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Original Article

Critical Wetting Phase Transition in a Dilute Ternary Bose-einstein Condensates

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Abstract: We investigated the possibility of a critical wetting phase transition in a dilute ternary Bose-Einstein condensate (BEC) using Gross-Pitaevskii theory within the framework of the double parabola approximation. By analytically determining the condensate wave functions, we derived the dependence of the surfactant layer thickness on the intrinsic atomic parameters. Our results revealed conditions under which a critical wetting transition may occur, highlighting a new aspect of interfacial phenomena in multi-component BEC.

Keywords: Ternary Bose-Einstein condensates, Wetting phase diagram, Degenerate points.

1. Introduction

The wetting phenomenon in Bose-Einstein condensates (BEC) was first theoretically predicted in 2004 [1], where it was shown that an immiscible two-component BEC confined by a hard-wall (optical wall) can exhibit adsorption at the interface, with one component preferentially wetting the hard-wall boundary. Subsequent research has extended this investigation to more detailed analyses of wetting behavior at both hard-wall and soft-wall boundaries [2], leading to the construction of a wetting phase diagram in the space of intrinsic atomic parameters within the framework of Gross-Pitaevskii (GP) theory. An analytical treatment was later presented in [3], employing the double-parabola approximation (DPA) introduced in [4] to provide a tractable analytical investigation of the wetting phenomenon. Recently, the prewetting phase has also been considered in very detail within the DPA [5] in order to have a deep insight into the wetting phase transition in the two-compoent BEC.

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As mentioned above, the wetting phenomenon in two-component BEC has been theoretically predicted for over two decades. However, its experimental observation remains a significant challenge. This difficulty is commonly attributed to the inability to realize an ideal hard-wall under experimental conditions. To circumvent this issue, Indekeu et al., [6] proposed a novel approach in which the hard or soft wall is replaced by a third component that serves as a surfactant, thereby mimicking the boundary conditions necessary for wetting. The introduction of this surfactant enriches the wetting phase diagram beyond that of conventional two-component BEC. In the absence of a physical wall, the wetting phase transition has been shown to exhibit either a strongly first-order or a critical wetting transition, depending on system parameters. This transition can be characterized by monitoring the variation in the thickness of the surfactant layer. In this work, we investigate the critical wetting phase transition in a three-component (ternary) BEC system.

2. Wave Functions of a Dilute Ternary BEC

Let us consider a dilute ternary BEC numbered by 1, 2 and 3 confined in a volume *V*. In the absence of any external field, our system is described by the grand potential takes the form [7]

$$\Omega=\sum_{i=1}^{3}\int_{V} d^3\vec{r}\left\{\psi_i^*(\vec{r})\left[-\frac{\hbar^2}{2m_i}\nabla^2-\mu_i\right]\psi_i(\vec{r})+\frac{g_{ii}}{2}\left|\psi_i(\vec{r})\right|^4\right\}+\sum_{i<j}g_{ij}\int_{V} d^3\vec{r}\left|\psi_i(\vec{r})\right|^2\left|\psi_j(\vec{r})\right|^2, \tag{1}$$

where $\hbar$ is the reduced Planck constant. For component *i* (*i* =1, 2, 3), m_i, μ_i denote the atomic mass and chemical potential, respectively. The condensate wave function $\psi_i(\vec{r})$ plays the role of the order parameter, is assumed to be real in the absence of flow. The inter- $(i \neq j)$ and intraspecies interactions ($i = j$) are charactered by coupling constant. For a dilute Bose gas mixtures, these coupling constants are linear in six scattering lengths a_{ij}

$$g_{ij}=2\pi\hbar^2\left(\frac{1}{m_i}+\frac{1}{m_j}\right)a_{ij}. \tag{2}$$

Minimizing the grand potential (1) with respect to the wave function yields the Gross-Pitaevskii (GP) equation [7],

$$-\frac{\hbar^2}{2m_i}\nabla^2\psi_i-\mu_i\psi_i+\sum_{i'=1}^{3}g_{ii'}\left|\psi_{i'}\right|^2\psi_i=0, \tag{3}$$

for component *i*.

