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Original Article

Location of Interface Bose-Einstein Condensate Mixtures in Semi-infinite Space under Neumann Boundary Condition

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Abstract: The location of interface plays a pivotal role in studying on wetting phase transition of Bose-Einstein condensates (BECs) mixture. Beside parameters of system, the position of the interface depends on the applied boundary condition. Using double-parabola approximation (DPA), we consider the dependence of position of interface on parameters in semi-infinite space under Neumann boundary condition.

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

1. Introduction

In two last decades, phase-segregated binary Bose-Einstein systems were observed experimentally [1- 4], and have opened up a new avenue for considering many interesting properties of BECs. Many theoretical studies of phase-segregated Bose–Einstein condensate (BEC) mixtures have been developing to consider static properties [5-8]. The static properties of BECs include the phase-segregation in ground state [6, 7], surface tension and interfacial tension [7, 8].

Despite their quite success, these researches have just investigated at the special limit of characteristic parameters. It is due to the nonlinear nature of the Gross–Pitaevskii (GP) equations, so the authors have no determination of the interface location of the system.

In this paper we use the double-parabolic approximation (DPA) described in [8] to investigate the dependency of the interface location of BECs on the parameters as number of particles, interactive constant.

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2. Research Content

Let's start from the GP Lagrangian

$$\pounds = \int d\vec{r} \left(P_1 + P_2 - g_{12} |\psi_1|^2 |\psi_2|^2 \right), \tag{1a}$$

$$\mathbf{P}_{j} = i\hbar\psi_{j}^{*}\frac{\partial\psi_{j}}{\partial t} + \frac{\hbar^{2}}{2m_{j}}\left|\nabla\psi_{j}\right|^{2} - \frac{g_{jj}}{2}\left|\psi_{j}\right|^{4},\tag{1b}$$

here ψ_j , m_j (j=1,2) are the wave function and the atomic mass of each species j, respectively. The coupling constant is given as

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

with a_{ii'}, being the s-wave scattering length between components j and j'.

Next, we consider two BEC components with translational symmetry in the x - y direction and without the external trapping potential (U_j = 0). From the Lagrangian (1) the GP equations are deduced straightforwardly [10]

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

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

Here the chemical potential μ_i of each species j, are determined by the relations:

$$\mathbf{N}_{j} = \int \left| \boldsymbol{\psi}_{j} \right|^{2} \mathbf{d}^{3} \vec{\mathbf{r}}, \tag{3}$$

with N_{j} the number of the j-th condensate atoms.

Now we apply to consider the system, which is restricted by a hard wall locates at z=0 and assuming that component 1 (2) occupies the region z > L (z < L). Here L denotes position of the interface. For this structure, Dirichlet boundary condition is applied for first component

$$\psi_1(0) = 0, \psi_1(\infty) = 1, \tag{4}$$

and for second component, Neumann boundary condition is applied at the wall

$$\psi_2(0) = 0,$$
(5)
and far from the wall we request
 $\psi_2(\infty) = 0.$
(6)

For simplicity, we therefore introduce the dimensionless quantities $\tilde{n} = z / \xi_1$ with $\xi_j = \hbar / \sqrt{2m_j g_{jj} n_{j0}}$ the healing length and n_{j0} the number density of condensate j in bulk Eqs. (3) are reduced to dimensionless form

$$-\partial_{\hat{n}}^2 \phi_1 - \phi_1 + \phi_1^3 + \mathbf{K} \phi_2^2 \phi_1 = 0, \tag{7a}$$

$$-\xi^2 \partial_{\tilde{n}}^2 \phi_2 - \phi_2 + \phi_2^3 + K \phi_1^2 \phi_2 = 0.$$
^(7b)

In these equations, the order parameters are normalized to their bulk density $\phi_j = \psi_j / \sqrt{n_{j0}}$ and $\xi = \xi_2 / \xi_1$. The chemical potential $\mu_j = g_{jj} n_{j0}$. The dimensionless quantity $K = g_{12} / \sqrt{g_{11}g_{22}}$ is an

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independent parameter and we restrict our considerations for two condensates are immiscible, i.e. K > 1 [8] and the miscible state K = 1.

In this way, the boundary conditions in (4) - (6) are in order

$$\phi_1(0) = 0, \phi_1(+\infty) = 1,$$
(8)

$$\phi_{2'}(0) = 0, \phi_2(+\infty) = 0. \tag{9}$$

In DPA, by expanding the order parameters about bulk condensate 1, $(\phi_1, \phi_2) = (1,0)$ for the half-space $\tilde{n} > \ell$ and bulk condensate 2, $(\phi_1, \phi_2) = (0,1)$ for the half-space $\tilde{n} < \ell$. Within DPA, GPEs (7) have the form

$$-\partial_{\hat{n}}^2 \phi_j + \alpha^2 (\phi_j - 1) = 0, \tag{10a}$$

$$-\xi^2 \partial_{\tilde{n}}^2 \phi_{j'} + \beta^2 \phi_{j'} = 0, \tag{10b}$$

in which
$$\alpha = \sqrt{2}, \beta = \sqrt{K-1}$$
 and $\ell = L / \xi_1$.

