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Concurrence and fidelity of a Bose–Fermi mixture in a one-dimensional optical lattice

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Abstract
We study the ground-state fidelity and entanglement of a Bose–Fermi mixture loaded in a one-dimensional optical lattice. It is found that the fidelity is able to signal quantum phase transitions between the Luttinger liquid phase, the density-wave phase, and the phase separation state of the system, and the concurrence, as a measure of the entanglement, can be used to signal the transition between the density-wave phase and the Ising phase.

(Some figures in this article are in colour only in the electronic version)

Ultra-cold atomic gases loaded in an optical lattice are attracting more and more attention as a way of gaining deep insight into some essential physical phenomena, such as quantum phase transitions (QPTs) [1], in condensed matter physics. The prediction [2] and successful observation [3] of a QPT from a superfluid to a Mott-insulator was one of the greatest achievements in this field. Quite recently, promising experimental progress has been made in the study of more non-trivial quantum phases in cold atomic systems. For example, bosonic and fermionic atoms can simultaneously be trapped in an optical lattice in a controllable way [4]. This ultra-cold atomic system, the so-called Bose–Fermi mixture, often reminds people of solid state systems including the electron–phonon interaction. The latter have been studied for a long time and have a complicated quantum phase diagram. So the exploration of possible new phases in Bose–Fermi mixtures becomes an interesting theoretical problem. Several works had been done on this [5–7, 9–14]. It is worthwhile mentioning that Pollet *et al* recently studied the ground-state phase diagram of a Bose–Fermi mixture loaded in a one-dimensional (1D) optical lattice by using quantum Monte Carlo (QMC) simulations [13]. Several phases, including a Luttinger liquid (LL) phase, a density-wave (DW) phase, a phase separation (PS) state, and an Ising phase, are predicted.

In recent years, some emerging concepts in quantum information theory [15] have been extensively used to study critical phenomena in quantum many-body systems. A typical example is entanglement. Many efforts have been made to understand the relation between entanglement and QPTs [16–19]. Quite recently, the fidelity, as a measure of similarity between states, was proposed as a means of studying the critical phenomena. The motivation is very simple: a dramatic change in the structure of the ground state around the quantum critical point should result in a great difference between the two ground states on the both sides of the critical point. Fidelity has been successfully applied in the study of spin, fermionic, and most recently bosonic systems [20–28]. Compared with entanglement, fidelity is a purely geometrical quantity; an obvious advantage is that in analyzing QPTs it does not require *a priori* knowledge of the order parameter and the symmetry of the system.

In this paper we study the ground-state fidelity and the entanglement of a Bose–Fermi mixture in a 1D optical lattice. The aim is to explore the role of fidelity and entanglement in a more realistic system. As shown in many examples [16, 17, 19], there exists a strong connection between entanglement and the QPT. However, the nature of the relation is still unclear so the current study will shed some light on this important issue. Following Pollet *et al* [13], we assume that a mixture of bosonic and fermionic atoms is loaded into a 1D optical lattice, and the temperature is low enough such that quantum degeneracy is achieved. The system is then described by a lowest-band Bose–Fermi Hubbard model,

$$H = -\sum_{i=1}^{N}(t_F c_i^\dagger c_{i+1} + t_B b_i^\dagger b_{i+1} + \text{H.c.}) + U_{BF}\sum_{i=1}^{N} c_i^\dagger c_i b_i^\dagger b_i + U_{BB}\sum_{i=1}^{N} b_i^\dagger b_i (b_i^\dagger b_i - 1), \quad (1)$$

where b_i ($b_i^\dagger$) and c_i ($c_i^\dagger$) are the bosonic and fermionic annihilation (creation) operators, respectively, at site i. Bosons (fermions) can hop from site i to the nearest neighbor site $i \pm 1$ with tunneling amplitude t_B (t_F). Furthermore, a large occupation of bosons on a single site is suppressed by the on-site repulsion interaction U_{BB}. Bosons and fermions can mutually repel or attract each other on each site depending on the sign of U_{BF}. In this paper, we choose $U_{BF} > 0$, and consider the case where both the bosons and the fermions have a density: $N_F = N_B = N/2$.