The system under consideration is assumed to be uniform in the *x* and *y* directions while along *z* axis, components 1 and 2 occupy in $z<0$ and $z>0$, respectively. The third component is located at the interface between 1-2. Therefore, the boundary conditions are

$$\begin{aligned}&\psi_1(-\infty)=\psi_2(\infty)=1,\\&\psi_1(\infty)=\psi_2(-\infty)=0,\\&\psi_3(-\infty)=\psi_3(\infty)=0.\end{aligned} \tag{4}$$

For convenience, we introduce the healing length

$$\xi_i = \frac{\hbar}{\sqrt{2m_i g_{ii} n_i}}, \tag{5}$$

and the relative strength of the interspecies interaction

$$K_{ij} = \frac{g_{ij}}{\sqrt{g_{ii}g_{jj}}} = \frac{m_i + m_j}{2\sqrt{m_i m_j}} \frac{a_{ij}}{\sqrt{a_{ii}a_{jj}}}, \tag{6}$$

which can be totally controlled in experiments. Assuming that the components 1 and 2 are in equilibrium with the equality of the bulk pressure

$$P_1 = P_2, P_i = \frac{\mu_i^2}{2g_{ii}}, \mu_i = g_{ii} n_i \, (i = 1, 2), \tag{7}$$

with the condensed density $n_i = \psi_i^2$. Now the surfactant is put into the interface 1-2 with condensed density $\bar{n}_3$ corresponding to the chemical potential $\bar{\mu}_3$. Naturally, the condition $\mu_3 \le \bar{\mu}_3, n_3 \le \bar{n}_3$ holds. We now introduce the dimensionless coordinate $\tilde{z} = z / \xi_2$ and reduced wave functions $\tilde{\psi}_1 = \psi_1 / \sqrt{n_1}, \tilde{\psi}_2 = \psi_2 / \sqrt{n_2}, \tilde{\psi}_3 = \psi_3 / \sqrt{\bar{n}_3}$. We ristrict our attention to the case in which components 1 and 2 are in the strong segregation, i.e. $a_{12} \to \infty$. In this regime, the wave functions of condensates 1 and 2 are mutually exclusive and do not overlap each other. Their interface formed by them is located at $z = 0$. In this regard, the GP equations (3) can be reformulated in dimensionless form, with the analysis carried out separately within two distinct domains. In the domain $\tilde{z} < 0$

$$\begin{aligned} \left(\frac{\xi_1}{\xi_2}\right)^2 \tilde{\psi}_1'' &= -\tilde{\psi}_1 + \tilde{\psi}_1^3 + K_{13}\tilde{\psi}_3^2\tilde{\psi}_1, \\ \tilde{\psi}_2 &= 0, \\ \left(\frac{\bar{\xi}_3}{\xi_2}\right)^2 \tilde{\psi}_3'' &= -\frac{\mu_3}{\bar{\mu}_3}\tilde{\psi}_3 + \tilde{\psi}_3^3 + K_{13}\tilde{\psi}_1^2\tilde{\psi}_3, \end{aligned} \tag{8}$$

and

$$\begin{aligned} \tilde{\psi}_1 &= 0, \\ \tilde{\psi}_2'' &= -\tilde{\psi}_2 + \tilde{\psi}_2^3 + K_{23}\tilde{\psi}_3^2\tilde{\psi}_2, \\ \left(\frac{\bar{\xi}_3}{\xi_2}\right)^2 \tilde{\psi}_3'' &= -\frac{\mu_3}{\bar{\mu}_3}\tilde{\psi}_3 + \tilde{\psi}_3^3 + K_{23}\tilde{\psi}_2^2\tilde{\psi}_3, \end{aligned} \tag{9}$$

in the domain $\tilde{z} > 0$.

