

Ground state of the dipolar Bose-Einstein condensate

T. F. Jiang*

Institute of Physics, National Chiao Tung University, Hsinchu, 300, Taiwan

W. C. Su

Department of Civil Engineering, National Chiao Tung University, Hsinchu, 300, Taiwan

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We present a variational method to study the ground state of the newly realized ^{52}Cr dipolar Bose-Einstein condensate. Besides the usual contact potential term in the mean-field equation, there is an additional long-range and anisotropic dipole-dipole interaction potential. We develop an efficient Newton-Raphson's scheme to solve the condensate state. The solution shows a double-peak feature in the loosely confined dimension. Compared to the existing single-peak calculations, the double-peak solution has lower energy and reflects the distinct property of the dipole-dipole interaction. Our method is easy and efficient to use for future investigations of the dipolar systems.

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I. INTRODUCTION

Since the realization of Bose-Einstein condensation (BEC) of alkali metal atoms in 1995 [1], its explosive progress has made an important impact on science. The contact atomic interaction has played a significant role in systems studied so far. Systems with long-ranged interaction were proposed a few years later [2]. The properties of dipole-dipole forces in an ultracold atomic systems were studied. Yi and You studied the properties of an electric field induced dipolar system [3]. The stability of a dipolar BEC system and the possible species for realization were discussed by Santos *et al.* and by Fischer [4]. Góral and Santos also studied the ground state and excitations of the dipolar BEC [5]. The collapse of dipolar BEC was discussed by Lushnikov [6]. Góral *et al.* studied the dipolar BEC in optical lattice [7]. Dipolar spinor BEC was also investigated recently [8]. Calculations through the quantum hydrodynamics model and by Thomas-Fermi approximations were also carried out [9].

Experimentally, Bose-Einstein condensation for systems with long-ranged interatomic interactions was first realized in 2005 by Stuttgart group with aligned chromium atoms [10]. The ^{52}Cr atom used has permanent magnetic dipole moment M of 6 bohr magneton. In their recent experiment [11], there are 10^5 condensate atoms in an anisotropic trap of frequencies $\omega_x:\omega_y:\omega_z=942:712.5:116.5$ (Hz). The atomic magnetic dipoles are aligned along the y direction by a dc magnetic field, and the s wave scattering wavelength a_s was measured to be 105 bohr radius. Under the mean-field theory, the Gross-Pitaevskii equation (GPE) that describes the BEC is written as

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\vec{r}) + Ng_c n(\vec{r}) + NV_{dd}(\vec{r})\right)\Psi(\vec{r}) = \mu\Psi(\vec{r}). \quad (1)$$

In the GPE, N is the number of condensate atoms, and m is the atomic mass. The trap potential is

$V_{\text{ext}} = \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$, $g_c = \frac{4\pi\hbar^2 a_s}{m}$. The order parameter is normalized as $\int |\Psi|^2 d^3\vec{r} = 1$, and $n(\vec{r}) = |\Psi(\vec{r})|^2$. The dipole-dipole potential V_{dd} with dipoles aligned along the y axis is written as follows:

$$V_{dd}(\vec{r}) = g_d \int \left[\frac{1}{|\vec{r} - \vec{r}'|^3} - \frac{3(y - y')^2}{|\vec{r} - \vec{r}'|^5} \right] |\Psi(\vec{r}')|^2 d^3\vec{r}', \quad (2)$$

where $g_d = \frac{\mu_0 M^2}{4\pi}$. We can see that the interaction potential among atoms becomes *nonlocal* instead of just the pseudo-potential of zero-ranged interaction.

In addition to the nonlocal property in the dipolar potential, the potential is also anisotropic. Along the polarization direction, the forces between dipoles are attractive and are repulsive in the directions perpendicular to the polarization axis. The effect was discussed by Pfau *et al.* [2] and the anisotropic nature was shown for a spherical trap case. The dipole-dipole interaction leads to the result of double-peak in the order parameter along the direction of the repulsive force. To our knowledge, no other theoretical calculations treated this property further because it is not easy to implement double-peak trial functions. In practical experiment [11], the trap is not spherical but is anisotropic. It is tightly confined in the x - and y -directions and loosely confined in the z -direction. Since the dipole-dipole force is much weaker than the confined forces in the x - and y -directions, the dipole-dipole effect is negligible. However, along the z -direction confinement is much weaker and the additional repulsive dipole-dipole force may exhibit double-peak feature in the order parameter under experimental conditions.