In (10) the labels j and j'comply with the following important convention, which we will henceforth maintain throughout this draft

$$(j,j') = \begin{cases} (1,2), & \tilde{n} > \ell; \\ (2,1), & \tilde{n} < \ell. \end{cases}$$
(11)

Solving (10) with boundary conditions (7a), (7b) we get

 $\phi_{1}(\tilde{n}) = 1 + A_{1} e^{-\sqrt{2}\tilde{n}}, \qquad (12a)$

$$\phi_{a}(\tilde{\mathbf{n}}) = \mathbf{A}_{a} \mathbf{e}^{-\frac{\beta \tilde{\mathbf{n}}}{\xi}},\tag{12b}$$

$$\psi_2(n) = N_2 c$$
,
for $\tilde{n} > \ell$ and

$$\phi_1(\tilde{n}) = 2B_1 \cosh[\beta \tilde{n}], \qquad (13a)$$

$$\phi_2(\tilde{\mathbf{n}}) = 1 + 2B_2 \cosh\left[\frac{\sqrt{2\tilde{\mathbf{n}}}}{\xi}\right],\tag{13b}$$

for $\tilde{n} < \ell$.

Within DPA we request that the wave functions and first derivative are continuous at the interface, e.g. $\partial \phi_{i,1}$ $\partial \phi_{i,1}$ (14)

$$\phi_{j}(\ell+) = \phi_{j}(\ell-), \frac{\partial \phi_{j}}{\partial \tilde{n}}\Big|_{\ell+} = \frac{\partial \phi_{j}}{\partial \tilde{n}}\Big|_{\ell-}.$$
(14)

Combining (12) and (13) with (14) yielding

$$A_{1} = -\frac{e^{\sqrt{2}\ell}\beta}{\beta + \sqrt{2} \operatorname{coth}[\ell\beta]}, A_{2} = \frac{2e^{\frac{\ell\beta}{\xi}}\left(-1 + e^{\frac{2\sqrt{2}\ell}{\xi}}\right)}{-2 + \sqrt{2}\beta + e^{\frac{2\sqrt{2}\ell}{\xi}}\left(2 + \sqrt{2}\beta\right)},$$
(15)
$$B_{1} = \frac{1}{2\operatorname{cosh}[\ell\beta] + \sqrt{2}\beta\operatorname{sinh}[\ell\beta]}, B_{2} = -\frac{\beta}{2\left(\beta\operatorname{cosh}\left[\frac{\sqrt{2}\ell}{\xi}\right] + \sqrt{2}\operatorname{sinh}\left[\frac{\sqrt{2}\ell}{\xi}\right]\right)}.$$

Now we calculate the number of particles corresponding to component 2, Eq. (3) now has the form

$$\mathbf{N}_2 = \xi_1 \int \phi_2^2 \mathbf{d}^3 \vec{\mathbf{r}},\tag{16}$$

or

$$N_{20} = \xi_1 \int_0^\infty \phi_2^2 d\rho,$$
(17)

in which N_{20} is the number of particles of component 2 per unit length along the Oz axis. From (12), (13) and (17) we have

$$N_{20} = \frac{2\xi \sinh\left[\frac{\sqrt{2}\ell}{\xi}\right]^2}{\beta\left(\sqrt{2}\beta \cosh\left[\frac{\sqrt{2}\ell}{\xi}\right] + 2\sinh\left[\frac{\sqrt{2}\ell}{\xi}\right]\right)^2} + \frac{X_1 + X_2}{8X_3^2},$$
(18)

here

$$X_{1} = 8\left(\ell\left(-1+\beta^{2}\right)+\beta\xi\right)+4\left(\ell\left(2+\beta^{2}\right)-2\beta\xi\right)\cosh\left\lfloor\frac{2\sqrt{2}\ell}{\xi}\right\rfloor,$$
$$X_{2} = \sqrt{2}\beta\left(8\ell-3\beta\xi\right)\sinh\left\lfloor\frac{2\sqrt{2}\ell}{\xi}\right\rfloor, X_{3} = \beta\cosh\left\lfloor\frac{\sqrt{2}\ell}{\xi}\right\rfloor+\sqrt{2}\sinh\left\lfloor\frac{\sqrt{2}\ell}{\xi}\right\rfloor$$

Using Eq. (18) we can investigate the dependency of the interface location on the system parameters such as the number of N_{20} particles, the K interaction constant and the characteristic length ratio ξ .



Figure 1. (Color online). The dependence of ℓ on the value $\frac{1}{K}$ with $N_{20} = 10\xi_1$. The red, green and blue lines correspond to $\xi = 1,0.6$ and 0.2. The solid lines (dashed lines) correspond to this Neumann boundary conditions (Dirichlet boundary conditions).

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Figure 2. (Color online). The dependence of ℓ on the value ξ at K = 3. The red, green and blue lines correspond to N₂₀ = 10 ξ_1 , 15 ξ_1 , 20 ξ_1 . The solid lines (dashed lines) corresponds to this Neumann boundary conditions (Dirichlet boundary conditions).



Figure 3. (Color online). The dependence of ℓ on the value N₂₀ at K=3. The red, green and blue lines correspond to ξ =1,0.6 and 0.2. The solid lines (dashed lines) corresponds to this Neumann boundary conditions (Dirichlet boundary conditions).

Figure 1 depicts the dependence of ℓ on the value $\frac{1}{K}$ with $N_{20} = 10\xi_1$. The results show that ℓ weakly depends on K, except for domain $K \rightarrow 1$. Figure 2 and Figure 3 depicts the dependence of ℓ on the value ξ and N_{20} at K=3. It is clear that this dependence is almost linear and the location of interface is sensitive to changes in parameters.

Moreover, from figure 1, 2, 3 we see the position of the interface depend on boundary conditions which we consider.

3. Conclusion

In the foregoing section, we presented the main results of our work. In scope of DPA we study the two-component BEC in semi-infinite system with a hard-wall. Our results are in order:

- We found analytical solutions for the ground state with Neumann boundary conditions.

- We investigated the location dependence of the interface on system parameters such as the number of N_{20} particles, the K interaction constant, the characteristic length ratio ξ and boundary conditions considered. These results allowed us to investigate in detail the wetting transition of the system [9].

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