Excited-state level crossing and quantum phase transition in one-dimensional correlated fermion models

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(Received 31 March 2003; published 13 June 2003)

We show that for a wide class of one-dimensional correlated fermion models, such as the extended Hubbard model, the global ground state is nondegenerate with proper boundary conditions. Consequently, energy level crossing in the ground state is absent. We also show that the continuous quantum phase transitions are actually caused by level crossing of the low-lying excited states of the system.

DOI: 10.1103/PhysRevB.67.245105 PACS number(s): 71.10.Fd, 71.10.Pm, 71.27.+a

Physics in one-dimensional correlated fermion systems have been one of the central focuses in condensed matter theory for decades,[1–3] especially after the discovery of high temperature superconductivity. As a good example, the one-dimensional extended Hubbard model (EHM), with on-site and nearest-neighbor Coulomb repulsions U and V, is a simple yet nontrivial model that exhibits rich ground state phase diagram.[1,3] In the $U,V>0$ regime at half filling, both strong-coupling analysis[4–6] and weak-coupling renormalization-group technique[1,2] have shown that there is a phase transition from the spin-density wave (SDW) to the charge-density wave (CDW) at $U=2V$. Some later studies showed that there exists also a bond-order-density wave-(BOW, or BCDW) phase between the SDW and the CDW phases.[7–13] It was claimed that, for example, as the coupling U and V increase, the continuous phase transition changes into the first-order one at a bicritical point around $(U,V)=(5.0t,2.3t)$ (see, for example, Ref. 13).

With the inclusion of additional terms in the EHM on different physics background, various one-dimensional correlated electronic models were actively studied recently[14–22] and many phase diagrams were obtained. Most of these studies applied analytical approaches, such as bosonization, and numerical techniques, such as exact diagonalization of the model Hamiltonian. However, the properties of phase transitions in these models have not been clearly spelt out yet. While it is worth the efforts to determine the phase boundaries, it is also important to understand the character of the transition between different phases based on some general but rigorous results.

In this work, we study the character of quantum phase transition in a class of one-dimensional correlated fermion models, where the off-diagonal Coulomb interactions, electron-phonon interactions, and alternating potential (the ionic Hubbard model[16–22]) are all included. We show that in most circumstances, the system ground state is nondegenerate. Thus, there is no energy level crossing in the ground state as long as fermion hopping is present. Implications of this result will be discussed.

To start, take a finite chain of lattice with L sites. For convenience, we shall assume that the lattice constant is unity and L is an even integer. We shall first impose the open boundary condition on the chain in order to avoid unnecessary mathematical nuisances. We then discuss the boundary effects. The generalized Hubbard Hamiltonian, which we shall consider, is of the following form:[16,23–26]

$$H=\sum_{i=1}^{L-1}\sum_{\sigma}T_i(\bar{\sigma})B_i(\sigma)+U\sum_{i=1}^{L}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}+V\sum_{i=1}^{L-1}\hat{n}_i\hat{n}_{i+1}+X\sum_{i=1}^{L-1}\sum_{\sigma}B_i(\sigma)(\hat{n}_{i\bar{\sigma}}+\hat{n}_{i+1,\bar{\sigma}})+W\sum_{i=1}^{L-1}\left(\sum_{\sigma}B_i(\sigma)\right)^2+\Delta\sum_{i=1}^{L}(-1)^i\hat{n}_i-\mu\hat{N}. \quad (1)$$

In Eq. (1), $\hat{c}^{\dagger}_{\mathbf{i}\sigma}$ ($\hat{c}_{\mathbf{i}\sigma}$) represents the fermion creation (annihilation) operator, which creates (annihilates) an itinerant electron of spin σ at lattice site i and $\hat{n}_i=\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow}$. $B_i(\sigma)$ is called the bond-charge operator, defined by

$$B_i(\sigma)=\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{i+1,\sigma}+\hat{c}^{\dagger}_{i+1,\sigma}\hat{c}_{i,\sigma}. \quad (2)$$

