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Original Article

Location of Interface Bose-Einstein Condensate Mixtures in Finite Space Under Neumann Boundary Condition

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Abstract: In this work we proposed a simple method to determine the coordinate of interface of two-component Bose-Einstein condensates (BECs) in double parabola approximation (DPA) under Neumann boundary conditions. Based on this idea, the static properties of BECs have been investigated totally in DPA.

Keywords: Bose-Einstein condensates, double-parabola approximation, interface, Neumann boundary condition.

1. Introduction

It is well-known that the ground state of a two-component Bose-Einstein condensate (BECs) is determined by coupled Gross-Pitaevskii (GP) equations [1, 2]. In case of an immiscible BECs, an interface is formed and a phase of separation is established [3].

The interface of BECs is characterized by several quantities, such as, thickness, position, penetration length, etc. These characteristics strongly affect to both statistical and dynamic properties of the system. We start here with the simplest quantity of the interface, which is the position. A question arises naturally is that how to determine the position of the interface of BECs? In a homogeneous BECs, which is recently created by a uniform (flat-bottom) optical-box traps [4], the position of interface can be easily chosen at the origin. In case of inhomogeneous BECs, for example, BECs in the finite [5] or semi-infinite space [6], the position of interface becomes a difficult problem.

The reason for this fact is that the GP equations cannot be solve analytically. The first solution to this problem is numerical computation [7, 8]. The disadvantages of this method are, of course, we cannot obtain an equation for position of the interface and therefore other quantities is also calculated

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numerically. Two noticeable approximate approaches were proposed to deal with this problem, namely, interpolation [9] and double parabola approximation (DPA) developed by Joseph et al., [10]. However, position of the interface was only determined for the symmetric case. In general case, the numerical computation was invoked. In this work, we introduced a simple way to find position of the interface within DPA under Neumann boundary condition.

2. Research Content

To begin with, we consider a system of BECs confined between two parallel plates. These plates are separated at distance $2h$ perpendicular to *z*-axis. Along to (*x*, *y*)-directions, system is translational invariance (Fig. 1).

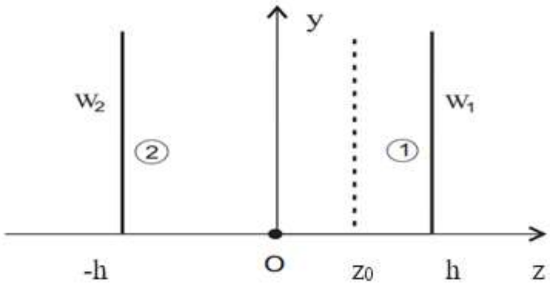

Figure 1. Two hard walls W_1, W_2 are located at $z = \pm h$ and the interface at $z = z_0$.

The stable criterion requires that the area A of each plate is very large compared with square of the distance between plates, i.e., $A : 4h^2$ [11]. As mentioned above, at zero temperature and without external field, the ground state can be described by coupled GP equations [2],

$$-\frac{\hbar^2}{2m_1}\frac{d^2\psi_1}{dz^2} - \mu_1\psi_1 + g_{11}\psi_1^3 + g_{12}\psi_1\psi_2^2 = 0, \tag{1a}$$

$$-\frac{\hbar^2}{2m_2}\frac{d^2\psi_2}{dz^2} - \mu_2\psi_2 + g_{22}\psi_2^3 + g_{12}\psi_1^2\psi_2 = 0. \tag{1b}$$

in which $\hbar$ is reduced Planck constant, m_j and μ_j are mass and chemical potential of component j, respectively. The coupling constants are defined as

$$g_{jj'} = 2\pi\hbar^2\left(\frac{1}{m_j} + \frac{1}{m_{j'}}\right)a_{jj'}, \tag{2}$$

with $a_{jj'}$ being the s-wave scattering length between components j and j' ($j, j' = 1, 2$).

