Transition from band insulator to Mott insulator in one dimension: Critical behavior and phase diagram

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(Dated: March 21, 2022)

We report a systematic study of the transition from band insulator (BI) to Mott insulator (MI) in a one-dimensional Hubbard model with an on-site Coulomb interaction $U$ and an alternating periodic site potential $V$. We employ both the zero-temperature density matrix renormalization group (DMRG) method to determine the gap and critical behavior of the system and the finite-temperature transfer matrix renormalization group (TMRG) method to evaluate the thermodynamic properties. We find two critical points at $U = U_c$ and $U = U_s$ that separate the BI and MI phases for a given $V$. A charge-neutral spin-singlet exciton band develops in the BI phase ($U < U_c$) and drops below the band gap when $U$ exceeds a special point $U_s$. The exciton gap closes at the first critical point $U_c$ while the charge and spin gaps persist and coincide between $U_c < U < U_s$ where the system is dimerized. Both the charge and spin gaps collapse at $U = U_s$ when the transition to the MI phase occurs. In the MI phase ($U > U_s$) the charge gap increases almost linearly with $U$ while the spin gap remains zero. These findings clarify earlier published results on the same model and offer new insights into several important issues regarding appropriate scaling analysis of DMRG data and a full physical picture for the delicate nature of the phase transitions driven by electron correlation. The present work provides a comprehensive understanding for the critical behavior and phase diagram for the transition from BI to MI in one-dimensional correlated electron systems with a periodic alternating site potential.

PACS numbers: 71.30.+h, 71.10.Pm, 77.80.-e

I. INTRODUCTION

The nature of the insulating ground state of interacting electron systems has been a subject of long-standing interest and debate in condensed matter physics. Because of strong quantum effects caused by spatial confinement and technical advantages for theoretical treatment, one-dimensional (1D) electron systems have been most extensively studied. Strong correlation effects in 1D lead to the separation (decoupling) of charge and spin degrees of freedom. Starting from a gapless phase with charge-spin separated excitations, interactions can drive the system into new phases of different characteristics with (i) gapful charge excitations only, (ii) gapful spin excitations only, or (iii) co-existing gapful charge and spin excitations. For phases with both charge and spin excitations gapful, the charge and spin degrees of freedom are rarely decoupled. Despite these findings, there remain important unresolved issues regarding the quantum nature of the insulating state in 1D interacting electron systems and the phase transitions driven by the electron correlation. The first issue concerns the establishment of an accurate phase diagram and the critical behavior near the phase boundaries. Secondly, a band insulator (BI) with quasi-particle excitations typically cannot be characterized by charge and spin excitations. A proper characterization scheme needs to be developed. Most importantly, the nature of the correlation-driven transition from BI to Mott insulator (MI) is still not fully understood.

There has been considerable recent interest in the study of a prototype one-dimensional model for ferroelectric perovskites for the understanding of the response of strongly correlated electron systems with lattice distortions. These efforts have raised and addressed some fundamental issues in the nature of the quantum phase transition and the related critical behavior in 1D interacting electron systems. Earlier works mainly deal with the effects of strong electron correlation on the electron-lattice interaction and the polarization effects in the insulator. Quantum phase transitions and the characterization of the insulating state are the focus of more recent work [6,7,8,9,10,11,12,13,14]. In particular, an issue of fascinating debate is the nature of the transition (or crossover) from the BI phase to the MI phases. Gidopoulos et al. showed that due to the reversal of inversion symmetry of the ground state from BI to MI, there is a critical point for spin excitations. However, for charge excitations the critical behavior is less clear. Recently, Fabrizio et al. developed an effective field theory for this problem and showed that there are two continuous transitions from BI to MI. One is a spin transition of the Kosterlitz-Thouless type at a critical point $U = U_s$, and the other is an exciton transition at an Ising critical point $U = U_c < U_s$ where the exciton gap closes. Between $U_c$ and $U_s$, the site-parity is spontaneously broken and the system is characterized by a doubly degenerate, dimerized ground state. These results raise interesting questions about the structure of the ground-state phase.
diagram of 1D interacting electron systems and the characterization of the critical behavior near the transition points from the BI phase to the MI phase.

The model Hamiltonian for the system of interest is defined in the Hubbard formalism at half-filling:

\[ H = \sum_{i\sigma} \left[ -t \left( c_{i\sigma}^\dagger c_{i+1\sigma} + \text{h.c.} \right) + V (-1)^i n_{i\sigma} \right] + U \sum_i \left( n_{i\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right), \]

where \( c_{i\sigma}^\dagger \) and \( n_{i\sigma} \) are the electron creation and number operators at site \( i \), \( U > 0 \) is the on-site Coulomb repulsion, and \( V \) is the staggered site chemical potential. This model captures the key ingredients of one-dimensional correlated insulators with mixed ionic-covalent characters, such as oxide dielectric materials and quasi-1D organic charge-transfer complexes. It incorporates covalency, ionicity, and strong electron correlation.