We now move to investigate within the DPA, in which the wave functions will be expanded either around their maximum or zero up to first-order of their deviations. This makes the fourth-order terms in Eq. (1) become second-order terms [4]. Let $\tilde{z}^-$ and $\tilde{z}^+$ be the coordinates of intersection points between $\tilde{\psi}_1$ and $\tilde{\psi}_3$ and $\tilde{\psi}_2$ and $\tilde{\psi}_3$, respectively. Along z-axis, the configuration of the system can be divided into 3 regions. Firstly, the region $-\infty \le \tilde{z} \le \tilde{z}^-$. Expanding $\tilde{\psi}_1$ around its bulk value and $\tilde{\psi}_3$ around zero, the GP equations (8) become

$$\begin{aligned}
&\left(\frac{\xi_1}{\xi_2}\right)^2 \tilde{\psi}_1'' = -2(1-\tilde{\psi}_1),\\
&\tilde{\psi}_2 = 0,\\
&\left(\frac{\bar{\xi}_3}{\xi_2}\right)^2 \tilde{\psi}_3'' = (K_{13} - \mu_3 / \bar{\mu}_3)\tilde{\psi}_3.
\end{aligned} \tag{10}$$

Solutions for Eqs. (10) have the form

$$\tilde{\psi}_1 = 1 - A_1 e^{\sqrt{2}\frac{\xi_2}{\xi_1}\tilde{z}}, \tilde{\psi}_2 = 0, \tilde{\psi}_3 = A_3 e^{\sqrt{K_{13}-\frac{\mu_3}{\bar{\mu}_3}\tilde{z}}}. \tag{11}$$

In region $\tilde{z}^- \le \tilde{z} \le \tilde{z}^+$, $\tilde{\psi}_1$ and $\tilde{\psi}_2$ deviate from zero whereas $\tilde{\psi}_3$ is expended around its maximum value $\sqrt{\mu_3 / \bar{\mu}_3}$. Combining (8) and (9) yields

$$\tilde{\psi}_1 = \begin{cases} 2B_1 \sinh\left(\sqrt{\frac{\mu_3}{\bar{\mu}_3} K_{13} - 1}\frac{\xi_2}{\xi_1}\tilde{z}\right), \tilde{z} < 0;\\ 0, \tilde{z} > 0, \end{cases} \tag{12}$$

$$\tilde{\psi}_2 = \begin{cases} -2C_2 \sinh\left(\sqrt{\frac{\mu_3}{\bar{\mu}_3} K_{23} - 1\tilde{z}}\right), \tilde{z} > 0;\\ 0, \tilde{z} < 0, \end{cases} \tag{13}$$

$$\tilde{\psi}_3 = \sqrt{\frac{\mu_3}{\bar{\mu}_3}} + B_3 e^{\sqrt{\frac{2\mu_3}{\bar{\mu}_3}}\frac{\xi_2}{\bar{\xi}_3}\tilde{z}} + C_3 e^{-\sqrt{\frac{2\mu_3}{\bar{\mu}_3}}\frac{\xi_2}{\bar{\xi}_3}\tilde{z}}. \tag{14}$$

The wave functions in the last domain $\tilde{z} \ge 0$ can be obtained by those in the first domain by alternating the subscripts in the wave functions

$$\tilde{\psi}_1 = 0, \tilde{\psi}_2 = 1 - D_2 e^{-\sqrt{2}\tilde{z}}, \tilde{\psi}_3 = D_3 e^{-\sqrt{K_{23}-\frac{\mu_3}{\bar{\mu}_3}}\frac{\xi_2}{\bar{\xi}_3}\tilde{z}}. \tag{15}$$

The wave functions of the components in DPA are shown in Eqs. (11)-(15), in which constants are determined by conditions for the continuity of the wave functions and their first derivatives at $\tilde{z}^-$ and $\tilde{z}^+$.

$$\begin{aligned}
&\tilde{\psi}_1(\tilde{z} \to \tilde{z}^- + 0) = \tilde{\psi}_1(\tilde{z} \to \tilde{z}^- - 0), \tilde{\psi}_3(\tilde{z} \to \tilde{z}^- + 0) = \tilde{\psi}_3(\tilde{z} \to \tilde{z}^- - 0),\\
&\tilde{\psi}_2(\tilde{z} \to \tilde{z}^+ + 0) = \tilde{\psi}_2(\tilde{z} \to \tilde{z}^+ - 0), \tilde{\psi}_3(\tilde{z} \to \tilde{z}^+ + 0) = \tilde{\psi}_3(\tilde{z} \to \tilde{z}^+ - 0),\\
&\tilde{\psi}_1'(\tilde{z} \to \tilde{z}^- + 0) = \tilde{\psi}_1'(\tilde{z} \to \tilde{z}^- - 0), \tilde{\psi}_3'(\tilde{z} \to \tilde{z}^- + 0) = \tilde{\psi}_3'(\tilde{z} \to \tilde{z}^- - 0),\\
&\tilde{\psi}_2'(\tilde{z} \to \tilde{z}^+ + 0) = \tilde{\psi}_2'(\tilde{z} \to \tilde{z}^+ - 0), \tilde{\psi}_3'(\tilde{z} \to \tilde{z}^+ + 0) = \tilde{\psi}_3'(\tilde{z} \to \tilde{z}^+ - 0).
\end{aligned} \tag{16}$$