We present in this paper a variational study for this property. We found that the double-peak in order parameter will lower down the total energy of the system in comparison with the single Gaussian wave function which has been popularly used in most previous related calculations. Due to the nonlocality, in addition to the nonlinearity in the GPE, the solution of the equation is not straightforward. We present a robust but simple way to obtain the variational solutions. We compare in detail the total energy, chemical potential, order parameter of single peak and double-peak

*Email address: tfjiang@faculty.nctu.edu.tw

trial solutions in the z -direction with experimental parameters. We show that the double-peak order parameter corresponds to the real experiment and it is quite different from the single-peak picture. The method is easy to apply for future dipolar BEC systems.

The layout of the paper is as follows. In Sec. II, we describe the energy variational formulation and introduce our method of calculations. In Sec. III we present our results. The discussion and conclusions are followed in Sec. IV.

II. FORMULATION AND METHOD OF CALCULATION

The GPE of Eq. (1) can be obtained by minimization of the following energy functional per particle with constraint $\int |\Psi|^2 d^3\vec{r} = 1$:

$$E[\Psi] = \int \left(\frac{\hbar^2}{2m} |\nabla\Psi|^2 + V_{ext}(\vec{r})|\Psi|^2 + \frac{Ng_c}{2} |\Psi|^4 + \frac{N}{2} V_{dd}(\vec{r})|\Psi|^2 \right) d^3\vec{r}. \quad (3)$$

In the following, we use $\hbar\omega_y$ as the energy unit, where $\omega_y = 2\pi \times 712.5$ Hz, and $L = \sqrt{\hbar/m\omega_y} = 0.52261$ μm as the length unit. To include the double-peak property in the z -direction, we employ the following trial functions:

$$\begin{aligned} \Psi(x, y, z) &= \phi_1(x)\phi_2(y)\phi_3(z), \\ \phi_1(x) &= (\pi\alpha_1^2)^{-1/4} \exp\left(-\frac{x^2}{2\alpha_1^2}\right), \\ \phi_2(y) &= (\pi\alpha_2^2)^{-1/4} \exp\left(-\frac{y^2}{2\alpha_2^2}\right), \\ \phi_3(z) &= c \exp\left(-\frac{(z-\alpha_4)^2}{2\alpha_3^2}\right) + c \exp\left(-\frac{(z+\alpha_4)^2}{2\alpha_3^2}\right), \end{aligned} \quad (4)$$

where α_i with $i=1,2,3,4$ are the four variational parameters and c is used to normalize $\phi_3(z)$. Here two Gaussian functions with peaks displaced at α_4 with the origin in the z -direction are assumed. To compare with the commonly used variational results, we also perform calculations with $\alpha_4=0$ and then there will be three variational parameters. It corresponds to the usual single-peak Gaussian trial solution. We denote the former calculation by *four-parameter* type and the latter by *three-parameter* type. In the variational calculations, we need to calculate the total energy functional $E[\alpha_i]$ and its derivatives. The minimization conditions are

$$\frac{\partial E}{\partial \alpha_i} = 0, \quad i = 1, 2, 3, 4. \quad (5)$$

To find out the optimum parameters, we need to calculate the energy functional. In the calculation of the kinetic energy term, we transform the trial function in Eq. (4) into momentum space and perform the integration by numerical quadrature. The calculations of trap potential energy and contact

energy terms are numerically straightforward, we use the Gauss-Legendre quadratures [12] for integrations. The calculation of the dipolar energy term in coordinate space is a six-dimensional integral and hence is not easy. To make it feasible, the dipolar energy term is transformed into the momentum space, and the integral becomes three-dimensional. With transformations

$$\begin{aligned} \rho(\vec{k}) &= \int |\Psi(\vec{r})|^2 e^{i\vec{k}\cdot\vec{r}} d^3\vec{r}, \\ V_{dd}(\vec{k}) &= \int V_{dd}(\vec{r}) e^{i\vec{k}\cdot\vec{r}} d^3\vec{r}, \end{aligned} \quad (6)$$

then the dipolar energy term is equal to

$$E_{dd} = \frac{N}{2} \frac{1}{8\pi^3} \int |\rho(\vec{k})|^2 V_{dd}(\vec{k}) d^3\vec{k}. \quad (7)$$

We can calculate the momentum space density function $\rho(\vec{k})$ directly by quadratures. The momentum representation of the dipole-dipole potential has been studied [2,13]. With the dipoles aligned along the y -axis and under the mean-field theory,

$$V_{dd}(\vec{k}) = 4\pi g_d \left[1 - \frac{3k_y^2}{k^2} \right] \left[\frac{\cos(ka)}{(ka)^2} - \frac{\sin(ka)}{(ka)^3} \right]. \quad (8)$$

With these efforts, the dipolar energy term can be calculated efficiently by Gauss-Legendre quadratures too.