We now briefly discuss the ground-state phase diagram of the model [13]. When the U_{BF} is small enough, the fermions behave as a LL, and interaction between them is induced by the bosons. At the same time, the bosons form an interacting liquid too. So we have a LL of fermions, which weakly interacts with a boson liquid. When U_{BB} is small and U_{BF} is large, the system is to first order unstable to the PS with hard domain walls; in other words the system is separated into two regions—a bosonic region and a fermionic region. When both U_{BB} and U_{BF} are very large, the bosons behave as fermions, which means that occupation by more than one boson at a single site is not allowed. The model can then be mapped into the 1D XXZ model: $H_{XXZ} = \sum_i J(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y) + J^z\sigma_i^z\sigma_{i+1}^z$, where $J = -(t_B t_F)/U_{BF}$ and $J^z = (t_B^2 + t_F^2)/(2U_{BF}) - t_B^2/(2U_{BB})$ [29]. This implies that there are three phases in this limit: the ferromagnetic phase, a gapless DW phase and a gapped Ising phase. In the ferromagnetic phase, boson–boson bonds and fermion–fermion bonds are favored compared with boson–fermion bonds due to the larger exchange interactions; this mechanism makes the system form two regions with hard domain walls. So the ferromagnetic phase corresponds to PS in the mixture. This mechanism is similar to the one appearing in the 1D asymmetric Hubbard model [30, 31] where PS also occurred when the system was away from half-filling. In the DW phase and Ising phase, the system always favors boson–fermion bonds. We would like to emphasize that the PS in the large U_{BB} limit and that in the small U_{BB} limit are different, since that the latter allows the occupation of more than one boson at a single site. In the whole PS region, with increasing of U_{BB}, the boson repulsion exerts a pressure such that the region occupied by the bosons will grow and at the same time the local density of bosons will decrease.

As mentioned before, the fidelity is the modulus of the overlap of two ground states relative to two different choices of the Hamiltonian parameters. In this paper, we mainly focus on these two:

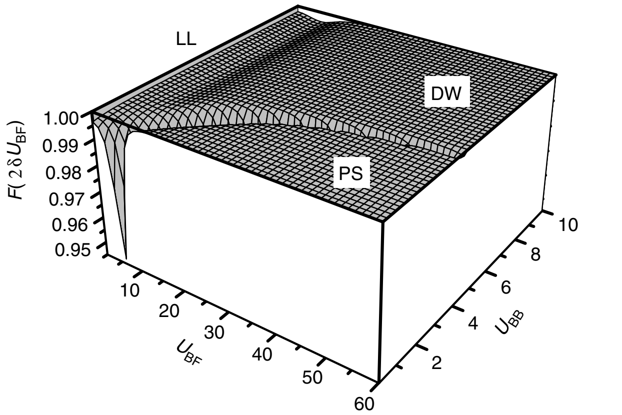

Figure 1. The obtained fidelity $F(2\delta U_{BF}, U_{BF}, U_{BB})$ when $t_F = 4.0$, $t_B = 1.0$, $\delta U_{BF} = 0.5$. It can be observed that there are two phase transition boundary lines indicated by the drop in the fidelity. Phases such as LL, DW and PS are identified by comparing this phase diagram with the one which was proposed earlier from the calculation of the correlation functions (see text). $N = 8$ (APBC).