Substituting Eqs. (11)-(15) into Eq. (16), one obtains 7 equations for 7 integral constants. Formulae for these constants are very long and, the most important thing is that, they do not provide any physical insights.

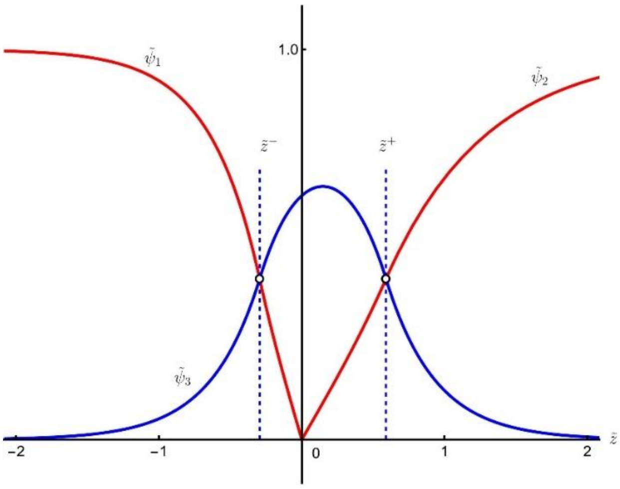

Figure 1. The wave functions of the condensates at $\mu_3 / \bar{\mu}_3 = 0.9, \xi_2 / \xi_1 = 2, \xi_3 / \xi_1 = 1$ and $K_{23} = K_{13}$.

The evolution of wave functions of condensates arround the interface 1-2 at $\mu_3 / \bar{\mu}_3 = 0.9$, $\xi_2 / \xi_1 = 2$, $\xi_3 / \xi_1 = 1$ and $K_{23} = K_{13}$. The red curves correspond to components 1 and 2, the blue curve corresponds to the surfactant.

3. Critical Wetting Phase Transition

In this section, we investigate the wetting phase transition in a dilute ternary BEC in the absence of confining walls. As discussed in [6], there are two distinct types of wetting phase transitions: a strongly first-order (discontinuous) transition and a critical (continuous) transition. The wetting transition occurs as the chemical potential approaches unity. The nature of this transition – whether it is strongly first-order or critical – depends on the behavior of the surfactant layer's thickness. The wetting phase transition is the strongly first-order if surfactant thickness layer has a jum from zero (without a layer of the surfactant) to infinity (macroscopic length). In case of the critical wetting phase transition, a layer of the surfactant is formed at the nucleation point. Thickness of this layer increases as the chemical potential ratio $\mu_3 / \bar{\mu}_3$ increases and becomes infinity (macroscopic length) at the three-phase coexistence, i.e., $\mu_3 / \bar{\mu}_3 = 1$.

We now consider the thickness of the surfactant layer in the critical wetting transition. Let us study in region of the wetting region and in three-phase coexistence. The thickness of the surfactant layer is defined as

$$L = \tilde{z}^+ - \tilde{z}^-. \tag{17}$$

Firstly, we find coordinate of the intersection point of wave functions corresponding to the components 1 and 3 in the region $\tilde{z} < 0$. The equality of the wave functions can be written as [8]