The next problem is to find out the variational parameters for a given number of trapped atoms N such that the total energy is minimum. The Newton-Raphson's scheme is useful for the purpose. Let $\alpha_i^{(n)}$ be the value of parameter α_i in the n th iteration, the next iteration value of α_i will be $\alpha_i^{(n+1)}$,

$$\alpha_i^{(n+1)} = \alpha_i^{(n)} - [J^{-1}]_{ij} \left[\frac{\partial E}{\partial \alpha_j} \right]_n; \quad i, j = 1, 2, 3, 4. \quad (9)$$

In the expression, repeated index means summation from 1 to 4. $[J]^{-1}$ is the inverse of the Jacobian matrix $[J]$, where in our problem, the matrix elements of $[J]$ are

$$[J]_{ij} = \frac{\partial^2 E[\Psi]}{\partial \alpha_i \partial \alpha_j}. \quad (10)$$

Even with the simple Gaussian trial functions with single-peak in the z -direction, the analytic expressions for the problem and the Newton-Raphson's scheme is still very hard. An example of an analytic expression of total energy in a cylindrical trap with a two-parameter Gaussian trial function can be found in Ref. [14]. With the double-peak Gaussian in the z -direction, the analytic expression for Newton-Raphson's method becomes even much harder. Our method to the problem is simply using a numerical central difference for the derivatives. For example,

$$\frac{\partial E[\Psi]}{\partial \alpha_i} = \frac{E(\alpha_i + \delta\alpha_i) - E(\alpha_i - \delta\alpha_i)}{2\delta\alpha_i}. \quad (11)$$

We have calibrated our quadrature results of the total energy with the three-parameter trial functions so that the analytic

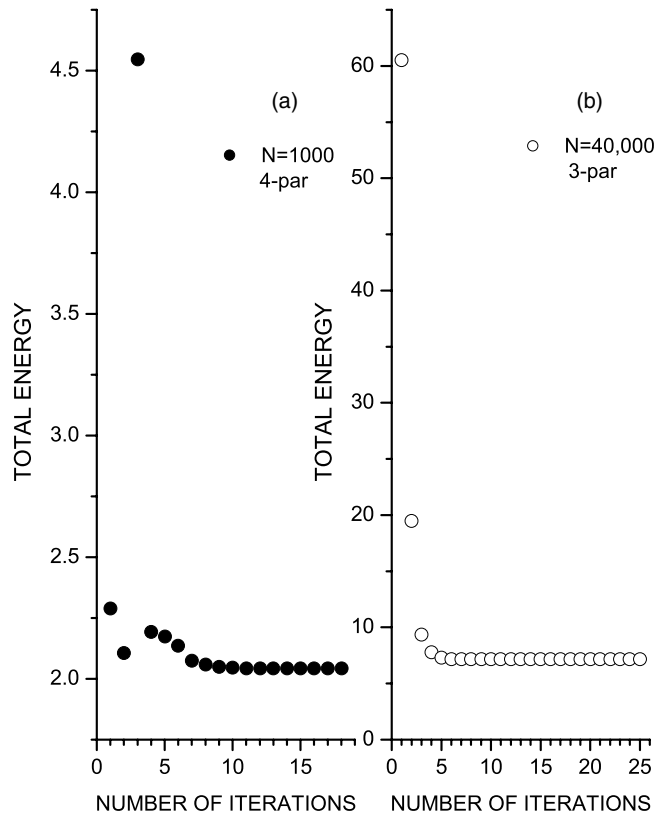


FIG. 1. Examples of convergence. (a) $N=1000$, four-parameter case, and (b) $N=40\,000$, three-parameter case.

results can easily be calculated. The accuracy of our numerical quadratures is to the fifth decimal place with 200 grids in the x - and y -axes, 400 grids in the z -axis. So the numerical derivatives work well. In Fig. 1, we show the examples of iterations for a case of four-parameter and another for three-parameter. Within a few iterations, the convergence is achieved.