$$F(2\delta U_{BF}, U_{BF}, U_{BB}) = |\langle\psi_{U_{BF}-\delta U_{BF}}|\psi_{U_{BF}+\delta U_{BF}}\rangle|, \quad (2)$$

$$F(2\delta U_{BB}, U_{BF}, U_{BB}) = |\langle\psi_{U_{BB}-\delta U_{BB}}|\psi_{U_{BB}+\delta U_{BB}}\rangle|, \quad (3)$$

in which $|\psi_\lambda\rangle$ stands for the ground state of the Hamiltonian (1) with the parameter λ, and is calculated by the Lanczos method for a finite sample. The Lanczos method is a numerical recipe, which is based on the Kylov subspace, for calculating some eigenvectors of a large sparse matrix. The basic idea of the Lanczos method is that a special basis can be constructed where the Hamiltonian has a tridiagonal representation. Once in this form the matrix can be diagonalized easily using standard library subroutines. One of the advantages of this technique is that ground-state properties can be obtained accurately well before the rest of the matrix eigenvalues are evaluated by systematically improving a given variational state that is used to represent the ground state of the system. Thus the method is very suitable for the analysis of the fidelity in this model. In spite of these advantages, memory limitations impose severe restrictions on the size of the clusters that can be studied with this method [32]. To avoid the ground-state level crossing, anti-periodic boundary conditions (APBCs) are applied for system size $N = 4n$ and periodic boundary conditions (PBCs) for $N = 4n + 2$, where n is an integer. According to the original idea of fidelity, a drop in the fidelity of two ground states separated by two slightly different parameters is expected to be a signature of a QPT.

In figure 1 we show one of our main results, i.e. the fidelity $F(2\delta U_{BF}, U_{BF}, U_{BB})$ defined on the U_{BB}–U_{BF} plane. Compare this figure with figure 4 of [13]; perfect similarity can be observed. The boundary lines of phase transitions between the LL, the DW and the PS are clearly indicated by a decreased fidelity. We would like to emphasize that the phase diagram presented here is obtained for a very small cluster and without any knowledge of the correlation properties of the system. It is also clearly observed that the drop of the fidelity along the phase transition line between the DW and PS phases becomes steeper and steeper as the interaction decreases. This phenomenon indicates that although the phase transition is within the same class but the similarity of the ground state is changing along this line.

However, the phase transition, as reported in [13], between the DW and the Ising phases is not indicated in figure 1. According to the effective model, i.e. the 1D XXZ model, this transition belongs to the KT universality class [13, 33]. Lode Pollet *et al* [13] did numerical calculations of the correlation functions in a somewhat larger system ($N \sim 30$) by QMC simulations and claimed that a true long-range order may exist in the Ising phase. It is very difficult for us to make a scaling analysis of the correlation functions by the Lanczos method. However, the 1D XXZ [34] model provides us with a clue to investigate this problem. It was reported that the concurrence [35], as a measure of entanglement between two qubits, reaches a maximum at the $SU(2)$ point [17] of the XXZ model. This maximum point corresponds to the transition point between the DW and the Ising phases.

The concurrence in the spin models can be calculated in the following way. Due to the global $SU(2)$ symmetry of the XXZ model, the z-component of the total spin of the system is a good quantum number and the reduced density matrix $\rho_{i,i+1}$ of two neighboring spins has the form

$$\rho_{i,i+1} = \begin{pmatrix} u^+ & 0 & 0 & 0 \\ 0 & w & z^* & 0 \\ 0 & z & w & 0 \\ 0 & 0 & 0 & u^- \end{pmatrix}, \tag{4}$$

in the spin basis $|\uparrow\uparrow\rangle$, $|\downarrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\downarrow\rangle$. The elements in the reduced density matrix $\rho_{i,i+1}$ can be obtained from the correlation functions

$$u^\pm = \tfrac{1}{4}(1 \pm 2\langle\sigma_i^z\rangle + \langle\sigma_i^z\sigma_{i+1}^z\rangle), \tag{5}$$

$$w = \tfrac{1}{4}(1 - \langle\sigma_i^z\sigma_{i+1}^z\rangle), \tag{6}$$

$$z = \tfrac{1}{4}(\langle\sigma_i^x\sigma_{i+1}^x\rangle + \langle\sigma_i^y\sigma_{i+1}^y\rangle + \mathrm{i}\langle\sigma_i^x\sigma_{i+1}^y\rangle - \mathrm{i}\langle\sigma_i^y\sigma_{i+1}^x\rangle). \tag{7}$$

All the information needed is contained in the reduced density matrix, from which the concurrence is readily obtained as [36]

$$C = 2\max\left[0, |z| - \sqrt{u^+u^-}\right], \tag{8}$$

which can be expressed in terms of the correlation functions and the magnetization by using equations (5)–(7).