In this paper, we present the results of extensive calculations for Hamiltonian (1) using both the zero-temperature density matrix renormalization group (DMRG) method and the finite-temperature transfer matrix renormalization group (TMRG) method. These methods have been demonstrated to be highly accurate for 1D interacting electron systems. Our aim is to systematically examine and clarify issues raised in recent work and to provide a comprehensive understanding for the transition from BI to MI in one dimension. We show detailed results on the gap and critical behavior. We find that a charge-neutral spin-singlet exciton band forms in the BI phase and drops below the band gap as \( U \) increases beyond a special point \( U_{c} \). With increasing \( U \), the excitons then condense and the system enters a dimerized phase, followed by the closure of the quasi-particle (both spin and charge) gap when the system enters the MI phase. We clarify basic concepts on charge and spin excitations studied in recent work. Our results support the conclusion of Fabrizio et al. on the existence of two critical points for the transition from BI to MI. We also present detailed results on the formation of the exciton band and the scaling behavior near the critical points. In addition, we carry out TMRG calculations to study thermodynamic properties to further elucidate the gap and critical behavior of the system.

II. LOW-ENERGY EXCITATIONS

To properly characterize the BI and MI phases and establish the phase diagram, we need to evaluate the behavior of several low-energy excitations, including the charge and spin excitations and an exciton excitation that will be used to characterize the BI phase. We calculate the following three excitation gaps defined on a finite 1D lattice of length \( L \) (chosen as an even integer) at half-filling: (i) the singlet exciton gap \( \Delta_{e}(L) \), (ii) the charge gap \( \Delta_{c}(L) \), and (iii) the spin-triplet gap \( \Delta_{s}(L) \),

\[ \Delta_{c}(L) = E_{1}(\frac{L}{2}, \frac{L}{2}) - E_{0}(\frac{L}{2}, \frac{L}{2}), \]

\[ \Delta_{s}(L) = E_{0}(\frac{L}{2} + 1, \frac{L}{2} + 1) + E_{0}(\frac{L}{2} - 1, \frac{L}{2}) - 2E_{0}(\frac{L}{2}, \frac{L}{2}), \]

\[ \Delta_{s}(L) = E_{0}(\frac{L}{2}, \frac{L}{2} + 1) - E_{0}(\frac{L}{2}, \frac{L}{2}), \]

where \( E_{0}(N_{\uparrow}, N_{\downarrow}) \) is the lowest energy of the system with \( N_{\uparrow} \) up and \( N_{\downarrow} \) down spin electrons, and \( E_{1}(N_{\uparrow}, N_{\downarrow}) \) is the lowest energy of the singlet excitations. For the charge gap \( \Delta_{c} \), there is an alternative definition

\[ \Delta_{c}(L) = E(\frac{L}{2} + 1, \frac{L}{2} + 1) - E(\frac{L}{2}, \frac{L}{2}). \]

For the model studied in this work, these two definitions on the charge gap give the same results in the thermodynamic limit. This is supported by our numerical calculations. However, since the numerical accuracy is much higher in calculating \( \Delta_{c} \) by using Eq. (9) than by using Eq. (6), we use Eq. (6) in all the reported calculations.

Although \( \Delta_{c} \) and \( \Delta_{s} \) are usually considered to be the charge gap and the spin gap, respectively, in the literature, \( \Delta_{c} \) in fact is the chemical potential jump for particles in the system. It measures the chemical potential jump of putting a particle into or taking a particle out of the system. Only when the charge and spin excitations are separated and the spin gap is zero, \( \Delta_{c} \) is equal to the charge excitation gap as, for example, in the standard Hubbard model (Eq. [1] with \( V = 0 \) or \( U \to \infty \)). When the charge and spin excitations are not separated, or when the spin gap is not zero, the chemical potential jump is not equal to the charge excitation gap.

At half-filling, the first excitation state can be either a spin singlet or a spin triplet and \( \Delta_{e} \) never exceeds \( \Delta_{s} \). When \( \Delta_{c} < \Delta_{s} \), the first excitation state must be a charge-neutral spin-singlet state; otherwise, \( \Delta_{c} \) equals \( \Delta_{s} \) and measures the excitation gap of an exciton band.

In the presence of a nonzero \( V \) in the Hamiltonian, the MI phase is reached when \( U \) is large (including the limit \( U \to \infty \)). In the MI phase, it is well understood that the charge gap is non-zero, but the spin gap is zero. Therefore \( \Delta_{c} \) is the charge excitation gap. Meanwhile, both \( \Delta_{s} \) and \( \Delta_{e} \) are zero and the gapless elementary excitations in the system are spinons.