Let origin be at the middle point between two plates, boundary condition for wave function is imposed:

- At hard wall $1\left(z = +h\right)$

$$\frac{\partial\psi_1(+h)}{\partial z} = 0, \tag{3a}$$

$$\psi_2(+h) = 0. \tag{3b}$$

- At hard wall 2 $(z=-h)$

$$\psi_1(-h)=0, \tag{3c}$$

$$\frac{\partial\psi_2(-h)}{\partial z}=0. \tag{3d}$$

To seek simplification, we introduce dimensionless coordinate $\tilde{z}=\dfrac{z}{\xi_1}$ with $\xi_j=h/\sqrt{2m_j g_{jj} n_{j0}}$ healing length, n_{j0} is bulk density of component j. The reduced order parameter $\phi_j=\psi_j/\sqrt{n_{j0}}$, $\xi=\xi_2/\xi_1$ are used.

At the two-phase coexistence, pressure in bulk of both components is equal, so that interspecies interaction can be characterized by a control parameter

$$K=g_{12}/\sqrt{g_{11}g_{22}} \tag{4}$$

Using Eqs. (2) and (4) one can rewrite GP equations (1) in dimensionless form

$$-\partial^2_{\tilde{z}}\phi_1-\phi_1+\phi_1^3+K\phi_2^2\phi_1=0, \tag{5a}$$

$$-\xi^2\partial^2_{\tilde{z}}\phi_2-\phi_2+\phi_2^3+K\phi_1^2\phi_2=0. \tag{5b}$$

and the boundary condition (3) reduces to

$$\frac{\partial\phi_1(+\tilde{h})}{\partial\tilde{z}}=0, \tag{6a}$$

$$\phi_2(+\tilde{h})=0. \tag{6b}$$

$$\phi_1(-\tilde{h})=0, \tag{6c}$$

$$\frac{\partial\phi_2(-\tilde{h})}{\partial\tilde{z}}=0. \tag{6d}$$

in which $\tilde{h}=h/\xi_1$.

Now we solve this problem in DPA. The condensate 1 is assumed to occupy the right half space and the remainder for component 2. Two components of condensate are separated by the interface locating at z_0. At this stage, we recall results for wave functions of ground state, which have found in [5]. Within DPA, Eqs. (5) have the form

$$-\partial^2_{\tilde{z}}\phi_1+\alpha^2(\phi_1-1)=0, \tag{7a}$$

$$-\xi^2\partial^2_{\tilde{z}}\phi_2+\beta^2\phi_2=0, \tag{7b}$$

in the right-hand side and in the left-hand side

$$-\partial^2_{\tilde{z}}\phi_1+\beta^2\phi_1=0, \tag{8a}$$

$$-\xi^2\partial^2_{\tilde{z}}\phi_2+\alpha^2(\phi_2-1)=0, \tag{8b}$$

in which $\alpha=\sqrt{2},\beta=\sqrt{K-1}$. It is obvious that Eqs. (7) and (8) are not couple. Solutions for Eqs. (7) with constraint of the boundary condition (6) have the form

$$\phi_1=1+A_1\left(e^{\sqrt{2}(2\tilde{h}-\tilde{z})}+e^{\sqrt{2}\tilde{z}}\right), \tag{9a}$$

$$\phi_2 = -2A_2 e^{\frac{\tilde{h}}{\xi}} \sinh\left[\frac{\beta\left(\tilde{h}-\tilde{z}_0\right)}{\xi}\right], \quad (9b)$$

Similarly, Eqs. (8) gives

$$\phi_1 = B_1 e^{-\beta\left(2\tilde{h}+\tilde{z}_0\right)}\left(-1+e^{2\beta\left(\tilde{h}+\tilde{z}_0\right)}\right), \quad (10a)$$

$$\phi_2 = 1 + B_2\left(e^{\frac{\sqrt{2}\tilde{z}_0}{\xi}} + e^{-\frac{\sqrt{2}\left(2\tilde{h}-\tilde{z}_0\right)}{\xi}}\right), \quad (10b)$$

Note that A_1, A_2, B_1 and B_2 in Eqs. (9) and (10) are integral constants. In principle, these constants can be evaluated by request that both the wave functions and their first derivatives to be continuous at $\tilde{z}_0$. The results are shown in Appendix.