The concurrence is only valid for a two-qubit system. For the Bose–Fermi Hubbard model, the double occupation of two particles is almost not allowed in the strong coupling limit, and the state of the two neighboring sites can be described by a four basis $|ff\rangle$, $|bf\rangle$, $|fb\rangle$, $|bb\rangle$ where f (b) represents that there is only one fermion (boson) on a single site. So we can associate a pseudo-spin 'up' ('down') with 'f'('b'). Then the equations described above can also be perfectly applied to the Bose–Fermi Hubbard model. In other words, if we calculate the trace of the reduced matrix of two nearest sites, which reads $T = \mathrm{Tr}\,\rho_{i,i+1}$, then T must equal to 1 in this limit. While T only approximately equals 1, when $U_{\rm BB}$ and $U_{\rm BF}$ are not infinite but large. As long as $(1 - T)$ is small enough, the concurrence calculated by equation (8) is a good characterization of entanglement between two sites. In this way, we are able to make an approximate calculation of the concurrence in the Bose–Fermi mixtures. This kind of treatment was also used by another group recently [37]. Obviously, as expected, a maximum is clearly observed in the behavior of the concurrence, which indicates a QPT point. It is important to point out that the variation of the concurrence is not dramatic in the whole DW region. Using the exact solution of the XXZ chain, a phase transition from the DW phase to the Ising phase should occur at $-J = J^z$, i.e. $U_{\rm BB} = 6.7$ for $t_{\rm F} = 4.0$, $t_{\rm B} = 1.0$, $U_{\rm BF} = 60$. But according to the obtained concurrence, the maximum point $U_{\rm BB}^{\max}$ equals approximately 7.7. The discrepancy may arise from two effects. One is that the hard-core limit is not fully satisfied in the whole DW phase region, so the phase transition point of the system is not exactly equal to the one indicated by the XXZ model. The other one is the size effect. From figure 2, it can be observed that the maximum point of concurrence is closer and closer to 6.7 when the system size is increased. As a result, we think that the phase transition point of the system is somewhere between 6.7 and 7.7.

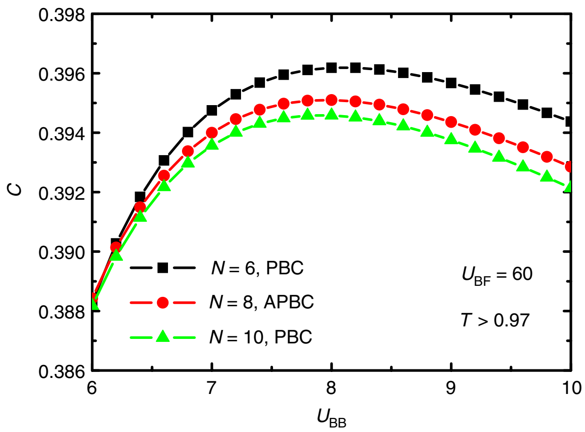

Figure 2. The obtained concurrence in the DW phase where $t_{\rm F} = 4.0$, $t_{\rm B} = 1.0$. The concurrence of $N = 6$ ($N = 8$) was been reduced by 0.029 (0.009) in order to make the results fall in the same region in the figure. T is defined as the trace of the reduced density matrix of two neighboring (pseudo-) spins (see text). All other parameters are indicated in the figure.