$$\tilde{\psi}_1(\tilde{z}^-) = \tilde{\psi}_2(\tilde{z}^-). \tag{18}$$

Inserting Eq. (11) into Eq. (18) one arrives at

$$\tilde{z}^- = \frac{1}{2\beta_{13}} \frac{\xi_1}{\xi_2} \ln F, \tag{19}$$

with

$$F = \frac{e^{-\frac{\sqrt{2}\xi_2\tilde{L}}{\xi_3}} \left[-2\beta_{13} e^{-\frac{\sqrt{2}\xi_2\tilde{L}}{\xi_3}} - 2\beta_{23} - \sqrt{2}\beta_{13}\beta_{23} + \sqrt{2}\beta_{13}\beta_{23} e^{-\frac{\sqrt{2}\xi_2\tilde{L}}{\xi_3}} \right]}{-2\beta_{13} - 2\beta_{23} e^{-\frac{\sqrt{2}\xi_2\tilde{L}}{\xi_3}} - \sqrt{2}\beta_{13}\beta_{23} + \sqrt{2}\beta_{13}\beta_{23} e^{-\frac{\sqrt{2}\xi_2\tilde{L}}{\xi_3}}}, \tag{20}$$

with $\beta_{ij} = \sqrt{K_{ij} - 1}$. Similarly, the equality of the wave functions at $\tilde{z}^+$ gives

$$\tilde{z}^+ = -\frac{1}{2\beta_{23}} \ln F. \tag{21}$$

In prewetting phase, Eqs. (19) and (21) can be evaluated

$$\begin{aligned} \tilde{z}^+ &\square -\frac{1}{2\beta_{23}} \ln \beta + \frac{1}{\sqrt{2}\beta_{23}} \frac{\xi_2}{\xi_3} \tilde{L}, \\ \tilde{z}^- &\square -\frac{1}{2\beta_{13}} \frac{\xi_1}{\xi_2} \ln \beta - \frac{1}{\sqrt{2}\beta_{13}} \frac{\xi_1}{\xi_3} \tilde{L}, \end{aligned} \tag{22}$$

where

$$\beta = \frac{\beta_{13}(\beta_{23} + \sqrt{2})}{\beta_{23}(\beta_{13} + \sqrt{2})}.$$

Plugging (22) into (17) one can find relation for thickness layer of surfactant

$$\tilde{L} = \frac{\frac{1}{2}\left(\frac{\xi_1}{\xi_2} \frac{1}{\beta_{13}} - \frac{1}{\beta_{23}} \right)}{1 - \frac{1}{\sqrt{2}} \left(\frac{\xi_1}{\xi_3} \frac{1}{\beta_{13}} + \frac{\xi_2}{\xi_3} \frac{1}{\beta_{23}} \right)}. \tag{23}$$

There is no doubt that the wetting phase transition takes place when the denominator of Eq. (23) vanishes, i.e.,

$$\frac{\xi_1}{\xi_3} \frac{1}{\beta_{13}} + \frac{\xi_2}{\xi_3} \frac{1}{\beta_{23}} = \sqrt{2}. \tag{24}$$

In space of the intrinsic atomic parameters, Eq. (23) exprresses the critical wetting line, which shows the continuous wetting phase transition.

The dependence of the surfactant layer thickness on K_{13}, as given by Eq. (23), is illustrated in Fig. 2 at the three-phase coexistence, with the same parameters in Fig. 1, i.e., $\xi_3/\xi_1=1$, $K_{23}=K_{13}$ $K_{23}=K_{13}$. As shown, the surfactant layer thickness increases monotonically with increasing K_{13}. A divergence occurs at $K_{13}=5.5$, indicating the presence of a wetting phase transition.

Fig. 3 displays the critical wetting line in the $(K_{13},\xi_3/\xi_1)-$plane for $\xi_3/\xi_1=1$, $K_{23}=K_{13}$. It is evident that the divergence point of the surfactant layer thickness in Fig. 2 corresponds to point M on the critical wetting line shown in Fig. 3.

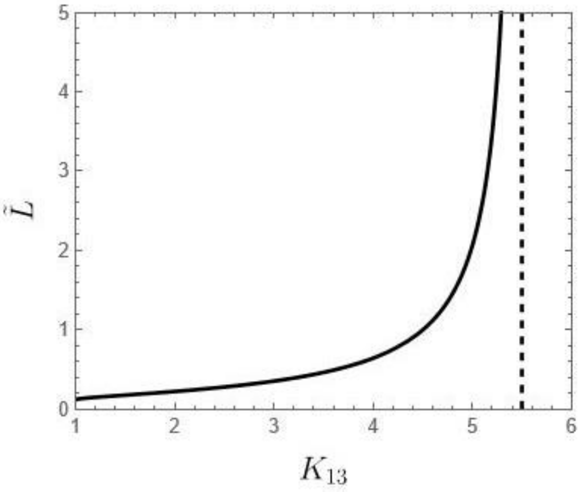

Figure. 2. The $K_{13}-$dependence of thickness of the surfactant layer at the three-phase coexistence and $\xi_2/\xi_1=2$, $\xi_3/\xi_1=1$, $K_{23}=K_{13}$.

