Comment on "Bose-Einstein condensation with magnetic dipole-dipole forces"

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The ground-state solutions of a dilute Bose condensate with contact and magnetic dipole-dipole interactions are examined. By lowering the value of the scattering length, Goral *et al.* [Phys. Rev. A **61**, 051601 (2000)] numerically predict a region of unstable solutions, accompanied by a neighborhood where the ground-state wave functions have internal structure. On the contrary, we find that the dipolar condensate has an intuitively located stability region, and ground-state solutions near the instability threshold that are without any unusual structure.

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A nonideal Bose-Einstein condensate in the presence of magnetic dipole-dipole forces was recently investigated [1]. For a magnetic moment equal to that for chromium and a typical value for the scattering length, all solutions were found to be stable and differed only in size from condensates lacking long-range interactions. Upon reducing the scattering length below a critical value, the dipolar condensate was found to become unstable, and for scattering length values just above the instability, a ''structured'' condensate was found (i.e., the density had several peaks instead of the ordinary single-peaked behavior). The purpose of this Comment is to report a disagreement in both the location of the instability threshold and the existence of the structured ground-state solutions.

The results of Ref. [1] were achieved by numerically solving the Gross-Pitaevskii equation for atoms in a cylindrical harmonic trap:

$$i\hbar\frac{\partial\Psi}{\partial t}=\left\{-\frac{\hbar^2\nabla^2}{2m}+\frac{1}{2}m\omega_0^2\left(x^2+y^2+\gamma^2z^2\right)+\frac{4\pi\hbar^2a}{m}N|\Psi|^2+N\int V\left(\mathbf{r}-\mathbf{r}'|\Psi\left(\mathbf{r}'\right)|^2d^3\mathbf{r}'\right\}\Psi. \tag{1}$$

Here Ψ is the condensate wave function, a is the s-wave scattering length, N is the number of atoms, and m is the mass of the atom. The long-range potential is due to the magnetic dipole-dipole interaction and is given by

$$V(\mathbf{r}-\mathbf{r}')=\frac{\mu_0}{4\pi}\frac{[\boldsymbol{\mu}_1(\mathbf{r})\cdot\boldsymbol{\mu}_2(\mathbf{r}')]-3[\boldsymbol{\mu}_1(\mathbf{r})\cdot\mathbf{u}][\boldsymbol{\mu}_2(\mathbf{r}')\cdot\mathbf{u}]}{|\mathbf{r}-\mathbf{r}'|^2}, \tag{2}$$

where $\mathbf{u}=(\mathbf{r}-\mathbf{r}')/|\mathbf{r}-\mathbf{r}'|$ and μ_0 is the magnetic permeability of the vacuum. All the magnetic moments are assumed to point in the same direction (z direction), i.e., $\boldsymbol{\mu}_1=\boldsymbol{\mu}_2=\boldsymbol{\mu}\hat{z}$. As explained in Ref. [1], the Gross-Pitaevskii equation (1) can be solved easily enough when one notices that the nonlocal (NL) term is a convolution, and is therefore local in k-space. This approach requires a Fourier transform of the dipole-dipole (DD) interaction, given in the limit of small atomic overlap distance as [1]

$$\mathcal{F}[V(\mathbf{r})]=-\tfrac{1}{3}\mu_0\mu^2(1-3\cos^2\alpha), \tag{3}$$

where α is the angle between $\mathbf{k}$ and $\boldsymbol{\mu}$.

Now, inspecting the formula (3), one thing seems intuitively clear: the first term will introduce an effective shift in the scattering length according to

$$U_0=4\pi\hbar^2aN/m-\mu_0\mu^2N/3, \tag{4}$$

and one would expect instability (roughly) when this becomes negative. A first approximation to the instability threshold is then

$$\overline{a}_c=m\mu_0\mu^2/12\pi\hbar^2. \tag{5}$$

Using the chromium parameters $\mu=6\mu_B$, $m=52u$ we get the estimate ($a_{\mathrm{Na}}=2.75$ nm)

$$\overline{a}_c/a_{\mathrm{Na}}\approx 0.291. \tag{6}$$

This simple estimate is about twice as big as the values given by Goral *et al.* [1] in their Fig. 2, and it also indicates a critical scattering length that is independent of particle number. To a certain extent, the kinetic energy (and possibly the anisotropic part of the dipole-dipole interaction) can stabilize the condensate in a manner similar to that for condensates with negative scattering lengths, but it seems unlikely that these would cause such a dramatic shift in the critical scattering length.