We now focus on herein main objective, which is how to determine position of the interface. No later than proposed, the DPA has been widely applied to investigate BEC(s) in both homogenous and inhomogeneous systems. In the homogenous BECs, the interface can always be chosen at the origin [10]. In a semi-infinite system of Bose gases, the position of interface was studied in both GP theory [12] and DPA [6]. In our previous work [5], this position was pointed out by solving numerically the coupled GP equations (5). It is obvious that those problems were not thoroughly solved. A simple method is proposed by Joseph et al., [13]. In this method, the wave functions are requested to be the same at thematching point $\tilde{z}_0$,

$$\phi_1(\tilde{z}_0) = \phi_2(\tilde{z}_0). \quad (11)$$

Plugging Eqs. (9) and (10) in to (11) one arrives at

$$1 + A_1\left(e^{\sqrt{2}\left(2\tilde{h}-\tilde{z}_0\right)} + e^{\sqrt{2}\tilde{z}_0}\right) + 2A_2 e^{\frac{\tilde{h}}{\xi}} \sinh\left[\frac{\beta\left(\tilde{h}-\tilde{z}_0\right)}{\xi}\right] = 0. \quad (12)$$

Using Eq. (12) we can investigate the dependency of the interface location on the system parameters such as the K interaction constant and the characteristic length ratio ξ.

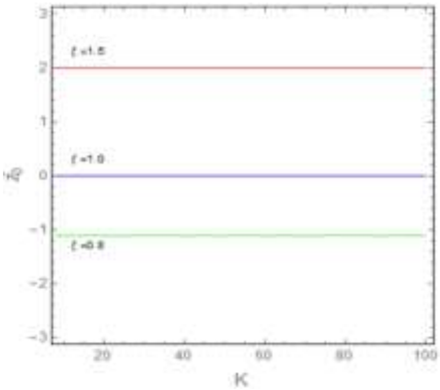

Figure 2. (Color online). The dependence of $\tilde{z}_0$ on the value K with $h=10$. The red, blue and green lines correspond to $\xi = 1.5, 1.0$ and 0.8.

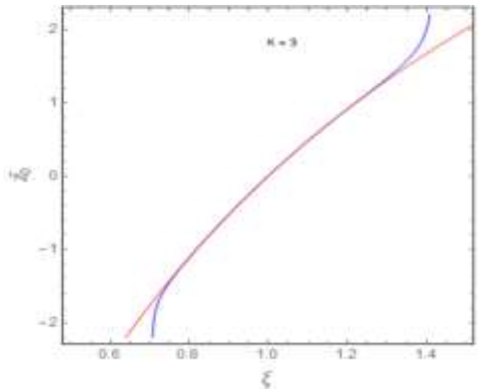

Figure 3. (Color online). The dependence of $\tilde{z}_0$ on the value ξ at $K = 3, h = 10.$ The blue and red lines correspond, respectively, to Neumann and Dirichlet BCs.

Figure 2 and 3 tell us that:

- Position of the interface depends weakly on the coupling constant K.
- Position of the interface depends strongly on the characteristic length ratio ξ.
- Position of the interface depend on boundary conditions which we consider.
- The symmetric case: this case is defined by unity value of the healing length ratio. The solid curve in Figure 2 shows that the interface locates at the middle with $\tilde{z}_0 = 0.$
- The asymmetric case: this happens for $\xi_1 \neq \xi_2$ the interface moves to the half-space corresponding to the component with smaller healing length.