In the BI phase, all the elementary excitations are gapful. Let \( u_{k\sigma}^\dagger \) and \( d_{k\sigma}^\dagger \) be the creation operators for particles in the upper conducting band and for the holes in the lower valence band. The Hamiltonian for free particles at \( U = 0 \) is

\[ H = \sum_{k\sigma} \varepsilon_{k} \left( u_{k\sigma}^\dagger u_{k\sigma} - v_{k\sigma}^\dagger v_{k\sigma} \right), \]

where \( k \) is the momentum, \( \sigma \) is the spin index, and \( \varepsilon_{k} = \sqrt{V^{2} + 4E^{2} \cos^{2} k} \). We have \( u_{k\sigma}(GS) = v_{k\sigma}^\dagger(GS) = 0 \) for the ground state (GS) at half filling with \( u_{k\sigma} \) being the annihilation operator for electrons in the conduction band, and \( v_{k\sigma}^\dagger \) the creation operator for electrons.
in the valence band. For particle-hole excitations with one particle and one hole in the system, it is clear that \( \Delta_s = \Delta_s = \Delta_e = 2V \).

When \( U \) is small in the BI phase, the particle or hole excitations become dressed quasi-particles, and \( \Delta_e \) measures the chemical potential jump of the particles. Since the charge and spin degrees of freedom are not separated, \( \Delta_e \) is not exactly the "charge gap" derived from the gapless charge-spin separated excitations in the field theoretical approach. If the particles and holes are not bounded, then \( \Delta_s = \Delta_s = \Delta_e = 0 \). However, the particle-hole excitations may bound to form excitons, and result in an exciton gap smaller than \( \Delta_e \). It is confirmed by our DMRG calculations shown below that \( \Delta_e \) equals \( \Delta_e \) when \( U \) is small, but becomes smaller than \( \Delta_e \) when \( U \) exceeds a special point \( U_c \), indicating the formation of singlet excitons. Meanwhile, the calculations show that \( \Delta_s = \Delta_e \) is always observed, indicating that there is no triplet exciton formation in the BI phase.

The DMRG calculations also show that in the BI phase the exciton gap and quasi-particle excitation gap decrease and approach zero with increasing \( U \) and the exciton gap closes at the first critical point \( U_c \). The exciton gap closes when \( \Delta_s = \Delta_s = \Delta_e = 0 \). When \( U \) exceeds \( U_c \), \( \Delta_s \) and \( \Delta_e \) remain zero but \( \Delta_e \) increases almost linearly with \( U \). Therefore, \( \Delta_s \) is the point where the quasi-particle excitation gap in the BI phase collapses, and spinons in the MI phase form. This picture is consistent with that of the recent field theoretical studies.

From the physical picture outlined above, it is clear that there are three special points \( U_e \), \( U_s \), and \( U_s \) along the \( U \) scale. Among them \( U_e \) and \( U_s \) are two critical points separating the BI and MI phases while \( U_e \) is a special point signaling the formation of the spin-singlet exciton band in the BI phase. In the thermodynamic limit for a given \( V \) the system can be divided into the following regions:

1. \( 0 < U < U_e \), \( \Delta_e = \Delta_e = \Delta_s \neq 0 \), gapful quasi-particle excitations only.
2. \( U_e < U < U_s \), \( 0 < \Delta_e < \Delta_e = \Delta_s \), gapful quasi-particle excitations coexist with singlet particle-hole excitations that bound to form excitons.
3. \( U = U_e \), \( \Delta_e = 0 \), \( \Delta_e = \Delta_e > 0 \), the system is critical for exciton excitations.
4. \( U_e < U < U_s \), \( \Delta_e < \Delta_e = \Delta_s \), excitons condense, and the system is dimerized.
5. \( U = U_s \), \( \Delta_e = \Delta_e = \Delta_s = 0 \), the system is critical for quasi-particle excitations.
6. \( U > U_s \), \( \Delta_e = \Delta_e = \Delta_s = 0 \), \( \Delta_e > 0 \), gapless spinon excitations in the MI phase; the particle-hole picture breaks down.

In the following we present the calculated results on the gap and critical behavior leading to the establishment of the phase diagram. In all reported calculations, free boundary conditions are used in the zero-temperature DMRG calculation. For a finite size system, we can show rigorously using the variational principle that the lowest energy state of the Hamiltonian \( H \) with free boundary conditions in each \( (N_\uparrow, N_\downarrow) \) subspace is non-degenerate except for an up-down spin degeneracy. Therefore there is no level crossing with the lowest energy state in the \( (N_\uparrow, N_\downarrow) \) subspace and \( E_0(N_\uparrow, N_\downarrow) \) is an analytic function of \( U \) and \( V \). From this property and Eqs. (3) and (4), we can further show that \( \Delta_e(L) \) and \( \Delta_s(L) \) are also analytic functions of \( U \) and \( V \). In this work we focus on two values of the staggered potential \( V = 0.3t \) and 1.0t and study the behavior of the three gaps introduced above in response to the on-site Coulomb repulsion \( U \).