To determine more accurately when the condensate is expected to turn unstable, we perform a variational calculation by assuming a trial wave function for the condensate density [2],

$$|\Psi|^2=\frac{1}{\pi^{3/2}\sigma^2\sigma_z}\exp[-(x^2+y^2)/\sigma^2]\exp(-z^2/\sigma_z^2). \tag{7}$$

The energy of the condensate is then $E=E_K+E_P+E_{\mathrm{NL}}+E_{\mathrm{DD}}$, where

$$E_K=(\hbar^2/2m)\,(1/\sigma^2+\tfrac{1}{2}\sigma_z^2), \tag{8}$$

$$E_P=(m\omega_0^2/2)\,(\sigma^2+\tfrac{1}{2}\gamma^2\sigma_z^2), \tag{9}$$

$$E_{\mathrm{NL}} = U_0/(2\pi)^{3/2}\sigma^2\sigma_z, \tag{10}$$

and

$$E_{\mathrm{DD}} = \frac{\mu_0\mu^2}{\sqrt{2}\pi^{3/2}\sigma^2\sigma_z}\left\{\frac{1}{2} - \frac{\sigma^2}{3\sigma_z^2}{}_2F_1\left(\frac{3}{2},2;\frac{5}{2};\left[1-\left(\frac{\sigma}{\sigma_z}\right)^2\right]\right)\right\}. \tag{11}$$

Here ${}_2F_1(\alpha,\beta;\zeta;z)$ is a hypergeometric function, and Eq. (3) has been used to calculate the anisotropic contribution (E_{DD}) to the energy. Minimizing this energy functional for a spherically symmetric trap with $\omega_0 = (2\pi)150$ Hz and $N = 300\,000$, we find that the energy becomes unbounded and the system unstable when $a/a_{\mathrm{Na}} \approx 0.94\overline{a_c}$. Additionally, the critical value is quite insensitive to the number of particles: for $N = 10^7$ it is $a/a_{\mathrm{Na}} \approx 0.95\overline{a_c}$. These values are in disagreement with the results of Ref. [1].

We also used a trial wave function

$$|\Psi|^2 = \frac{3}{4\pi z_0\sigma^2}\left[1-\left(\frac{z}{z_0}\right)^2\right]\exp[-(x^2+y^2)/\sigma^2]. \tag{12}$$

At the threshold of instability, this trial wave function seems better justified than the Gaussian trial. Due to the $\cos^2\alpha$ factor in Eq. (3), there is extra repulsion in the z direction, so inverted parabola seems to be a natural guess. In the xy plane, the interaction terms vanish so a Gaussian profile is expected. For the function (12), the kinetic energy diverges so it was left out from the optimization process. Thus this approach is valid only at the Thomas-Fermi limit, i.e., at large particle numbers. We were not able to evaluate all the integrals analytically, so a numerical integration was performed. With this wave function, we estimate that for $N = 300\,000$ the critical value is $a/a_{\mathrm{Na}} \approx 0.96\overline{a_c}$, again quite close to the simple estimate given before.

In Fig. 1, we show the instability threshold calculated with three different methods. It can be seen that each method gives about the same results at large particle numbers. The missing kinetic-energy term for the parabolic-Gaussian trial results in a nonphysical behavior at small particle numbers, but the Gaussian trial gives fairly satisfactory results for all particle numbers. Figure 1 should be contrasted with Fig. 2 of Ref. [1].

Finally, we address the existence of structured dipolar condensates by solving Eq. (1) numerically using the method outlined in Ref. [1]. The largest grid we used had a size $128\times128\times128$, but the results obtained with this grid were not very different from those in a grid with a size $64\times64\times64$. For $N = 300\,000$, we estimate the critical value of the scattering length to be $a/a_{\mathrm{Na}} \approx 0.92\overline{a_c}$. Near the instability threshold, the ground-state wave functions looked roughly parabolic along the z axis and Gaussian in the xy plane. Solutions in the neighborhood of the Ref. [1] instability were consistently found to be unstable, although *transient* structure was observed en route to collapse (at least) when the kinetic-energy term was artificially removed.

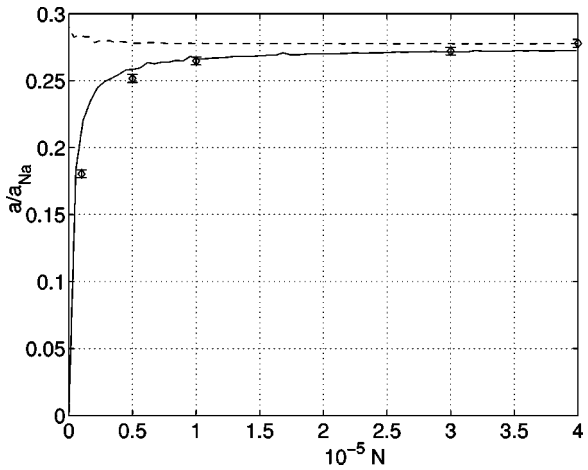

FIG. 1. Instability threshold as a function of the number of particles for a nonideal dipolar condensate of chromium atoms in a spherically symmetric trap with $\omega_0 = (2\pi)150$ Hz. The solid line is based on a Gaussian trial and the dashed line is based on a parabolic-Gaussian trial. Individual data points are numerical solutions of the Gross-Pitaevskii equation with error bars indicated. (The small amount of noise present in the figure is due to the Monte Carlo method used for minimization.)

While it is true that a variational wave function will not deliver any more physics than is already present in the trial wave function, our analytical and numerical results strongly indicate that the numerical instability threshold of Ref. [1] is dubious; furthermore, their structured solutions are not numerically reproducible. In conclusion, we therefore contend that, upon lowering the strength of the contact interaction, a nonideal dipolar BEC reveals an instability threshold that is largely independent of N and given to a good approximation by the intuitive result (6), and the ground-state wave functions at and near this threshold have a simple, single-peak profile.

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