$T_i(\bar{\sigma})$ is the occupation-dependent electron hopping amplitude from site i to $i+1$, given by

$$T_i(\bar{\sigma})=t_{AA}(1-\hat{n}_{i,\bar{\sigma}})(1-\hat{n}_{i+1,\bar{\sigma}})+t_{BB}\hat{n}_{i,\bar{\sigma}}\hat{n}_{i+1,\bar{\sigma}}+t_{AB}[\hat{n}_{i,\rangle\bar{\sigma}}(1-\hat{n}_{i+1,\bar{\sigma}})+\hat{n}_{i+1,\bar{\sigma}}(1-\hat{n}_{i,\bar{\sigma}})]. \quad (3)$$

The three parameters t_{AA}, t_{BB}, and t_{AB} stand for electron hopping from a singly occupied site to an empty site, from a doubly occupied site to a singly occupied site, and from a doubly occupied site to an empty site (and the opposite process), respectively. We shall require that they have the same sign, either positive or negative. Rest of the terms represent electron-electron interactions.[23–25] U and V denote, respectively, the on-site and the nearest-neighbor interactions between electrons. In general, they are positive parameters for the Coulomb interaction. However, as we shall show in the following, their signs do not matter as far as the degeneracy of the global ground state of Hamiltonian (1) is concerned. The W term can be either the off-diagonal Coulomb interaction with $W>0$ or be induced by phonon-electron interactions with $W<0$.[27–29] The X term is another off-diagonal Coulomb interaction whose magnitude is smaller than the hopping integrals. Parameter Δ was originally proposed[26] to study the neutral-ionic transition in mixed-stack donor-accepted organic crystals.[30]

In fact, Hamiltonian (1) represents several models, which have been and are currently under intensive studies. For instance, when $t_{AA}=t_{BB}=t_{AB}$ and $W=X=\Delta=0$, H is the well-known EHM Hamiltonian, and with $W<0$, $t_{AA}=t_{BB}=t_{AB}$, and $X=\Delta=0$, H represents an effective Hamiltonian of the famous Su-Schrieffer-Heeger model[31] at the antiadiabatic limit with $W<0$.[27–29] For $W=X=0$, H represents the so-called ionic Hubbard model, which is now vigorously investigated by many physicists.[16–22] These models have different kinds of phases in different regions of the parameter space. Consequently, quantum phase transitions will take place as these parameters vary.

With the above preparations, we now proceed to prove the following fact.

Theorem. Under the conditions $W\leqslant 0$ and $|X|<|t_{AA}|,|t_{AB}|,|t_{BB}|$, the global ground state $\Psi_0(N)$ of Hamiltonian (1) on an open chain is nondegenerate for any admissible even number of electrons. The same conclusion also holds true if $N=4n+2$ with the periodic boundary condition (PBC) or $N=4n$ with the antiperiodic boundary condition (APBC).

To prove the theorem, we shall apply a simplified version of Lieb and Mattis' method in proving the absence of ferromagnetism in one-dimensional itinerant electron lattice models.[32] In the present case, the occupation-dependent hopping of electrons and the W-interaction term in Hamiltonian (1) needs to be dealt with care.

In the following, for definiteness, we assume that all the parameters t_{AA}, t_{BB}, and t_{AB} appearing in the occupation-dependent hopping amplitude $T_i(\overline{\sigma})$ are negative nonzero quantities. This assumption can be relaxed for a bipartite lattice with nearest-neighbor hopping, since we can always apply a unitary transformation to Hamiltonian (1), which maps $\hat{c}_{i\sigma}$ into $(-1)^i\hat{c}_{i\sigma}$, thus $T_i(\overline{\sigma})$ is mapped into $-T_i(\overline{\sigma})$, while other terms of the Hamiltonian keep unchanged.