III. EXCITATION GAPS

For fermion systems, the truncation error of DMRG iterations is generally much smaller than that of spin systems when the same number of optimal states are retained. The efficiency of the finite system DMRG method is related to the truncation error; the bigger the truncation error is, the larger the improvement of the finite lattice sweeping can make. We used both finite and infinite lattice DMRG algorithms in testing calculations. We find that the improvement of the ground-state energy made with the finite lattice sweeping is very small when a large number of states are retained. A better way to increase the accuracy of the results is using the infinity lattice approach by retaining more states.

Figure (a) shows the behaviors of \( \Delta_e \), \( \Delta_e \), and \( \Delta_e \) as a function of \( 1/L \) for different \( U \) at \( V = 1.0t \). For \( V = 0.3t \), similar results can be drawn but the \( V = 1.0t \) case is more accurate because most of the features can be seen when the chain length is short, while in the \( V = 0.3t \) case, very long chains need to be used to obtain the same results. Figure (b) presents the results for \( U = 2.0t \) and clearly shows that the three gaps converge to the same finite value in the thermodynamic limit. The difference between these gaps shown in Fig. (b) also displays this feature clearly. When the chain length is short, the exciton gap is larger than the spin gap, and level crossing happens at a finite chain length where the exciton gap drops lower thereafter. The exciton gap decreases continually and reaches a minimum when the chain length increases further; it then starts to increase and converge to the value of the spin and charge gaps. For \( U = 3.0t \), in Fig. (c) and (d), the spin gap and charge gap still converge to the same value in the thermodynamic limit, but the exciton gap goes to a different value lower than the other two gaps. In short chains, the exciton gap is still larger than the spin gap, but after they cross each other, the exciton gap decreases monotonically. One can also see that the second state in the singlet sector also crosses
the spin and charge gap and converges to the lowest state when $L \rightarrow \infty$. In our calculations, we also see that more states in the singlet sector cross the spin and charge gap with increasing chain length. This shows that the whole spectrum of the exciton sector decreases in value and the exciton gap is indeed different from the other two gaps. For the case of $U = 4.0t$, shown in Fig. 1(e) and (f), no level crossing for different chain length is detected. All three gaps decrease monotonically when the chain length increases. The exciton gap and the spin gap approach zero at infinite chain length, indicating that there is no gap for the exciton and spin sectors. Meanwhile, the charge gap approaches a finite value in the thermodynamic limit.

For all the cases we have studied, $\Delta_c$ decreases monotonically with increasing $L$. However, the size dependence of $\Delta_s$ is more complicated. In certain ranges of $U/t$ and $V/t$ close to the critical regimes, including the case shown in Fig. 1(a) and (c), $\Delta_s$ and $\Delta_c$ vary non-monotonically and their minima are located at a finite $L = L_{\text{min}}$ rather than at $L = \infty$. In a recent work\textsuperscript{20}, the authors studied the same model Hamiltonian $\mathbf{(1)}$ using the DMRG method but did not observe such non-monotonically behavior, and suggested that such a behavior may be due to the loss of accuracy in DMRG calculations when the chain length is increased or due to some intrinsic length scale for the spin degree of freedom. We have carefully examined this issue by carrying out extensive scaling analysis. We demonstrate that the non-monotonical behavior is not due to the lack of accuracy of the calculations, instead the behavior is a true feature of Hamiltonian $\mathbf{(1)}$ with the open boundary condition (OBC). Figure 2 shows the chain length dependence of the spin gap for $U = 2.5t$ and $V = 1.0t$ calculated by retaining different numbers of optimal states $m = 300, 400, 500,$ and $800$. One can see that the minimum occurs at $L \sim 30$; at this length the accuracy of the DMRG calculations are still very high. More significantly, the results for different $m$ fall onto the same curve (except for the cases of $L > 100$ and $m = 300$). It shows unambiguously the existence of the minimum of $\Delta_s$ in its dependence on the chain length. For the exciton gap $\Delta_e$, the situation is the same. In fact the occurrence of a gap minimum at a finite $L$ is not an uncommon feature for a system with incommensurate low-lying excitations. It suggests that the spin excitations of the model Hamiltonian $\mathbf{(1)}$ maybe incommensurate with a characteristic wave vector defined by $2\pi/L_{\text{min}}$ (or $\pi - 2\pi/L_{\text{min}}$) in some area of the phase space.