III. RESULTS

We present in Table I the results of double-peak, four-parameter calculations, and results of single-peak, three-parameter calculations. In the calculations, we vary the number of atoms from 1000 to 10^5 with experimental parameters of trap frequencies, g_c and g_d . As expected, the tabulated α_1 and α_2 show not much differences in widths of $\phi_1(x)$ and $\phi_2(y)$ for both three-parameter and four-parameter calculations because the dipole-dipole effect is relatively smaller than the confined potential and the contact potential. But the widths in $\phi_3(z)$ do show notable differences; and through the wide range of particle numbers, the total energies of double-peak calculations are lower than the single-peak calculations. However, the difference is not drastic. This is because the energy of trap potential and contact energy terms are an order of magnitude larger than the dipole-dipole term. Here we just perform simulations according to the real experimental parameters. We can expect that if we lower down the trap frequencies and tune the scattering length to a smaller value by the Feshbach resonance method [15], the more dominant

TABLE I. Results of variational calculations. α_1, α_2 are widths of Gaussian density in the x - and in the y -directions, respectively. α_3 in three-parameter calculation is the width of density in the z -direction, while in four-parameter calculations, it is the width of the single Gaussian in a sum of double Gaussians separated at a distance of $2\alpha_4$. The numbers of atoms are from 1000 to 100 000.

$N/1000$	Four-parameter					Three-parameter			
	Etotal	α_1	α_2	α_3	α_4	Etotal	α_1	α_2	α_3
1	2.044	1.031	1.306	3.826	3.995	2.062	1.035	1.313	6.253
5	3.297	1.236	1.679	5.544	5.881	3.338	1.243	1.691	9.180
10	4.202	1.369	1.905	6.452	6.858	4.260	1.378	1.919	10.699
15	4.874	1.462	2.057	7.035	7.483	4.943	1.471	2.073	11.672
20	5.428	1.535	2.174	7.475	7.954	5.505	1.545	2.191	12.405
25	5.905	1.595	2.270	7.832	8.335	5.991	1.606	2.287	12.999
30	6.330	1.648	2.352	8.135	8.659	6.423	1.659	2.370	13.503
35	6.716	1.694	2.424	8.399	8.941	6.814	1.706	2.443	13.942
40	7.070	1.736	2.489	8.633	9.191	7.174	1.748	2.507	14.332
45	7.400	1.774	2.547	8.845	9.417	7.509	1.786	2.566	14.684
50	7.708	1.808	2.600	9.038	9.623	7.822	1.821	2.620	15.006
55	7.999	1.841	2.650	9.216	9.814	8.118	1.854	2.670	15.302
60	8.274	1.871	2.695	9.382	9.991	8.397	1.884	2.716	15.577
65	8.537	1.899	2.738	9.537	10.156	8.664	1.913	2.759	15.835
70	8.787	1.925	2.779	9.683	10.311	8.919	1.939	2.800	16.076
75	9.028	1.950	2.817	9.820	10.457	9.163	1.965	2.838	16.304
80	9.259	1.975	2.853	9.949	10.595	9.397	1.989	2.875	16.520
85	9.482	1.997	2.887	10.075	10.729	9.623	2.012	2.910	16.725
90	9.697	2.019	2.920	10.192	10.854	9.842	2.034	2.943	16.921
95	9.905	2.040	2.952	10.303	10.973	10.053	2.055	2.974	17.109
100	10.106	2.060	2.982	10.411	11.088	10.258	2.075	3.005	17.288

