On the applicability of the classical dipole-dipole interaction for polar Bose-Einstein condensates.

Vladimir V. Konotop

Departamento de Física e Centro de Física da Matéria Condensada, Universidade de Lisboa, Complexo Interdisciplinar, Av. Prof. Gama Pinto, 2, Lisbon, P-1649-003 Portugal

Víctor M. Pérez-García

Departamento de Matemáticas, E.T.S.I. Industriales, Universidad de Castilla-La Mancha, Avda. Camilo José Cela, 3, Ciudad Real, 13071 Spain.

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We argue that the classical form of the dipole-dipole interaction energy cannot be used to model the interaction of the bosons in a dilute Bose-Einstein condensate made of polar atoms. This fact is due to convergence of integrals, if no additional restrictions are introduced. The problem can be regularized, in particular, by introducing a hard sphere model. As an example we propose a regularization consistent with the long range behavior of the effective potential and with the scattering amplitude of the fast particles.

The first clear observation of pure Bose-Einstein condensation was done using a ultracold gas of neutral bosonic atoms[1]. After these remarkable experiments an explosive growth of the interest on the subject happened[2]. Following the experimental guidelines, the theoretical analysis of the problem concentrated on condensates made of alkaline atoms (neutral and nonpolar) interacting collisionally through s-wave spherically symmetric effective potentials, which lead to an interaction proportional to the local atomic density.

Although this description of the problem captures most of what has been done experimentally up to now, very recently there has been increased interest on other, more complex, interactions. Specifically, there has been some interest on nonlocal interactions (see e.g. [2] and references therein). In fact any realistic interaction should always be nonlocal due to the fact that the range of interaction is not zero. Another situation corresponds to nonsymmetric and nonlocal interactions considered in Refs. [3–7], such as those which appear when the bosons inside the condensate are polar molecules (with permanent or externally induced dipole moments). The possibility of finding condensates with nonsymmetric interactions is very interesting since it would lead to a bunch of new phenomena and many possibilities for control.

In all the previously cited cases the model for the dynamics of the system is the zero temperature mean field theory, i.e. a Gross-Pitaevskii equation, for the condensate dynamics

\[ \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \Psi + \frac{1}{2} m \omega_0^2 (x^2 + y^2 + \gamma^2 z^2) \Psi \\
+ \frac{4\pi \hbar^2 a}{m} |\Psi|^2 \Psi + \left( \int V(r, r') |\Psi(r')|^2 \, dr' \right) \Psi. \]

where \( \Psi \) is the condensate wavefunction normalized to the total number of particles,

\[ N = \int dr |\Psi(r)|^2, \]

\( a \) is the s-wave scattering length and \( V \) is a real function taking into account the nonlocal part of the interactions. Of course, \( V \) vanishes or is very small when the interactions are purely local. When the interactions are mediated by dipoles, they are supposed to be long range. In such situation it is proposed that the interaction is ruled by a potential of the type \[ \frac{\mu_0}{4\pi} \frac{d(r)d(r') - 3(d(r)e_r)(d(r')e_r)}{|r - r'|^3} \]

where \( e_r = (r - r')/(|r - r'|) \) and \( d(r) \) is the dipole moment at point \( r \). The simplest version of Eq. (3), where \( d(r) \equiv d \) is homogeneous and the potential can be considered as a function of relative distances only, has the form

\[ V(r - r') = \frac{\mu_0 d^2}{4\pi} \frac{1 - 3 \cos^2 \theta}{|r - r'|^3}, \]

where \( \cos \theta = e_d \cdot e_r \). In some cases [8], instead of the simple angular dependence \( 1 - 3 \cos^2 \theta \), which is proportional to the spherical harmonic \( Y_{20} \) more complex dependencies in the form of a finite combination of spherical harmonics may appear.

It is our intention in this brief report to show that all those potentials lead to a singular (in mathematical sense) interaction which must be regularized to give physically acceptable results. This situation is not surprising if one takes into account that even in classical theory (i) Eq. (3) is an asymptotics of the dipole-dipole interactions (see e.g. [8]) and thus fails in the near zone, and (ii) Eq. (3) displays the realistic dipole-dipole interaction while \( V(r) \) in [3] is an effective potential obtained within the mean field theory.