Comparing Fig. 1(a) and (c), it is clear that there is a special point $U_e$, where the exciton gap begins to deviate from the spin gap (for $V = 1.0t$, $2.0t < U_e < 3.0t$). In both cases, all three excitations are gapful. The system is in the same (BI) phase as the $U = 0$ case, where $\Delta_s = \Delta_e = \Delta_c = 2V$ in the thermodynamic limit. Here particle-hole excitations bound into excitons by the Coulomb interaction at $U > U_e$. Fig. 3 shows the difference $\Delta_s - \Delta_e$ for $V = 1.0t$ and $0.3t$. The fitting to DMRG results gives the critical value $U_e = 2.264t$ for $V = 1.0t$ and $U_e = 1.276t$ for $V = 0.3t$.

For finite $L$ we find that $\Delta_e$ is always larger than $\Delta_s$. In
the MI phase, $\Delta_c$ is finite but $\Delta_s$ approaches zero in the thermodynamic limit. In the BI phase, $\Delta_s$ and $\Delta_e$ always approach the same value in the thermodynamic limit. This can be seen either from the asymptotic behaviors of $\Delta_s$ and $\Delta_e$ in the limit $L \to \infty$ [Fig. 1(a) and (c)] or from the $1/L$ dependence of the difference $\Delta_s - \Delta_e$ (Fig. 1(b) and (d)). For all the cases we have studied, we find that $\Delta_s - \Delta_e$ drops monotonically and approaches zero in the limit $1/L \to 0$ even when $\Delta_s$ changes non-monotonically.

For a given $V$, this result holds from $U = 0$ up to a critical regime where both $\Delta_e$ and $\Delta_s$ become smaller than truncation errors. It suggests that $\Delta_c$ and $\Delta_s$ are equal in the thermodynamic limit in the entire BI phase.

When $\Delta_s$ changes non-monotonically with $L$, the extrapolation for the spin gap in the limit $1/L \to 0$ becomes subtle. If the data with $L < L_{\text{min}}$ are used in the extrapolation, the extrapolated value of $\Delta_s$ will certainly be smaller than the true value. However, if the data with $L > L_{\text{min}}$ is used but $L$ is still not large enough to reach the regime where $\Delta_s$ begins to saturate, the extrapolated value of $\Delta_s$ will be smaller than the true value (this seems to be the case in Ref. [27]). For the data shown in Fig. 1(a) and (c), these two kinds of extrapolations result in $\Delta_c > \Delta_s$ and $\Delta_c < \Delta_s$, respectively. Both are incorrect.

To correctly extrapolate $\Delta_s$ in the limit $1/L \to 0$, data with $L$ much larger than $L_{\text{min}}$ must be used.

For the $U = 4.0t$ case shown in Fig. 1(e), $\Delta_c$ is finite but $\Delta_s$ becomes zero in the thermodynamic limit. This indicates that the system is in the same phase as that for $U \to \infty$, namely the MI phase. In the MI phase, the chain length dependence of the three gaps are monotonical; in addition, there is no crossing between $\Delta_s$ and $\Delta_e$ when the chain length varies. In the $L \to \infty$ limit the spin gap $\Delta_s$ is zero in the MI phase suggesting that there is a critical point that separates the MI phase from the BI phase. At this critical point $U_s$, the spin gap vanishes. Because the charge gap is equal to the spin gap in the BI phase, the charge gap will also vanish at the same point $U_s$. However, when $U$ increases further, the charge gap increases with $U$ while the spin gap remains zero. Considering that the exciton gap is lower than the spin gap in the BI phase at $U > U_s$, $\Delta_e$ may vanish before the spin gap and charge gap do. In that case, there should be another critical point $U_c$ signaling the collapse of the exciton gap.

In Fig. 4 we show the $U$ dependence of the three gaps for $V = 0.3t$ [(a) and (b)] and $V = 1.0t$ [(c) and (d)]. For both cases, there are indeed two critical points $U_c$ and $U_s$ although they are very close. When $U < U_c$, $\Delta_e = \Delta_s = \Delta_c$, and the three gaps decrease almost linearly with increasing $U$. At $U_s$, the exciton gap splits off and drops below the other two gaps. At the critical point $U_c$,...
the exciton gap collapses while the spin and charge gaps still coincide and remain finite until the second critical point $U_s$, where they both collapse. At $U > U_s$, the charge gap increases with increasing $U$ while the spin gap and the exciton gap remain zero in the thermodynamic limit. Although the accuracy of our DMRG calculations do not allow a direct assessment of the behavior of the exciton gap for $U_c < U < U_s$, we believe that $\Delta_c$ is finite in this region (see more detailed discussion on this point in the following section). The extrapolation of the gap behavior leads to $U_c \sim 2.225t$ and $U_s \sim 2.265t$ for $V = 0.3t$, while $U_c \sim 3.675t$, $U_s \sim 3.71t$ for $V = 1.0t$.