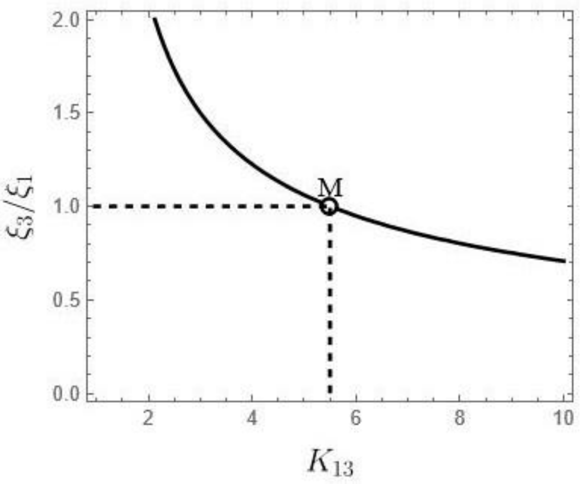

Fig. 3. The critical wetting line in $(K_{13},\xi_3/\xi_1)-$plane at $\xi_2/\xi_1=2$, $K_{23}=K_{13}$.

4. Discussion

Our analytical results for the wave functions more accurately capture the ground states of a dilute ternary BEC. This demonstrates the advantage of the DPA compared to the original GP theory, as previously established for binary BEC in [4].

In the context of wetting phase transitions, the thickness of the wetting layer plays a crucial role. A wetting transition is said to occur when this thickness diverges to a macroscopic scale. Our result for the surfactant layer thickness under the three-phase coexistence condition, $(\mu_3/\bar{\mu}_3=1)$, as presented in Eq. (23), enables the determination of the condition under which the critical wetting transition occurs.

The criterion for the critical wetting line, as given in Eq. (24), shows that the onset of the critical wetting phase is governed by the intrinsic atomic parameters of the three components. These include the atomic masses and scattering lengths characterizing both interspecies and intraspecies interactions. Remarkably, as shown in Eq. (24), the dependence of the wetting condition on these parameters can be reformulated in terms of the dimensionless relative coupling constants K_{13}, K_{23} and the healing length ratio

$$\frac{\xi_i}{\xi_j} = \left(\frac{m_j a_{jj}}{m_i a_{ii}} \right)^{1/4}. \tag{25}$$

In summary, the phase diagram space is characterized by four dimensionless parameters, $K_{13}, K_{23}, \xi_1 / \xi_3$ and ξ_2 / ξ_3. The presence of these additional degrees of freedom enriches the structure of the critical wetting phase diagram compared to the binary BEC case [1-5]. Experimentally, these parameters can be tuned either independently or simultaneously in BEC mixtures composed of either two hyperfine states of a single atomic species or two distinct atomic species [9, 10]. The use of a third component opens up new experimental avenues.

5. Conclusion

In the preceding sections, we have analyzed the wetting phase transition in a dilute ternary BEC in the absence of external confinement, employing GP theory within the framework of the DPA. Our main results are as follows:

- The condensate wave functions of the three components have been obtained within the DPA, which provides a quantitatively accurate and analytically tractable approximation.
- For the case of a critical wetting transition, the locations of the matching points have been explicitly determined.
- The thickness of the surfactant layer has been evaluated under the assumption of critical wetting and is shown to diverge as the transition is approached.
- Compared to the two-component system, the increase in the number of parameters in the phase diagram space from two to four in the three-component system renders the phase diagram more diverse, thereby offering experimentalists a wider range of options for observing wetting phase transitions.

It is noteworthy that these results have been derived under the assumption that the surfactant layer grows continuously from zero at the nucleation point to a macroscopic thickness. This continuous behavior of the surfactant layer thickness is indicative of the wetting phase transition, which is called the critical wetting transition as discussed in [6].

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