To simplify the analysis, let us first consider the solution of the Gross-Pitaevskii equation with an interaction
term of the form $\frac{1}{r}$. Then the nonlinear nonlocal term is proportional to the integral

$$I(r) = \int d\mathbf{r}' \frac{1 - 3 \cos^2 \theta}{|\mathbf{r} - \mathbf{r}'|^3} J(\mathbf{r}')$$

being $J(\mathbf{r}') = |\Psi(\mathbf{r}')|^2$. Taking into account that due to the presence of the trap and the finite norm of the solution the wave function decays as $|\mathbf{r}| \to \infty$, the only point where the integral may lead to a singular behavior is $\mathbf{r}' = \mathbf{r}$, thus we will employ spherical coordinates and estimate the integral in the $\epsilon$-vicinity of $\mathbf{u} \equiv \mathbf{r} - \mathbf{r}'$. To do so we split (hereafter $d\Omega = \sin \theta d\theta d\phi$)

$$I(r) = \left( \int_0^\epsilon + \int_\epsilon^\infty \right) \frac{du}{u} \int d\Omega (1 - 3 \cos^2 \theta) J(u + r)$$

$$= I_e(r) + Q(r).$$

(6)

The singular behavior, if present, may only be due to the contribution of $I_e(r)$ for which we have the following set of estimates

$$I_e = \int_0^\epsilon \frac{du}{u} \int d\Omega (1 - 3 \cos^2 \theta) J(u + r)$$

$$= \int_0^\epsilon \frac{du}{u} \int d\Omega (1 - 3 \cos^2 \theta) \left[ J(r) + (u \nabla) J(r) + O(u^2) \right]$$

$$= \int_0^\epsilon \frac{du}{u} \int d\Omega (1 - 3 \cos^2 \theta) J(r) + O(1).$$

(7)

Taking into account that $J(r)$ does not depend on the integration variable one gets an indetermination of type $0 \times \infty$ which cannot be avoided because the order of integration is not defined (and should not be relevant in a physically meaningful model). This is the first indication that there may be problems with the type of nonlocal interaction kernels considered.

To rule out the possibility that the singular behavior previously found is a product of the specific orientation of the dipoles chosen (i.e. all of them parallel) we consider now a general situation. Let us first define a new function

$$\Delta(\mathbf{r}, \mathbf{u}) = \mathbf{d}(\mathbf{r} + \mathbf{u}) - \mathbf{d}(\mathbf{r}).$$

(8)

With this definition we may write

$$I(r) = \int d\mathbf{u} J(r + \mathbf{u})$$

$$= \int d\mathbf{u} \frac{\mathbf{d}(\mathbf{r})(\mathbf{d}(\mathbf{r} + \mathbf{u}) - 3(\mathbf{d}(\mathbf{r})\mathbf{e}_r)(\mathbf{d}(\mathbf{r} + \mathbf{u})\mathbf{e}_r)}{u^3}$$

$$= \int \frac{du}{u^3} J(r + \mathbf{u}) \left[ \mathbf{d}(\mathbf{r})\mathbf{d}(\mathbf{r}) - 3(\mathbf{d}(\mathbf{r})\mathbf{e}_r)(\mathbf{d}(\mathbf{r})\mathbf{e}_r) \right. $$

$$+ \Delta(\mathbf{r}, \mathbf{u}) \mathbf{d}(\mathbf{r}) - 3(\Delta(\mathbf{r}, \mathbf{u})\mathbf{e}_r)(\mathbf{d}(\mathbf{r})\mathbf{e}_r) \right].$$

(9)