It is clear that the $U$ dependence of the three gaps is similar for $V = 0.3t$ and $V = 1.0t$. It is expected that the same picture is valid for all $V$. Furthermore, $U_c$, $U_e$, and $U_s$ all approach the same point $U_{\infty} = 2V$ in the $V \to \infty$ limit.

IV. CRITICAL BEHAVIOR

![Graphs showing critical behavior](image)

**FIG. 5**: The behavior of the charge gap in the vicinity of $U_s$ for $V = 0.3t$. (a) The chain length dependence of the charge gap at $U = 2.22t$ for different numbers of optimal states retained: $m=200$ (filled circles), 250 (empty squares), 300 (empty circles) and 400 (filled squares); (b) The dependence of the charge gap on the number of the retained states at $L=300$ with $U = 2.22t$; (c) The charge gap for $m \to \infty$ with different chain lengths: $L = 300$ (empty circles), 400 (filled circles), 500 (empty squares) and 600 (filled circles) in the vicinity of the critical region; the fitting lines using eq. (8) are also shown; (d) The chain length dependence of $\Delta_{c,\min}(L)$; (e) The chain length dependence of $U_{s,L}/t$; (f) The chain length dependence of $\alpha_{c,L}$.

From the gap behavior presented in the previous section, it is clear that there are two critical points $U_c$ and $U_e$ for Hamiltonian $H$ for a given $V$. It is important to study the detailed critical behavior near the critical points for the understanding of the nature of the BI-to-MI transition. In the following we study the critical behavior of the system by examining (i) the evolution of the gap behavior near the critical points and (ii) the behavior of the ground-state energy of the system.

A. Analysis of the gap behavior

The $U$ dependence of the gaps shows that the charge instability occurs at the same point as that for the spin transition. To determine the critical points for the charge and spin excitations, we examine when $\Delta_c$ and $\Delta_s$ become zero in the limit $L \to \infty$. Since the numerical errors are larger than the magnitude of $\Delta_c$ or $\Delta_s$, in the vicinity of the critical points, it is difficult to determine accurately the critical behavior simply from the values of the energy gaps. To resolve this issue, we analyze the scaling behavior of $\Delta_c(L)$ around its minimum with respect to $U$. However, the DMRG results of $\Delta_c(L)$ depend the number of states $m$ retained during the iterations. When the chain length is long enough, the difference due to retaining different number of states show clearly. In Fig. 5 (a), we show the chain length dependence of the charge gap at $U = 2.22t$ and $V = 0.3t$ by keeping different $m$. The difference is obvious. This problem can be solved by employing the extrapolation in the limit of $m \to \infty$. For given $U$ and $V$, the charge gap at chain length $L$ and by keeping $m$ states is $\Delta_c(m, L)$. By extrapolating to the infinite $m$ limit, more accurate result of the charge gap at chain length $L$ can be obtained,

$$\Delta_c(\infty, L) = \lim_{m \to \infty} \Delta_c(m, L).$$

In Fig. 5 (b), we show the $1/m$ dependence and the extrapolation procedure of the $\Delta_c(m, L)$ for $L=300$ at $U = 2.22t$ and $V = 0.3t$. The extrapolated result $\Delta_c(\infty, L)$ is considered the exact charge gap $\Delta_c(L)$ at chain length $L$.

The extrapolated charge gap $\Delta_c(\infty, L)$ is a function of $U$ and chain length $L$ at a given $V$. By applying the same procedure shown in Fig. 5 (b), we obtain $\Delta_c(\infty, L)$ for different values of $U$ near the critical point $U_s$ for a serial of selected $L$. In Fig. 5 (c), we show the $U$ dependence of $\Delta_c(L)$ ($\Delta_c(\infty, L)$) in the vicinity of the critical point $U_c$ at chain length $L = 300, 400, 500,$ and 600, respectively, for $V=0.3t$. A gap minimum at finite chain length is clearly seen. Assuming $\Delta_{c,\min}(L)$ to be the minimum of $\Delta_c(L)$ located at $U_{s,L}$, then around this minimum we can expand $\Delta_c(L)$ to the leading order of the parameter $u = U - U_s$ as

$$\Delta_c(L) = \Delta_{c,\min}(L) + \alpha_c(L) u^2 + O(u^3).$$

Since $\Delta_c(L)$ is an analytic function of $U$, both $\Delta_{c,\min}(L)$ and $\alpha_c(L)$ should be finite. The critical behavior of
satisfies $c(U) - U_{\text{c}}$ in the limit $L \to \infty$. If $\Delta_{c,\text{min}}(L) \to 0$ in the limit $L \to \infty$, the charge excitation is critical at $U_s = U_{\text{c},\infty}$, which would be consistent with the discussion in the previous section. However, if $\Delta_{c,\text{min}}$ remains finite in the limit $L \to \infty$, then there is no critical point for charge excitations and the ground state is insulating in the entire parameter space.