We calculated the fidelity $F(2\delta U_{\rm BB}, U_{\rm BF}, U_{\rm BB})$ which is also able to signal the transition between the PS phase and the DW phase. As one can see in figures 3(a) and (b), the most dramatic drop in the fidelity is in correspondence with the phase transition point between the PS state and the DW phase. The critical point found here is consistency with the one found in figure 1. In addition, more drops in the fidelity can be observed in the PS region. These drops are related to the changing rate of the local density of the boson. To show this, we define the local density of the boson as,

$$D_{\rm B} = \left\langle \frac{1}{N}\sum_{i=1}^{N} b_i^\dagger b_i (b_i^\dagger b_i - 1) \right\rangle, \tag{9}$$

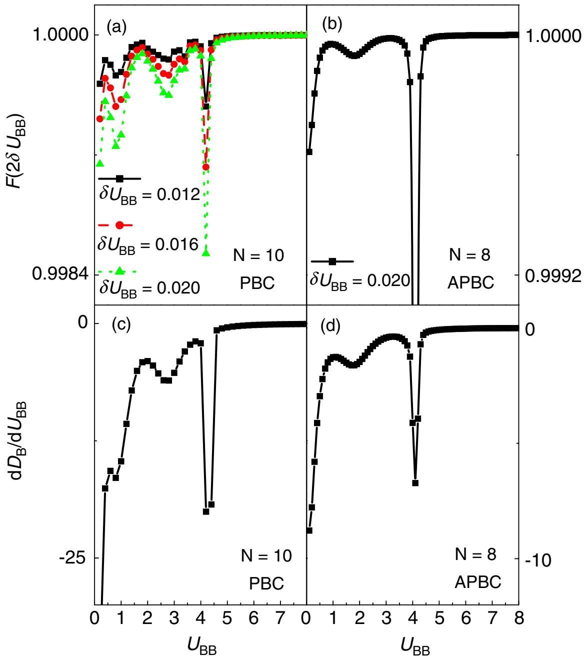

Figure 3. The obtained fidelity $F(2\delta U_{BB}, U_{BF}, U_{BB})$ ((a), (b)) and the first order derivative of the local density of boson (see text) ((c), (d)) when $t_F = 4.0$, $t_B = 1.0$, $U_{BF} = 60.0$. All other parameters are indicated in the figure.

and calculate its first order derivative. Comparing figures 3(a) and (b) with figures 3(c) and (d), respectively, it can be seen that every drop in the fidelity is accompanied by a drop in the derivative of the local density of bosons. This relation can be understood by considering that the dramatic change of the local density of bosons leads to a big change in the ground-state wavefunction, and then makes the fidelity decrease greatly. These observations imply that the transition between PS phase and the DW phase is within the Landau symmetry breaking theory. Furthermore, it is easy to notice that the drops found in the PS phase is strongly affected by the system size and the boundary conditions, while the phase transition point between PS phase and DW phase is not. We may conclude that these drops are size effects and cannot be identified as phase transition points. However, the transition between the DW phase and the Ising phase is still not indicated.

By careful analyzing the data we have, the missing phase transition signature in the fidelity between the DW phase and the Ising phase can be attributed to two reasons. The first is that this kind of transition is actually a very weak one, which means that the change in the ground state around the critical point is not dramatic, at least in a finite-sized system. The second is that, as reported before, the fidelity may not be a good indicator of infinite order phase transitions, such as the KT transition [24].

In summary, we have calculated the fidelity $F(2\delta U_{BF}, U_{BF}, U_{BB})$ and $F(2\delta U_{BB}, U_{BF}, U_{BB})$ of the 1D Bose–Fermi Hubbard model, which can be used to describe low-temperature physics of atomic Bose–Fermi mixtures loaded in 1D optical lattices. It was shown that the fidelity may be a good tool with which to study the complicated phase diagram without *a priori* knowledge of the order parameter and the symmetry of the system. However, caution is called for when one deals with the KT-like phase transition, for which the fidelity may not signal the transition, for example, the transition between the DW phase and the Ising phase in this system. We also calculated the concurrence in the DW phase. The result indicated that a QPT may exist in the DW phase.

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