predictions within experimental resolution. In the same work the internal energy was measured during ballistic expansion and found to be significantly higher in the BEC phase than predicted by the ideal-gas model. While the increase is easily understood as a consequence of the interatomic repulsions, a quantitative estimate is still lacking.

In this work we present a two-fluid mean-field model which is able to explain the above-mentioned effects, giving results in agreement with experiment for both the condensate fraction and the internal energy as functions of temperature.

We describe the condensate by means of the Gross–Pitaevskii (GP) equation for its wave function $\Psi(r)$,

$$-\frac{\hbar^2\nabla^2}{2m}\Psi(r) + V^{\mathrm{ext}}(r)\Psi(r) + 2gn_1(r)\Psi(r) + g\Psi^3(r) = \mu\Psi(r) \qquad (1)$$

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where $g = 4\pi\hbar^2 a/m$, a being the scattering length, $V^{\rm ext}(\boldsymbol{r}) = m\omega^2(x^2 + y^2 + \lambda^2 z^2)/2$ is the confining potential and $n_1(r)$ is the average non-condensed particle distribution. The factor 2 in the third term arises from exchange [12] and we neglect the term involving the off-diagonal density of non-condensed particles. Following Bagnato *et al* [13] we treat the non-condensed particles as non-interacting bosons in an effective potential $V^{\rm eff}(r) = V^{\rm ext}(r) + 2gn_1(r) + 2g\Psi^2(r)$. Thermal averages are computed with a standard semiclassical Bose–Einstein distribution in chemical equilibrium with the condensate, i.e. at the same chemical potential μ. In particular, the density $n_1(r)$ is

$$n_1(r) = \frac{1}{(2\pi\hbar)^3}\int \frac{{\rm d}^3 p}{\exp\{(p^2/2m + V^{\rm eff}(r) - \mu)/k_B T\} - 1} = \frac{(mk_B T)^{3/2}}{(2\pi)^{3/2}\hbar^3}\sum_{j\geqslant 1}\frac{1}{j^{3/2}}\exp\{-j(V^{\rm eff}(r) - \mu)/k_B T\}. \tag{2}$$

We fix the chemical potential from the total number of particles N:

$$N = N_0 + \int \frac{\rho(E)\ {\rm d}E}{\exp\{(E-\mu)/k_B T\} - 1} \tag{3}$$

where $N_0 = \int \Psi^2(r)\ {\rm d}^3 r$ and the semiclassical density of states is

$$\rho(E) = \frac{(2m)^{3/2}}{4\pi^2\hbar^3}\int_{V^{\rm eff}(r)<E}\sqrt{E - V^{\rm eff}(r)}\ {\rm d}^3 r. \tag{4}$$

This completes the self-consistent closure of the model.

Equation (1) can be solved analytically in the experimentally relevant situation $N \sim 10^4$–10^5 and $a/a_\perp \sim 10^{-2}$, where $a_\perp = \sqrt{\hbar/m\omega}$. Except for in a small region close to the phase transition, the interaction parameter $N_0 a/a_\perp$ entering the GP equation is large and the kinetic energy can be neglected. This yields

$$\Psi^2(r) = \frac{\mu - V^{\rm ext}(r) - 2gn_1(r)}{g}\theta(\mu - V^{\rm ext}(r) - 2gn_1(r)) \tag{5}$$

where $\theta(x) = 0$ (1) for $x < 0$ ($x > 0$). The present strong-coupling solution neglects the condensate zero-point energy $E_0^c = \hbar\omega(1 + \lambda/2)$. As Giorgini, Pitaevskii and Stringari [11] pointed out, finite-size effects are thereby excluded.

Before presenting the complete numerical solution of the self-consistent model defined by equations (2)–(5) and comparing its predictions with existing experimental data [5], we display perturbative solutions at zero and first order.

An approximate semi-analytical solution can be obtained by treating perturbatively interactions involving the 'dilute gas' of non-condensed particles. To zero order in $gn_1(r)$, we have

$$N_0 = \left(\frac{2\mu}{\hbar\omega}\right)^{5/2}\frac{a_\perp}{15\lambda a} \tag{6}$$

and equation (4) gives

$$\rho_0(E) = \frac{1}{\pi\lambda(\hbar\omega)^3}\left[2\sqrt{\mu}(E-\mu)^{3/2} + E^2\arctan\sqrt{\frac{E-\mu}{\mu}} + (2\mu - E)^2\ln\frac{\sqrt{|E-2\mu|}}{\sqrt{\mu} + \sqrt{E-\mu}}\right] \tag{7}$$

for $\mu > 0$ and

$$\rho_0(E) = \frac{E^2}{2\lambda(\hbar\omega)^3} \tag{8}$$

for $\mu < 0$. The self-consistent zero-order solution is then completed by equation (3). We remark that no assumption of weak interactions *within the condensate* has been made.