Figure 5(d) shows the calculated $\Delta_{c,\text{min}}(L)$ as a function of $1/L$. The solid curve is a least-square fit of the data and given by $\Delta_{c,\text{min}}(L) \approx 17.894/L - 729.785/L^2$. Within numerical errors, we find that $\Delta_{c,\text{min}}(L)$ is indeed 0 in the limit $1/L \to 0$. Figure 5(e) shows the $L$ dependence of $U_{s,L}$. It changes almost linearly with $1/L$. Within numerical errors, we find that the data of $U_{s,L}$ are well fitted by $U_{s,L}/t = 2.265 - 22.532/L$. Thus the critical point is at $U_{c}/t = 2.265t$, in full agreement with the value obtained by fitting the gap directly in the previous section.

We now turn to the critical behavior of $\alpha_c(L)$. Figure 4(f) shows the $1/L$ dependence of $\alpha_c(L)$ for the case $V = 0.3t$. The fitting curve (solid line) is given by $-0.323 + 0.0091L$. The divergence of $\alpha_c(L)$ suggests that the derivative of $\Delta_c(L)$ is singular at $U_{c}$ and the leading term in $\Delta_c$ in the thermodynamic limit is linear rather than quadratic in $u$, i.e., $\Delta_c(U) \sim |U - U_s|$.

### B. Analysis of the ground-state energy

The ground-state energy as the zero-temperature free energy can also provide evidence for the critical behavior. However, singularities in the ground-state energy are of higher order derivatives with respect to the model parameter for continuous phase transitions. As a result, evidence for critical behavior derived from the ground-state energy is not as strong as that from the gap behavior, this despite the higher accuracy of the ground-state energy per site for $U < U_c$.

We have calculated the ground-state energy in the critical region by retaining $m=800$ states and up to chain length $L=1000$. For Hamiltonian (1), with open boundary conditions, the ground-state energy per site $e_0(L)$ satisfies

$$e_0(L) = \frac{E_0(L)}{L} = e_0 + \frac{e_b}{L} + \frac{c}{L^2} + O(\frac{1}{L^3}),$$  

where $E_0(L)$ is the ground-state energy for a chain of length $L$, $e_0$ the ground-state energy per site for $L \to \infty$, $e_b$ is the boundary energy (surface energy) due to the free boundary condition, and $c = v \pi$ where $v$ is the spin wave velocity. When $U > U_{c}$, the system is gapful and $c$ should approach zero when the chain length is much larger than the correlation length $\xi$.

The $V = 0.3t$, $L > 200$ ground-state energy results are fitted directly by

$$e_0(L) = e_0 + \frac{e_b}{L} + \frac{c}{L^2},$$  

and the obtained results are shown in Fig. 4(a), (b) and (c). $e_0$ and $e_b$ are analytic functions of $U$. For $c$, Fig. 4(c) shows that it is not only non-zero for $U < U_c$ but also has a fairly large value. This is due to the finite chain length effect. The value of $c$ depends very sensitively on the chain length range used for fitting.

To analyze the chain length dependence of $c$, we fit the ground-state energy for $L = 20$, $L = 100$ and vary $L$ from 24 to 980. Each fitting gives the exact result of $e_0(L)$, $e_b(L)$ and $c(L)$. In Fig. 4(d), we show the $L$ dependence of $c(L)$ for $U = 1.5t$, $U = 2.0t$ and $U = 2.2t$. It is clear that for $U = 1.5t$ and $2.0t$, $c(L)$ becomes zero when $L \to \infty$. The result of $U = 2.2t$ shows a minimum at $L \sim 90$, and the $c(L)$ begins to approach zero after the minimum. For $U = 2.2t$, a minimum is also clearly seen. A comparison of these results leads to the conclusion that for $L \to \infty$, $c(L)$ will approach zero. The largest chain length used in the calculation is not long enough to obtain correct $c(L)$ values. However, the obtained $e_0(L)$ and $e_b(L)$ may display the critical behavior of $U_c$.

In Fig. 4(e) and (f), we show the results of $e_0(L) - e_0(L_0)$ and $e_b(L) - e_b(L_0)$ for $L_0 = 100$. These results show the existence of the critical point $U_c$. $L_0$ can be viewed as a characteristic length of the critical region.

From the $U$ dependence of $e_0$, it is possible to examine...
the type of transition at the critical points. A problem is that the fitting results shown in Fig. 6(a) include extra errors induced by the fitting method. To avoid this, we analyze the \( U \) dependence of the ground-state energy using a different approach.

