Comment on “Phase separation in a two-species Bose mixture”

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In an article in 2007, Mishra, Pai, and Das [Phys. Rev. A 76, 013604 (2007)] investigated the two-component Bose-Hubbard model using the numerical DMRG procedure. In the regime of inter-species repulsion \( U^{ab} \) larger than the intra-species repulsion \( U \), they found a transition from a uniform miscible phase to phase-separation occurring at a finite value of \( U \), e.g., at around \( U = 1.3 \) for \( \Delta = U^{ab}/U = 1.05 \) and \( \rho_a = \rho_b = 1/2 \). In this comment, we show that this result is not correct and in fact the two-component Bose-Hubbard model is unstable to phase-separation for any \( U^{ab} > U > 0 \).

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In an article in 2007, Mishra et al. [1] studied the two-component Bose-Hubbard model and phases that can be described by this model with their modified form of the finite-size density matrix renormalization group (FS-DMRG) method. The studied lattice has a density of \( \rho_{a(b)} \) bosons of species \( a(b) \) per site, with intra-species repulsion \( U \), and inter-species repulsion \( U^{ab} \) while the tunneling coefficient \( t \) is chosen as the energy unit. One of their results is that for any fixed \( \Delta = U^{ab}/U > 1 \) the system undergoes a transition from a miscible phase at small \( U \) to phase-separation at large \( U \). Unfortunately, we find this conclusion is invalid and the system is phase separated whenever \( \Delta > 1 \), for all values of \( U > 0 \).

We show this by perturbation analysis, where the miscible phase is unstable at first order for any density profile and \( U > 0 \), \( \Delta > 1 \). As an example, we also perform iDMRG calculation for the density profile \( \rho_a = \rho_b = 1/2 \) with \( \Delta = 1.05 \), which is one of the three studied density profiles in Ref. [1]. Moreover, by finite DMRG simulation with the above set of parameters, we point out that a plausible reason for the mistake of Mishra et al is they have not done a sufficient number of sweeps in their finite-size DMRG algorithm.

When \( U < t \), we can prove by a first-order perturbation theory in the thermodynamic limit that the phase-separated energy per site is always lower than that of the miscible phase. The Hamiltonian is comprised of the kinetic term and the on-site repulsion term,

\[
H = H_T + H_U.
\]  (1)

On \( L \) sites with periodic boundary conditions, these terms take the form in the momentum space as

\[
H_T = -2t \sum_{q=0}^{L-1} \cos(2\pi q/L)(a_q \hat{a}_q + b_q \hat{b}_q),
\]  (2)

\[
H_U = \frac{U}{2L} \sum_{q_1, q_2, q_3, q_4=0}^{L-1} \delta_{q_1+q_2, q_3+q_4} (a_{q_1} \hat{a}_{q_2} a_{q_3} + b_{q_1} \hat{b}_{q_2} b_{q_3})
+ \frac{U^{ab}}{L} \sum_{q_1, q_2, q_3, q_4=0}^{L-1} \delta_{q_1+q_2, q_3+q_4} a_{q_1} \hat{a}_{q_2} b_{q_3} b_{q_4},
\]  (3)

where the operator in momentum space is defined as

\[
a_{q} \hat{a}_{q} = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{i(2\pi q/L)} a_{j} \hat{a}_{j},
\]  (4)

creating a species \( a(b) \) boson with momentum \( 2\pi q/L \).

In the ground state of the miscible phase with \( U = 0 \), all the bosons are in the \( q = 0 \) level, therefore we have

\[
| \text{miscible} \rangle = \frac{1}{\sqrt{n_a!n_b!}} (a_{q=0}^{\dagger})^{n_a} (b_{q=0}^{\dagger})^{n_b} |0\rangle,
\]  (5)

where \( n_a(b) = \rho_a(b)L \) is the number of species \( a(b) \) bosons.

In the phase-separated regime, the system will split into two domains, each with momentum \( q \rightarrow 0 \) in the thermodynamic limit. Each domain only has one species.

\[
\begin{align*}
\text{FIG. 1: (Color online) The total energy per site obtained from finite DMRG (black dashed), infinite DMRG for a miscible phase (red dash-dotted), and for phase-separation (blue solid).}
\end{align*}
\]
The same conclusion can be drawn from the calculation of the ground state energy per site of a one-component Bose-Hubbard model using an infinite DMRG (iDMRG) \cite{2}. A ground state with the density $\rho = 1/2$ simulates a state in the miscible phase and with the density $\rho = 1$ it simulates a phase-separated state.

In Fig. 1 we compare the total energy per site for the miscible phase and the phase-separation. We can find when $U$ is comparable to $t$ the miscible phase apparently has a higher energy than the phase-separation. In addition, the finite DMRG gives a slightly higher total energy. The tiny extra energy should stem mainly from the open boundary and from the domain wall between two domains in the phase-separated state. We also verified that for $\Delta = 1$, the DMRG calculation produces a miscible phase as expected.

When the energy difference between miscible and phase-separated states is small, it may take a lot of iterations for DMRG to converge to the correct state. For instance, we recognize the imbalance in occupations near the boundaries in Fig. 3 of Ref. \cite{1} with $U = 1$ is a precursor to a fully phase-separated state. We have carried out DMRG calculations for an example parameter set $\rho_a = \rho_b = 1/2$, $\Delta = 1.05$, to verify that DMRG does reproduce the expected phase separated state. This is shown in Fig. 2 where we start from a random wavefunction. The randomness can be seen in the occupation expectations $n^a_i$ and $n^b_i$ in Fig. 2(a). After around 20 sweeps, $n^a_i$ and $n^b_i$ evolve to a pattern displayed in Fig. 2(b), where we find the phase-separation also starts from the boundaries. After another about 200 sweeps, the occupation expectations are clearly phase-separated as shown in Fig. 2(c).

In conclusion, we have shown through a perturbation analysis that the two-species Bose mixture is unstable to phase separation whenever $\Delta > 1$, for any $U > 0$. Additionally, we have also carried out DMRG calculations for an example parameter set to verify that DMRG does reproduce the expected phase-separated state. We can easily see in Fig. 3(a) and (b) that even when $U$ is very small, two species of bosons could not coexist and two domains are formed when enough sweeps have been done. Therefore, the erroneous conclusion in Ref. \cite{1} is likely due to an insufficient number of sweeps.

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[1] T. Mishra, R. V. Pai, and B. P. Das, Phys. Rev. A 76, 013604 (2007).

[2] I. P. McCulloch, arXiv:0804.2509 (2008).