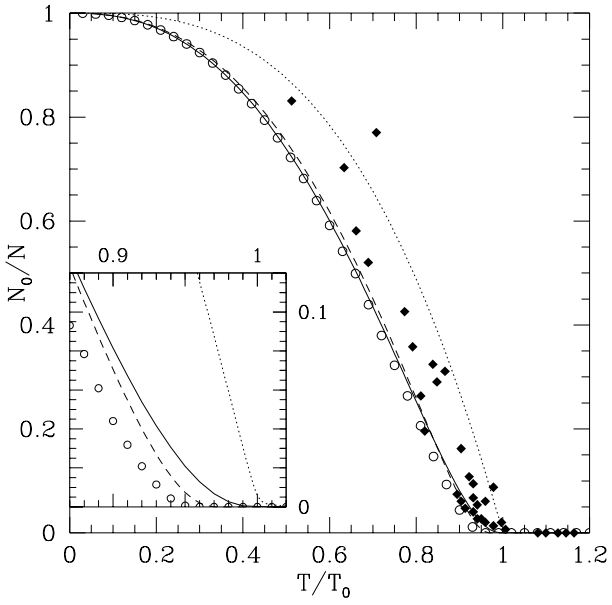

Figure 1. The condensate fraction obtained in the two-fluid model compared with the experimental data of Ensher *et al* [5] (diamonds) and with the ideal-gas result (dotted curve). We present results obtained from the zero-order solution (full curve), from the first-order perturbative treatment (dashed curve) and from the complete numerical solution (circles). The inset is an enlargement of the region around T_c.

We now proceed to compute the first-order correction to the above zero-order solution. We take

$$\Psi^2(r) = \frac{\mu - V^{\rm ext}(r) - 2gn_1(0)}{g}\theta(\mu - V^{\rm ext}(r) - 2gn_1(0)) \tag{9}$$

and expand equation (4) to first order in $g[n_1(r) - n_1(0)]$. The choice of the expansion parameter $g[n_1(r) - n_1(0)]$ ensures that the perturbative expansion is regular, since the correction to ρ vanishes where the zero-order term vanishes. With the additional approximation $g\Psi^2(r) \simeq \mu\theta(\mu)$ in the first-order term we get

$$\rho(E) = \rho_0(E - 2gn_1(0)) + \delta\rho_1(E - 2gn_1(0) - \mu\theta(\mu)) \tag{10}$$

where

$$\delta\rho_1(E) = \frac{4}{\sqrt{2\pi}\lambda}\frac{a}{a_\perp}\left(\frac{k_BT}{\hbar\omega}\right)^{3/2}\sum_{j\geqslant 1}\frac{E{\rm e}^{j\mu\theta(-\mu)/k_BT}}{j^{3/2}(\hbar\omega)^2}\left[1 - {}_1F_1\left(\frac{3}{2}, 2, -j\frac{E}{k_BT}\right)\right] \tag{11}$$

where ${}_1F_1$ is the Kummer confluent hypergeometric function. The self-consistent first-order solution is then completed by equation (3).

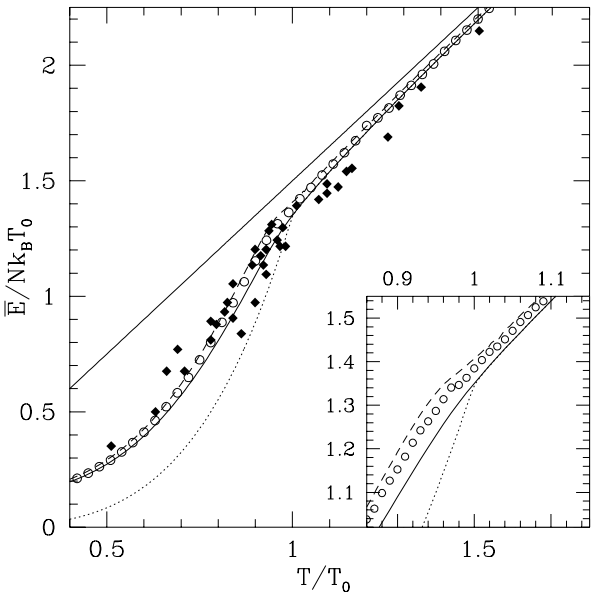

Figure 2. The sum of kinetic and interaction energy, as defined in the text, obtained in the two-fluid model, compared with the experimental data of Ensher *et al* [5] (diamonds) and with the ideal-gas result (dotted curve). We present results obtained from the zero-order solution (full curve), from the first-order perturbative treatment (dashed curve) and from the complete numerical solution (circles). The straight line is the classical Maxwell–Boltzmann result. The inset is an enlargement of the region around T_c.

We have solved numerically the simplified two-fluid model, first treating the parameter $gn_1(0)$ to all orders (equations (2)–(5)), then to zero order (equations (3) and (6)–(8)) and finally to first order (equations (3) and (9)–(11)). Each case involves solving the integral equation (3) to obtain μ as a function of N and T; the non-perturbative solution also involves the local non-linear problem posed by equations (2) and (5). The small differences between our three results justify *a posteriori* a perturbative treatment. The experimental parameters are taken from the work of Ensher *et al* [5]: $\lambda = \sqrt{8}, N = 40\,000$ and $a/a_\perp = 0.0062$. We have verified numerically that our results depend weakly on N in the region explored in the experiments and therefore have used a fixed $N = 40\,000$ in all of our computations. We use as energy units the semiclassical ideal-gas critical temperature $k_B T_0 = \bar{h}\omega(N\lambda/\zeta(3))^{1/3}$, $\zeta(3) \simeq 1.202$ being the Riemann zeta function.