Let us formally split this integral into two parts, $I(r) = I_0(r) + I_1(r)$. The first one

$$I_0(r) = \int \frac{du}{u^3} J(r + \mathbf{u}) \left[ \mathbf{d}(\mathbf{r})\mathbf{d}(\mathbf{r}) - 3(\mathbf{d}(\mathbf{r})\mathbf{e}_r)(\mathbf{d}(\mathbf{r})\mathbf{e}_r) \right]$$

$$= d^2(r) \int \frac{du}{u} d\Omega J (r + \mathbf{u}) \left[ 1 - 3 \cos^2 \theta \right]$$

(10)

is of the same type as Eq. (5) and leads to an indetermination. The second contribution to $I(r)$ is

$$I_1(r) = \mathbf{d}(\mathbf{r}) \int \frac{du}{u} d\Omega J (r + \mathbf{u}) \left[ \Delta(\mathbf{r}, \mathbf{u}) - 3(\Delta(\mathbf{r}, \mathbf{u})\mathbf{e}_r)(\mathbf{d}(\mathbf{r})\mathbf{e}_r) \right].$$

(11)

Let us define

$$I_2(r) = \int \frac{du}{u} d\Omega J (r + \mathbf{u}) \Delta(\mathbf{r}, \mathbf{u}).$$

(12)

Then we may write

$$I_1(r) = \mathbf{d}(\mathbf{r}) \left[ I_2(r) - 3(I_2(\mathbf{r})\mathbf{e}_r)(\mathbf{d}(\mathbf{r})\mathbf{e}_r) \right].$$

(13)

Thus if $I_2$ is convergent one may ensure convergence of $I_1$ or equivalently $I_0$. Assuming that $\mathbf{d}(\mathbf{r})$ is a differentiable function and expanding in Taylor series we find that $\Delta(\mathbf{r}, \mathbf{u}) = O(u)$ and thus the singular behavior for small $u$ values is avoided. Thus the convergence of the integral depends on the contribution of $I_0(r)$. This means that the consideration in what follows can be restricted to the model (6) without restriction of generality.

As we have commented above the integral $I_0(r)$ is not well defined. Let us show, however that the problem may be regularized. Indeed, assuming that the dipole-dipole interaction is cut off at some distance $a_c$ one has to substitute the lower limit in (6) by $a_c$ what will lead to the result of integration which is not divergent at $a_c \to 0$.

Mathematically

$$I_0(r) = d^2(r) \int_{a_c}^\infty \frac{du}{u} \int d\Omega J (r + \mathbf{u}) \left[ 1 - 3 \cos^2 \theta \right]$$

is uniformly bounded with respect to $r$. The contribution of the small scale of the integral can be estimated as before by expanding $J(\mathbf{r})$ as

$$\int_{a_c}^\epsilon \frac{du}{u} \int d\Omega (1 - 3 \cos^2 \theta) J(r) + O(1)$$

$$= J(r)(\log a_c) \int d\Omega (1 - 3 \cos^2 \theta) + O(1) = O(1),$$

(15)

In fact one may easily prove that the result may be expanded in power series of $a$ as

$$I_0(r) = I_0^r(r) + a_c I_0^c(r) + ...$$

(16)

so that, in the limit $a_c \to 0$ one gets a finite value for $I_0(r)$.

The fact that the integral is well behaved when a cutoff is used is the reason why no divergences were observed in numerical studies (6) (7). The use of any computational mesh introduces a cutoff related to the mesh size which is effectively equivalent to introducing the hard sphere radius.

The cut-off model, although the most straightforward way of avoiding singularities of the problem is not the
most natural one, from the physical point of view. Indeed, this is not properly a “hard sphere” model which is often used in physics, since the respective cut-off is not introduced in the self-interaction term. Thus such a cut-off corresponds to zero dipole-dipole interaction at small distances which is not correct from the physical point of view.