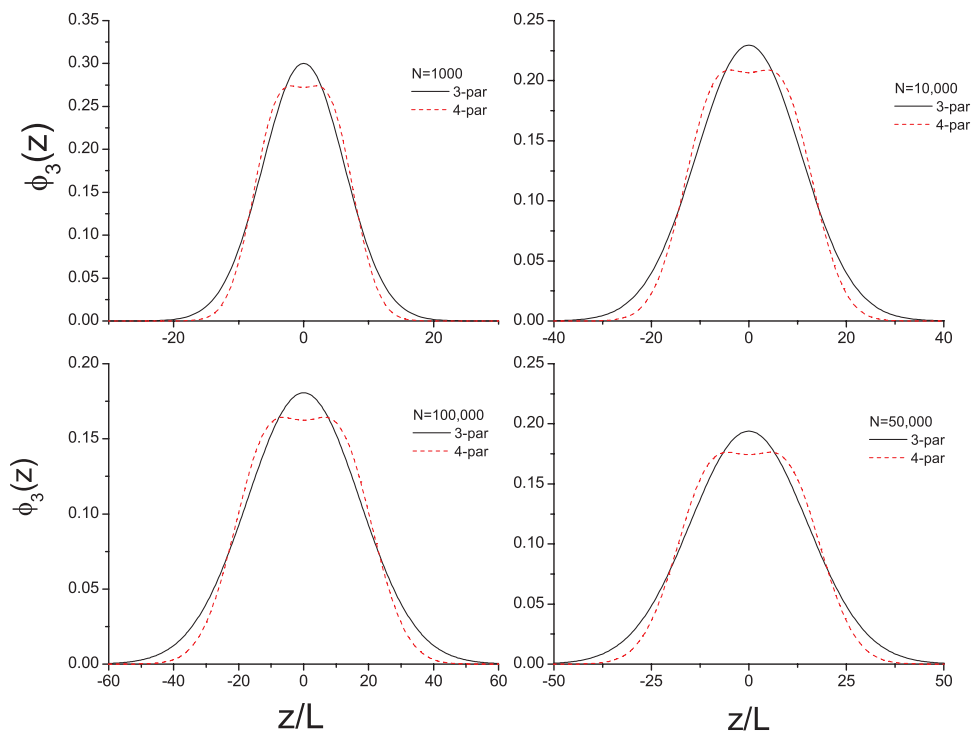


FIG. 2. (Color online) The comparisons of $\phi_3(z)$ for three-parameter (solid line) and four-parameter (dashed line) results with $N=1000$, 10 000, 50 000, and 100 000. The horizontal axis is z in units of $L=0.522\ 61\ \mu\text{m}$, vertical axis is $\phi_3(z)$.

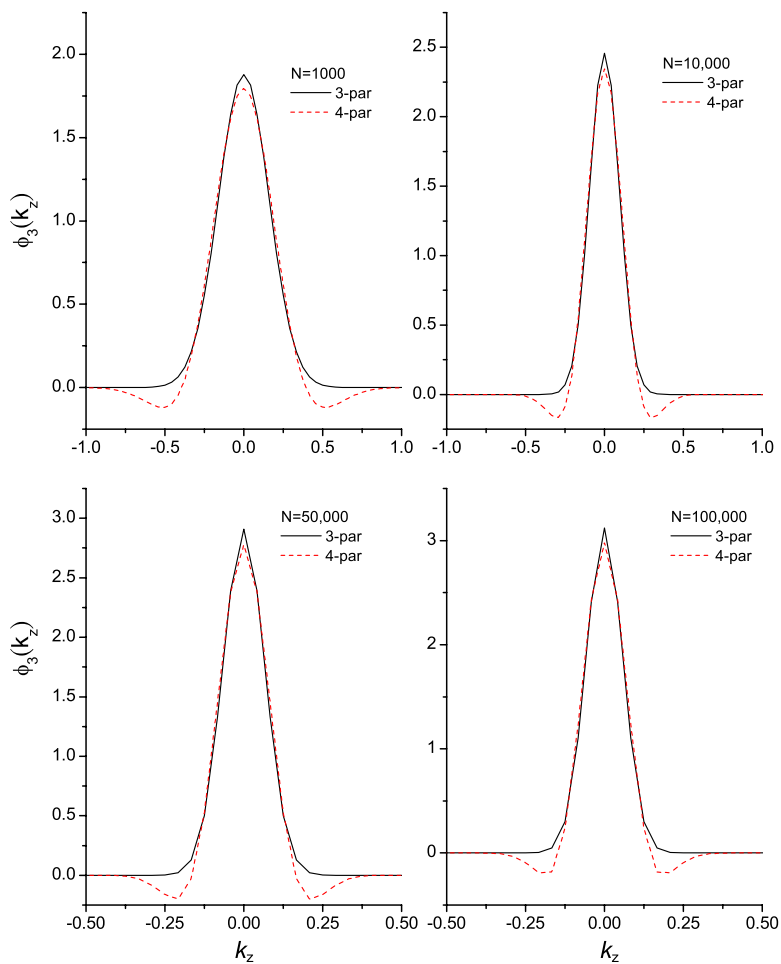


FIG. 3. (Color online) The comparisons of momentum space $\phi_3(k_z)$ for three-parameter (solid line) and four-parameter (dashed line) results with $N=1000$, 10 000, 50 000, and 100 000. The horizontal axis is k_z , and the vertical axis is $\phi_3(k_z)$.