It is easy to check that Hamiltonian (1) commutes with the total electron number operator $\hat{N}$, the total spin operators $\hat{S}$ and $\hat{S}_z$. Hence, the Hilbert space $V(N)$ of N electrons can be decomposed into separate subspaces

$$V(N)=\sum_{M=0}^{N}\oplus V(N_\uparrow=N-M,N_\downarrow=M). \tag{4}$$

Furthermore, in each subspace $V(N-M,M)$, we observe that, under the open boundary condition, *the up-spin and the down-spin fermion operators can be properly arranged in such a way that the action of Hamiltonian 1* does not violate their orderings. More precisely, one can choose a natural basis of configurations of $V(N-M,M)$ by

$$\phi_\alpha=(\hat{c}^\dagger_{i_1,\uparrow}\cdots\hat{c}^\dagger_{i_{N-M},\uparrow})(\hat{c}^\dagger_{j_1,\downarrow}\cdots\hat{c}^\dagger_{j_M,\downarrow})|0\rangle, \tag{5}$$

where $|0\rangle$ is the vacuum state. $(i_1<i_2<\cdots<i_{N-M})$ and $(j_1<j_2<\cdots<j_M)$ denote the positions of the up-spin and the down-spin electrons on the lattice chain, respectively. In terms of these vectors, Hamiltonian (1) can be rewritten into a Hermitian matrix $\mathcal{H}$. We notice that, when $W\leqslant 0$ and $|X|\leqslant|t_{AA}|,|t_{AB}|,|t_{BB}|$, all of its off-diagonal elements, such as $W\langle\phi_\beta|[\Sigma_\sigma B_i(\sigma)]^2|\phi_\alpha\rangle$, are nonpositive quantities. Furthermore, $\mathcal{H}$ is also irreducible in the following sense: For any pair of indices m and n, there is a positive integer K such that the matrix element $(\mathcal{H}^K)_{mn}$ is nonzero; that is, due to the fact that electron can move from one site of the open chain to any other site by a sequence of hoppings. Therefore, any pair of configurations ϕ_α and ϕ_β in subspace $V(N-M,M)$ are connected by $\mathcal{H}^K$ with an appropriate integer K.

To such a Hermitian matrix, we are able to apply the well-known Perron-Fröbenius theorem.[33] It tells us that *the ground-state wave function of $\mathcal{H}$ in $V(N-M,\rangle M)$ is a linear combination of $\{\phi_\alpha\}$ with positive coefficients and, hence, is nondegenerate*. In particular, since each eigenstate of Hamiltonian (1) has a representative in subspace $V(N/2,N/2)$, the ground state of $\mathcal{H}$ in this subspace is actually the global ground state $\Psi_0(N)$ of Hamiltonian (1), and is nondegenerate.

To go further, we let parameters W,X,U,V, and Δ tend to zero. In this limit, $\Psi_0(N)$ keeps nondegenerate, but the Hamiltonian is reduced to that of a noninteracting electron chain. Its ground state is nondegenerate and has spin $S=0$ when the electron number N is an even integer. Therefore, by the continuity argument, $\Psi_0(N)$ must also have $S=0$ for nonzero parameters.

If the periodic rather than the open boundary condition is imposed on the lattice, some mathematical ambiguities may arise. In particular, due to electron hopping between boundary sites, the off-diagonal matrix elements of $\mathcal{H}$ in an arbitrary $V(N-M,M)$ can be either positive or negative; this makes the Perron-Fröbenius theorem invalid. Fortunately, for our purpose, we need only to consider the subspace $V(N/2,N/2)$, which contains the global ground state. In this subspace, when electron number $N=4n+2$, it is easy to check that all the off-diagonal elements of $\mathcal{H}$ in terms of the basis vectors given in Eq. (5) are still nonpositive. Therefore, the global ground state $\Psi_0(N)$ is also nondegenerate and has spin $S=0$.

However, when $N=4n$, a little algebra shows that electron hopping between boundary sites produce several positive off-diagonal matrix elements. As a result, the Perron-Fröbenius theorem cannot be applied. To avoid this situation, one may deliberately impose the antiperiodic boundary condition on the lattice. The extra minus sign created by this boundary condition will eliminate the problem and make the global ground state nondegenerate again. This completes our proof of the theorem, and some remarks are in order.

