Comment on "Phase separation in a two-species Bose mixture"

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In an article in 2007, Mishra *et al.* [Phys. Rev. A **76**, 013604 (2007)] investigated the two-component Bose-Hubbard model using the numerical density-matrix renormalization-group procedure. In the regime of interspecies repulsion U^{ab} larger than the intraspecies 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 (DMRG) method. The studied lattice has a density of $\rho_{a(b)}$ bosons of species $a(b)$ per site with intraspecies repulsion U and interspecies 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 that 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 an infinite DMRG (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 performed a sufficient number of sweeps in their finite-size DMRG algorithm.

When $U \ll t$, 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 composed of the kinetic term and the on-site repulsion term,

$$H = H_T + H_U. \tag{1}$$

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

$$H_T = -2t \sum_{q=0}^{L-1} \cos(2\pi q/L)(a_q^\dagger a_q + b_q^\dagger b_q), \tag{2}$$

$$H_U = \frac{U}{2L} \sum_{\substack{q_1,q_2,\\q_3,q_4=0}}^{L-1} \delta_{q_1+q_2,q_3+q_4}\left(a_{q_1}^\dagger a_{q_2}^\dagger a_{q_3} a_{q_4} + b_{q_1}^\dagger b_{q_2}^\dagger b_{q_3} b_{q_4}\right)$$
$$+ \frac{U^{ab}}{L} \sum_{\substack{q_1,q_2,\\q_3,q_4=0}}^{L-1} \delta_{q_1+q_2,q_3+q_4} a_{q_1}^\dagger b_{q_2}^\dagger a_{q_3} b_{q_4}, \tag{3}$$

where the operator in momentum space is defined as

$$a_q^\dagger (b_q^\dagger) = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{i(j 2\pi q/L)} a_j^\dagger (b_j^\dagger), \tag{4}$$

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

$$|\text{miscible}\rangle = \frac{1}{\sqrt{n^a! n^b!}} (a_{q=0}^\dagger)^{n^a} (b_{q=0}^\dagger)^{n^b} |0\rangle, \tag{5}$$

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 $q \to 0$ in the thermodynamic limit. Each domain only has one species present, therefore, we can write the wave function in this region, e.g., with only species a present, as

$$|\text{phase-sep.}\rangle = \frac{1}{\sqrt{n^a!}} (a_{q=0}^\dagger)^{n^a} |0\rangle, \tag{6}$$

and similarly for species b.

Both states give the same kinetic energy per site, $E^K = -2t(\rho_a + \rho_b)$. But the first-order perturbation gives different corrections: For the miscible state, we have

$$E_{\text{miscible}}^U = \frac{U}{2}\left(\rho_a^2 + \rho_b^2 + 2\,\Delta \rho_a \rho_b\right). \tag{7}$$
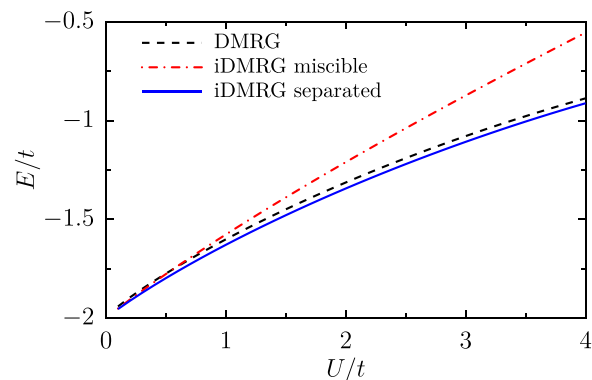

FIG. 1. (Color online) The total energy per site obtained from finite DMRG (black dashed line), infinite DMRG for a miscible phase (red dashed-dotted line), and for phase separation (blue solid line).
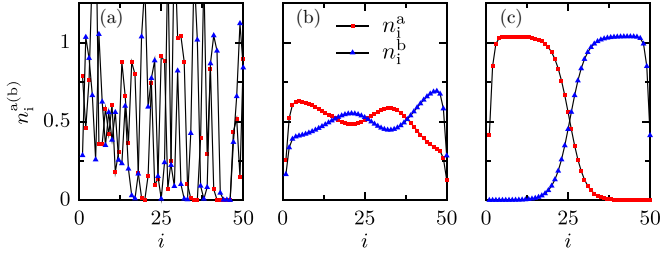
FIG. 2. (Color online) The expectations n_i^a and n_i^b for (a) an initial random wave function, (b) the wave function after about 20 sweeps, and (c) after about another 200 sweeps when $U = 1$.

FIG. 3. (Color online) The expectations n_i^a and n_i^b when (a) $U = 0.1$ and (b) $U = 0.2$, respectively (symbols used as in Fig. 2).

On the other hand, we have

$$E_{\text{phase-sep.}}^U = \frac{U}{2}(\rho_a + \rho_b)^2. \tag{8}$$

In consequence, as long as $\Delta > 1$, the phase-separated energy per site is lower than the miscible phase.

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 iDMRG [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 the DMRG to converge to the correct state. For instance, we recognize the imbalance in occupations near the boundaries in Fig. 3 of Ref. [1] with $U = 1$ is a precursor to a fully phase-
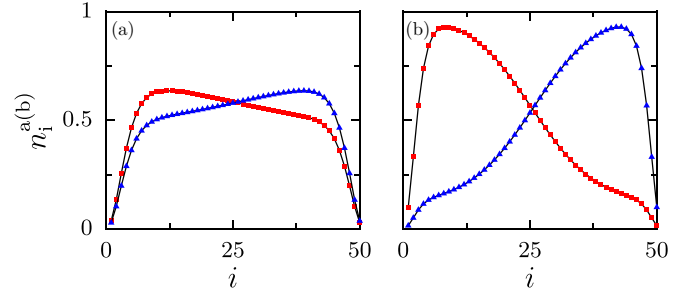
separated state. We have carried out DMRG calculations for an example parameter set $\rho_a = \rho_b = 1/2$, $\Delta = 1.05$, to verify that the DMRG does reproduce the expected phase-separated state. This is shown in Fig. 2 where we start from a random wave function. The randomness can be seen in the occupation expectations n_i^a and n_i^b in Fig. 2(a). After around 20 sweeps, n_i^a and n_i^b evolve to a pattern displayed in Fig. 2(b) where we find the phase separation also starts from the boundaries. After about another 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 the DMRG does reproduce the expected phase-separated state. In Figs. 3(a) and 3(b), we can easily see that, even when U is very small, two species of bosons could not coexist and two domains are formed when enough sweeps have been performed. Therefore, the erroneous conclusion in Ref. [1] is likely due to an insufficient number of sweeps.

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

[2] I. P. McCulloch, arXiv:0804.2509.