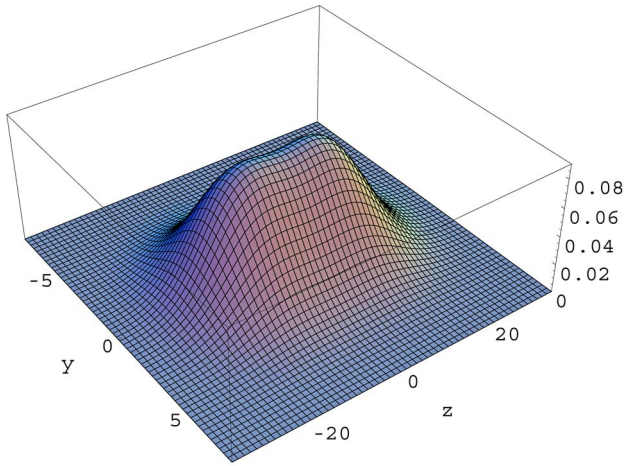


FIG. 4. (Color online) The three-dimensional density plot for the experimental case. The number of atoms is 100 000 and trap frequencies and scattering length were described in Ref. [11]. The dipoles are aligned along the y direction. The coordinates are in units of $\sqrt{\hbar/m\omega_y}=0.522\ 61\ \mu\text{m}$.

role of dipole-dipole effect will emerge from the adjustment.

In Fig. 2, we plot the comparison of order parameter $\phi_3(z)$ for four- and three-parameter calculations with $N=1000$, 10 000, 50 000, and 100 000. The four-parameter results are combinations of two Gaussian functions. The difference in order parameters at $z=0$ is mainly due to the result of the dipole-dipole effect. Also, Fig. 3 shows the corresponding order parameter in momentum space. There are negative values of $\phi_3(k_z)$ for four-parameter results which are very different from three-parameter results. Corresponding to the experimental case with 100 000 ^{52}Cr atoms trapped and aligned in the y direction [11], we plot the density as a function of y and z (see Fig. 4). The trap is far more loosely confined in the z direction and the dipole-dipole repulsions among atoms exhibit the notable double-peak structure in density. This is a

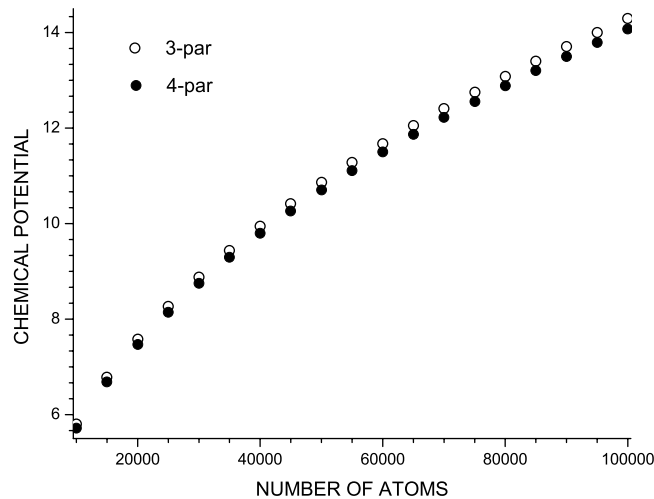


FIG. 5. The chemical potential as a function of number of condensate atoms. Solid dots are results of four-parameter calculations while empty dots are three-parameter results.