This theorem tells us that level crossing of the global ground state is absent in the region of parameter space for $W\leqslant 0$ with nonzero electron hoppings. Therefore, physical quantities of the system associated only with the ground-state at temperature $T=0$, such as the ground-state energy and momentum, should be smooth functions of these parameters for any finite-size chains. In particular, the symmetries of the ground state should not change as these parameters vary. However, as the system size increases toward the thermodynamic limit, this smoothness may be violated. We shall later discuss on this issue.

Here, we should point out that energy level crossing could

be induced by *boundary conditions*. In fact, in some studies of Hamiltonian (1), say, the EHM in regions around $U=2V$, ground-state energy level crossing were observed and used to determine transition point. In most numerical studies, including exact diagonalization and quantum Monte Carlo simulation, $4n$ electrons with PBC were used, which violates the condition of our theorem as we discussed above. Consequently, a level crossing of the global ground state may happen at some special point $(U_0,V_0,W_0,X_0,\Delta_0)$ in the parameter space. It is well known that for $4n$ electrons with PBC, and $4n+2$ electrons with APBC, the ground state is degenerate at noninteracting limit, $U=V=W=X=\Delta=0$. This is an example of *accidental degeneracy*,[36] which induces observed level crossing in some existing numerical simulations. In fact, as noticed by several authors,[11,18,22] when ''improper'' boundary conditions were intentionally used, the global ground state and the first excited state of the system could be degenerate at the border between different phases. Generally, these (two) degenerate states have different symmetries and when parameter varies, the global ground state undergoes a symmetry crossover, and that defines (some kind of) phase transition. From the numerical point of view, such tactics may be a clever way to determine phase transition point. Nevertheless, the ground-state properties should not depend on the choice of boundary conditions in the thermodynamic limit. Introducing intentionally such accidental degeneracy may mislead us.

With regard to the quantum phase transition when the ground state is known to be nondegenerate, we would like to point out that, *these transitions are actually caused by the level crossing of excited states of the Hamiltonian*. This issue has been discussed by several authors in the framework of bosonization and renormalization group techniques, suitably dealing with weak-coupling cases.[11,34] In the following, we shall provide a more general and straightforward argument.

We start with the following well-known identity in the many-body theory:

$$\langle\Psi_0|[\hat{O}^\dagger,[H,\hat{O}]]|\Psi_0\rangle=\sum_n (E_n-E_0)(|\langle\Psi_0|\hat{O}|\Psi_n\rangle|^2 + |\langle\Psi_0|\hat{O}^\dagger|\Psi_n\rangle|^2), \tag{6}$$

where $\hat{O}$ is an arbitrary operator. The sum on the right-hand side of Eq. (6) is over all the eigenvectors Ψ_n of the Hamiltonian. We observe that, when $\langle\Psi_0|\hat{O}|\Psi_0\rangle=0$, this sum is larger than $[E_1(\hat{O})-E_0]\langle\Psi_0|\hat{O}^\dagger\hat{O}|\Psi_0\rangle$, where $E_1(\hat{O})$ denotes the energy of the first excited state Ψ_1, which contributes a nonzero matrix element $\langle\Psi_1|\hat{O}|\Psi_0\rangle$. Now, we take $\hat{O}$ for the SDW, CDW, or BOW ordering operators. It is easy to check that the left-hand side of Eq. (6) is actually a quantity of order $O(1)$ in the thermodynamic limit since the hopping and the interaction terms in Hamiltonian (1) are short ranged. This fact implies that, if the system has a certain type of ordering, say the SDW ordering, and the corresponding correlation function diverges in the thermodynamic limit, then the energy difference $E_1(\hat{O})-E_0$ must tend to zero. Therefore, in different ordered phases, the low-lying excited states of Hamiltonian (1) should have different symmetries, which are required by the selection rules of the corresponding ordering operators.