In order to propose another way of regularization in the case at hand we take into account that in the field theory dipoles appear as an artifact of the energy expansion with respect to a small parameter \( r_d/r \) where \( r_d \) is a characteristic dimension of the dipole (for the next terms of the expansion one has to compute multipolar terms). The complete potential energy is just made of two-particle Coulomb interactions. This imposes the first requirement: the singularity of the potential must be of the \( 1/r \)-type when the distance between two particles goes to zero. The second requirement is a “free” parameter which describes the size of the transition region between \( 1/r \) and \( 1/r^3 \) laws (this is the parameter which substitutes the scattering length arising in the theory including only local interactions). The third requirement is that in the limit \( r \to \infty \) the potential must acquire the form (3). Finally, the potential must be differentiable in the whole space (except the origin). A simple form which satisfies all these requirements is

\[
V(r) = -\frac{\mu_0 d^2}{4\pi} \left( \exp\left(\frac{r^2}{a_d^2}\right) - 1 \right) \frac{1 - 3 \cos^2 \theta}{r^3}
\]  

where \( a_d \) is a constant.

A natural question which appears after the regularized potential is introduced is how it affects the results obtained, so far. First of all we mention that (4) with the potential (17) without cutoff does not allow plane wave solutions, just because the respective integrals diverge (and not because of instability). Introducing a cutoff does not change the situation since it makes the equation explicitly spatially dependent and so it still has no plane wave solutions.

It is easy to see that one of the main effects of regularization is the effect on the collapse or blow-up phenomenon. Namely, we are going to show now that any kind of cutoff prevents collapse. First however, we point out a heuristic argument in favor of our statement. The model (3), which is not regularized, is formally invariant with respect to the renormalization \( \Psi \to \Psi/L, r \to Lr, t \to L^2 t \) (see e.g. (11)) while any kind of regularization breaks this symmetry indicating the possibility of existence of a ground state solution. Such a solution (if any) will be stable if the respective Hamiltonian has a lower bound at constant number of particles.

So we now proceed to prove that such a bound in the case of positive (or zero) scattering length exists (12). As a matter of fact after introducing a regularized potential the proof of the stability is reduced to one given in (11). Indeed considering Eq. (11) and using appropriate dimensionless variables one can write down an associated Hamiltonian in the form

\[
H = \int \left( |\nabla \psi|^2 + |\psi|^4 + V(r)|\psi|^2 \right) dr - \int dr \int dr' |\psi(r)|^2 |\psi(r')|^2 \frac{f(r-r')}{|r-r'|} \]

Any regularization satisfying the conditions imposed above satisfies also the constraint

\[
|f(r)| \leq f_0 < \infty,
\]

where \( f_0 = \text{const.} \) For instance this condition is strictly satisfied by regularization (17). We would like to stress the essential fact that the particular function \( f(r) \) used to regularize is not essential provided Eq. (19) is satisfied (for example, the cut-off model also satisfies this requirement, as well).

Finally

\[
H \geq \|\nabla \psi\|^2_2 - 2f_0 \|\nabla \psi\|_2 \|\psi\|^2_2 \geq -f_0^2 N^3,
\]

and thus the Hamiltonian is bounded below, i.e. strict collapse is not possible. Of course some tendency of the system to compress would be observed in the dynamics.

To conclude, in this report we have shown that the classical dipole-dipole interaction given by Eq. (3) is not consistent and must be regularized somehow to take into account the divergence near the origin. Fortunately the model is well behaved in the sense that it is possible to regularize in several reasonable (and physically meaningful) ways. In fact the usual numerical treatment of the problem includes implicitly a regularization which is why previous works with this interactions did not show up the bad-possessed of the nonregularized model.

Finally we have shown that any reasonable choice of the regularization leads to a suppression of the collapse in the sense that the ground state of Eq. (11) exists. Of course the effect of other physical terms should be taken into consideration and depending on the scale at which collapse is stopped the tendency to shrink the solutions could lead to an effective depletion of the condensate even in this case in which strict collapse is not possible.

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+ Electronic address: konotop@cii.fc.ul.pt

* Electronic address: vperez@ind-cr.uclm.es

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[12] This results means that the instability and collapse reported in [3] and [5] are related to the anomalously strong singularity (of 1/r^3 type) of the potential at the origin. As we have commented before this behavior is nonphysical for small r and collapse would probably be stopped. This fact does not rule out however the possible existence of some shrinking tendency of the atomic cloud for some spatial scales.