Figure 1 compares the temperature dependence of the condensate fraction N_0/N with the experimental results of Ensher *et al* [5]. Lowering of the transition temperature due to interactions is clearly visible, even if the smoothness of our results around the transition prevents a precise assessment of an interaction-induced shift in T_c from the numerical solution. It should be noticed that the strong-coupling solution of the GP equation is not valid for T close to T_c, since it requires $N_0 \gg a_\perp/a \simeq 160$, and that our mean-field model does not include critical fluctuations. As both effects are relevant only in a narrow window around T_c [11], we expect our results to be meaningful over most of the temperature range. Recently Giorgini *et al* [11] solved numerically the Popov approximation to the finite-temperature generalization of the GP equation within a semiclassical WKB approximation. Their results for the temperature dependence of the condensate fraction are in very good agreement with

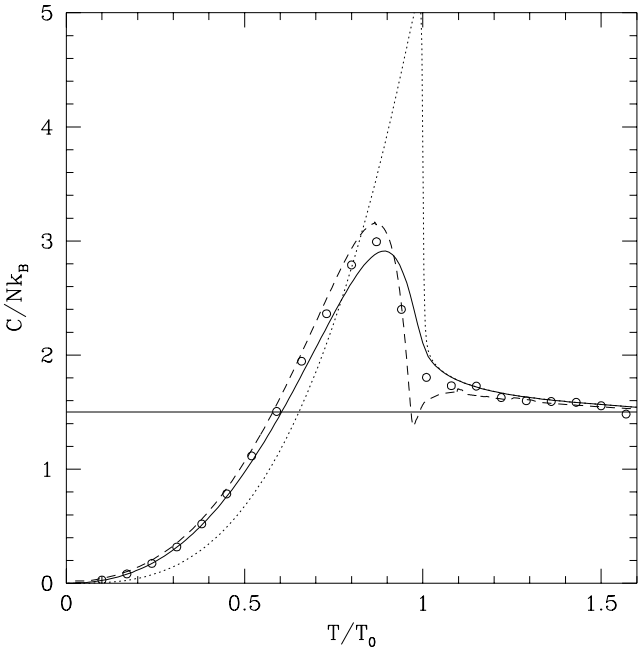

Figure 3. The specific heat $C = \mathrm{d}\bar{E}/\mathrm{d}T$ obtained in the two-fluid model compared with the ideal-gas result (dotted curve). We present results obtained from the zero-order solution (full curve), from the first-order perturbative treatment (dashed curve) and from the complete numerical solution (circles). The straight line is the classical Maxwell–Boltzmann result. The anomalous behaviour obtained from the first-order perturbative solution near T_c is an artifact.

the predictions of our more naive model except for when $|T - T_c|/T_c < 0.05$, where they find a sharp change in the slope of $N_0(T)$. Their result for the interaction-induced shift in critical temperature $\delta T_c/T_c \simeq -1.33N^{1/6}a/a_\perp \simeq -0.048$ is also in good agreement with our curves.

Figure 2 reports our results for the temperature dependence of the internal energy. We remark that the experimentally measured quantity is the sum of the kinetic energy and the interaction energy, not including the confinement potential energy due to the rapid switching off of the trapping potential [14]. The average single-particle energy

$$\langle E\rangle_{\mathrm{nc}} = \int E\rho(E)\ \mathrm{d}E/\{\exp[(E-\mu)/k_BT] - 1\}$$

obtained from the semiclassical density of states contains twice the interaction energy, and—assuming that on average the kinetic and potential energy terms are equal—is twice the measured quantity. The kinetic energy of condensed atoms is negligible in our strong-coupling limit and their interaction energy per particle is

$$\langle E\rangle_{\mathrm{c}} = \frac{1}{2}g\int \Psi^4(r)\ \mathrm{d}^3r.$$

The quantity directly comparable to the experimental data is therefore $\bar{E} = (\langle E\rangle_{\mathrm{nc}}(N - N_0)/2 + \langle E\rangle_{\mathrm{c}})/N$, which we plot in figure 2, obtaining good agreement with the measured values. The calculated internal energy does not contain any sharp feature at the transition, paralleling the result discussed above for the condensate fraction. Correspondingly, the

rapid rise in the specific heat is considerably smoothed with respect to the ideal-gas result (see figure 3). Apart from this small region around the transition, our results on $\bar{E}(T)$ above and below T_c imply a significant reduction of the increase in specific heat across the phase transition.

In conclusion, we have presented a mean-field, semiclassical two-fluid model and discussed its perturbative and non-perturbative solution in the experimentally relevant parameter range. Our results on the temperature dependence of the condensate fraction and of the internal energy are in agreement with recent experimental measurements, accounting for the pronounced increase in internal energy with respect to the non-interacting boson case measured below T_c. We have also verified that our model reproduces the results obtained for the condensate fraction with a more refined theory given by Giorgini *et al*.

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