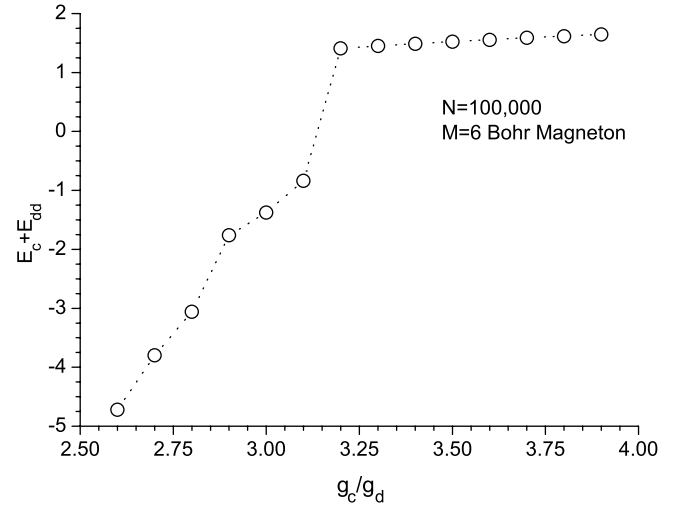


FIG. 6. The interaction energy of the dipolar BEC vs the ratio of g_c/g_d . For a ratio less than 3.2, the interaction energy becomes negative and instability may happen. The parameter g_d is fixed with the atomic magnetic dipole moment of a chromium atom. g_c is adjusted by the Feshbach resonance technique.

very unique feature of dipolar BEC that does not appear in BEC systems without the long-ranged interaction.

We show in Fig. 5 the chemical potentials from both calculations. The chemical potential can be derived as

$$\mu = \int \left(\frac{\hbar^2}{2m} |\nabla\Psi|^2 + V_{ext}(\vec{r})|\Psi|^2 + Ng_c|\Psi|^4 + NV_{dd}(\vec{r})|\Psi|^2 \right) d^3\vec{r}. \quad (12)$$

We can see that there are visible differences for double-peak and single-peak results for all N . The double-peak chemical potential is smaller than single-peak for each N . It means variationally that the four-parameter results are better than the three-parameter ones.

One question that naturally happens is how reliable is the simple double-peak trial function? To shed some light on this, we perform many-Gaussian trial functions for the cases of $N=1000$ and $N=10^5$. We make an expansion with three sets of four-parameter Gaussian trial functions:

$$\Psi(x, y, z) = \phi_1(x)\phi_2(y)\phi_3(z),$$

$$\phi_1(x) = \sum_{i=1}^3 a_i \exp\left(-\frac{x^2}{2\alpha_i^2}\right),$$

$$\phi_2(y) = \sum_{i=1}^3 b_i \exp\left(-\frac{y^2}{2\beta_i^2}\right),$$

$$\phi_3(z) = \sum_{i=1}^3 c_i \left[\exp\left(-\frac{(z-\gamma_i)^2}{2\delta_i^2}\right) + \exp\left(-\frac{(z+\gamma_i)^2}{2\delta_i^2}\right) \right]. \quad (13)$$

We obtain the value of total energy as 2.043 83 compared to the single set of four-parameter 2.0443 for $N=1000$, and to-

tal energy of 10.0708 vs 10.1063 for $N=100\,000$. Thus we conclude that the four-parameter model is satisfactory for dipolar BEC.

With the method described above, we now turn to the instability problem of the dipolar BEC system. As shown in [1], the instability will occur when the mutual atomic interaction becomes attractive. Then due to the increase of three-body collisional loss, the BEC may collapse. In the ^{52}Cr dipolar system, the contact interaction energy $E_c = \frac{1}{2}Ng_c \int |\Psi|^4 d^3\vec{r}$ is repulsive with positive g_c , while the dipole-dipole energy term E_{dd} is attractive. A predicted criterion of the instability, $g_c/g_d < 4\pi/3$ can be found in [2,6] for instance. Since the scattering length can be tuned by the Feshbach resonance technique, we perform our calculation with experimental g_d and adjust the scattering length near the criterion region. In Fig. 6, we show the results with 100 000 atoms (which is in the Thomas-Fermi regime). The total interaction energy $E_c + E_{dd}$ becomes negative for $g_c/g_d < 3.2$. This is quite close to the estimated criterion condition while the calculation here is in realistic experimental parameters.

IV. DISCUSSIONS AND CONCLUSIONS

In the past few years, simple single-peak Gaussian trial functions are used to model the order parameter of dipolar BEC. From our study, we find that the double-peak order parameter is a special property of dipolar BEC. We present a simple but efficient method to perform the variational calculation of its ground state. Our simulation results agree with the real experimental parameters. Due to the relatively larger trap potential and contact potential in comparison to the dipole-dipole potential, the double-peak property does emerge but is not drastically dominant. For the future dipolar systems, the dipole-dipole effect may become dominant if the physical conditions are adjusted. The method can be applied to future systems straightforwardly.

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