3. Conclusion

In forgoing section, the ground state of two-component BECs is totally determined by DPA with Neumann boundary conditions. A progress is archived by DPA is that the position of interface by requiring that at the matching point, not only the wave functions and their first derivative are continuous, but also the wave functions are the same value. By this way, the ground state of a two-component BECs can be completely considered by DPA. Comparing with the same problem investigated before where the position of interface was investigated by numerical computation, our work can be seen as an achievement. By the way, we should note that in our previous work, the position of interface was found by numerical calculation, in which the particle number is fixed, i.e. the canonical ensemble was employed, whereas only grand canonical ensemble was invoked in this work.

In this work, we investigated the location dependence of the interface on system parameters such as the K interaction constant, the ξ characteristic length ratio, boundary condition. These results allowed us to investigate in detail the wetting transition of the system.

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Appendix: Integral constants

The continuity of the wave functions and their first derivative is

$$\left(\frac{d\phi_j}{d\zeta}\right)_{\zeta=\zeta_0-0} = \left(\frac{d\phi_j}{d\zeta}\right)_{\zeta=\zeta_0+0}. \quad \text{(A1)}$$

$$\phi_j(\zeta_0-0) = \phi_j(\zeta_0+0). \quad \text{(A2)}$$

Substituting Eqs. (9a, 9b, 10a, 10b) into Eqs. (A1, A2) we finds

$$A_1 = -\frac{\sqrt{2}\mathrm{e}^{\sqrt{2}l+h\beta}\left(1+\mathrm{e}^{2(h+1)\beta}\right)\beta}{\sqrt{2}\mathrm{e}^{h\beta}\left(\mathrm{e}^{2\sqrt{2}h}+\mathrm{e}^{2\sqrt{2}l}\right)\left(1+\mathrm{e}^{2(h+1)\beta}\right)\beta+4\mathrm{e}^{l\beta}\left(\mathrm{e}^{2h\left(\sqrt{2}+\beta\right)}-\mathrm{e}^{2\sqrt{2}l+2h\beta}\right)\sinh\left[\left(h+1\right)\beta\right]},$$

$$A_2 = \frac{\mathrm{e}^{-\frac{h\beta}{\xi}}\left(1-\mathrm{e}^{\frac{2\sqrt{2}(h+1)}{\xi}}\right)}{\sqrt{2}\left(1+\mathrm{e}^{\frac{2\sqrt{2}(h+1)}{\xi}}\right)\beta\cosh\left[\frac{(h-1)\beta}{\xi}\right]+2\left(-1+\mathrm{e}^{\frac{2\sqrt{2}(h+1)}{\xi}}\right)\sinh\left[\frac{(h-1)\beta}{\xi}\right]},$$

$$B_1 = \frac{2\mathrm{e}^{(3h+1)\beta}\left(\mathrm{e}^{2\sqrt{2}h}-\mathrm{e}^{2\sqrt{2}l}\right)Csch\left[\left(h+1\right)\beta\right]}{4\mathrm{e}^{(2h+1)\beta}\left(\mathrm{e}^{2\sqrt{2}h}-\mathrm{e}^{2\sqrt{2}l}\right)+\sqrt{2}\mathrm{e}^{h\beta}\left(\mathrm{e}^{2\sqrt{2}h}+\mathrm{e}^{2\sqrt{2}l}\right)\left(1+\mathrm{e}^{2(h+1)\beta}\right)\beta Csch\left[\left(h+1\right)\beta\right]},$$

$$B_2 = -\frac{\sqrt{2}\left(\mathrm{e}^{\frac{\sqrt{2}(2h+1)}{\xi}}+\mathrm{e}^{\frac{\sqrt{2}(4h+3l)}{\xi}}\right)\beta\cosh\left[\frac{(h-1)\beta}{\xi}\right]}{\sqrt{2}\left(1+\mathrm{e}^{\frac{2\sqrt{2}(h+1)}{\xi}}\right)^2\beta\cosh\left[\frac{(h-1)\beta}{\xi}\right]+2\left(-1+\mathrm{e}^{\frac{4\sqrt{2}(h+1)}{\xi}}\right)\sinh\left[\frac{(h-1)\beta}{\xi}\right]}.$$