As a result, when level-crossing of the global ground state is absent, a quantum phase transition can only be induced by a reconstruction of low-excitation spectrum of the system. Take the extended Hubbard model, for example. In the SDW insulating phase, it is known that the spin-triplet eigenstates are low-lying excitations. On the other hand, the CDW ordering is caused by a low-lying excitation spectrum of spin-singlet states. Consequently, these low-lying excitation states must cross over each other at the border between the SDW phase and the CDW phase. Other interesting examples are the ionic Hubbard model[16–22] and some exactly soluble two-dimensional quantum spin models.[35] In the former model, as the on-site Coulomb repulsion U changes, the system undergoes transition from band insulator to spontaneously dimerized and to Mott insulating phases. While at the same time, one observes that the first excited state varies from spin triplet to spin singlet and to spin triplet.[16,17,22] In the latter models, we found that, at the phase transition point, the first excited state changes from triplet to singlet, while the ground state remains to be a nondegenerate and completely dimerized state.[35] As one expects, the change of symmetries of the low-lying excitation states in these cases are commanded by the selection rules of the ordering operators characterizing the corresponding phase. In other words, the accidental degeneracies of these low-lying excitation states, which are caused by the existence of a higher symmetry of the Hamiltonian,[36] determine the quantum phase-transition points.

Here, we would like to make a remark on the previous result on the Kosterlitz-Thouless (KT)-type quantum phase transition observed in some one-dimensional systems. In some limiting cases, such as $W=0$, $\Delta=0$ or $W=0$, $X=0$, Hamiltonian (1) can be mapped into a Sine-Gordon model, by taking the continuum limit and applying the bosonization transformation.[11,34] A KT-type quantum phase transition is observed. By the definition of bosonization, the Sine-Gordon model actually describes the excitation spectrum of the system, so it is the change in the excited states that causes the phase transition. This conclusion is completely consistent with our general theorem proved in this work. On the other hand, not all quantum phase transitions appear in the model Hamiltonian (1), especially with correlated hopping interactions, could be correctly described by the Sine-Gordon model even qualitatively.

Another important and related issue, which we would like to discuss briefly, is whether the phase transitions in these models are always continuous, like the XXZ model at the isotropic Heisenberg point. A careful investigation shows that, although their ground states are nondegenerate on finite-size chains, a cusp on the curve of E_0 may still develop in the thermodynamic limit, as shown in Fig. 10 of Ref. 12. It is caused by the so-called avoided level-crossing phenomenon.[37] Notice that the curve of E_0 approaches to that of the first excited state energy without crossing in this limit, as we showed above. On the other hand, the latter has a cusp at the transition point since an excited states level

crossing occurs there. Consequently, a cusp may also be squeezed out on the former at the same point as the chain tends to infinity.

Finally, we would like to emphasize that, except the conditions on parameters W and X, connectivity of the lattice as well as the configurations $\{\phi_\alpha\}$ by electron hopping is also of fundamental importance in establishing the nondegeneracy of the global ground state. Therefore, one expects that this theorem could be violated in either the case of $W>0$ or the atomic limit with $T_i(\overline{\sigma}),\rangle X$, and W tending to zero. Under these circumstances, the global ground state $\Psi_0(N)$ of H in a specific subspace $V(N)$ may be degenerate for some parameters U_0, V_0, and Δ_0, and accompanied by a first-order phase transition.[25] We should also mention that our theorem does not apply to some one-dimensional fermion models, especially to those integrable models as discussed in Refs. 38–41. These models usually posses higher symmetries that induce degeneracy and level crossing in its eigenvalue spectrum, and consequently, quantum phase transitions at corresponding integrable points. On the other hand, our theorem does apply to the one-dimensional Hubbard model, which is integrable.

To summarize, in the present work, we show that, in a wide class of one-dimensional correlated fermionic models, such as the extended Hubbard model and the ionic Hubbard model, the global ground state of the system is nondegenerate under a properly chosen boundary condition. Consequently, all the physical quantities change continuously as parameters vary and there exists no energy level crossing. We emphasize the important role played by level crossing of the low-lying excited states in inducing the quantum phase transition in the systems.

We are grateful to A. W. Sandvik and D. K. Campbell for helpful comments. G. S. Tian wishes to thank the department of physics at the Chinese University of Hong Kong for its hospitality and the support of this work through the ''Incentive Fund Program.''

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