![Graph](image1)

**FIG. 7:** (a) \( d^2e_0/dU^2 \) versus \( U \) for \( L = 500 \) (filled circles), 600 (filled squares), 800 (empty circles), 1000 (empty squares). The solid line is an extrapolation of the data to the limit \( L \rightarrow \infty \). Inset: Enlarged figure in the vicinity of the critical point \( U_c \). (b) The dependence of the \( d^2e_0/dU^2 \) with \( \ln(1/L) \) at \( U = 2.21t \) (empty squares), 2.25t (filled circles), 2.27t (empty circles). The solid fitting -0.00997 + 0.009ln(1/L) is the least square fitting for the \( U = 2.225t \) case.

At a finite chain length \( L \), the ground-state energy per site \( e_0(L) \) is also a function of \( U \). Here \( e_0(L) \) contains only the errors from the DMRG truncation. We can examine the derivatives of \( e_0(L) \) with respect to \( U \) and analyze their chain length dependence. In Fig. 7(a), we show the second derivative of \( e_0(L) \) with \( U \) for \( L = 500, 600, 800, \) and 1000. At each chain length, there is a minimum near \( U_c \) in the \( U \) dependence of the second derivative. When the chain length increases, the position of the minimum moves towards larger \( U \) and approaches \( U_c \) which is the critical point in the thermodynamic limit; meanwhile, the shape of the minimum becomes sharper. Fig. 7(b) shows the chain length dependence of the second derivative. It is clear that for \( U = 2.225t \sim U_c \), the second derivative diverges logarithmically with the chain length, but for other values of \( U \) the second derivative does not diverge. These observations suggest that the phase transition at \( U_c \) is of the second order. No singularity is found in the first derivative or the second derivative near the critical point \( U_c \). This means that the transition at \( U_c \) is higher than second order. These results are consistent with those reported by Fabrizio et al.

V. TMRG STUDY OF SPIN SUSCEPTIBILITY AND SPECIFIC HEAT

To gain more insight into the physics of the BI-to-MI transition, we have studied the thermodynamic properties of the model using the TMRG method which is implemented in the thermodynamic limit and can evaluate very accurately the thermodynamic quantities at low temperature for quasi-1D systems. In our calculations, we kept 250 optimal states. The calculated specific heat \( C_v \), charge susceptibility \( \chi_c \), and spin susceptibility \( \chi_s \) for \( U/t = 1.0, 2.25, 5.0 \) and \( V/t = 0.3 \) as a function of temperature are shown in Fig. 8.

![Graph](image2)

**FIG. 8:** Temperature dependences of (a) the spin susceptibility \( \chi_s \), (b) the charge susceptibility \( \chi_c \), and (c) the specific heat \( C_v \). (\( t \) is set to 1).

We find that \( \chi_c \) decreases exponentially at low temperatures in both the BI and MI phases, while \( \chi_s \) shows activated behavior only in the BI phase. In the MI phase, there are two broad peaks in \( C_v \), probably due to the charge-spin separation. Near the critical point, \( U = 2.25t \), since both the charge and spin energy gaps are very small, the exponential decays in both \( \chi_c \) and \( \chi_s \) show up only
at very low temperatures. These results support the conclusions of the DMRG calculations presented in previous sections.

VI. PHASE DIAGRAM

The overall $U$ dependence of the charge, spin and exciton gaps shown in Fig. 4 give a lot of information on the phase diagram of Hamiltonian $\mathbf{1}$. The charge and spin gaps coincide in the BI phase. Above $U_s$, $\Delta_c$ increases with $U$ but $\Delta_s$ remains zero. The exciton gap $\Delta_e$ collapses at $U_c < U_s$, and when $U > U_s$, the exciton gap should also be zero. However, from Fig. 4 it is unclear whether the exciton excitations are gapful or gapless in the regime between the two critical points, $U_c < U < U_s$. Even if the exciton excitations are gapful in this regime, the gap would be too small to detect numerically.

**Figure 9:** (a) Chain length dependence of the dimerization order parameter $D$ for $U = 2.21t$ (empty squares), $U = 2.29t$ (filled circles) and $U = 2.29t$ (empty circles). The straight fitting line is $0.045 + 3.886/L$. (b) $D(L)$ in the critical regime for $L=200$ (empty circles), 300 (filled circles), 400 (empty squares), and 500 (filled squares). The dotted lines indicate the two critical points.

When the exciton gap collapses, the excitons can condense into the ground state $\mathbf{15}$. In this case, the system is expected to be dimerized $\mathbf{15}$. Here we evaluate the dimerization order parameter

$$ D = \frac{1}{L} \sum_{i\sigma} (-1)^i (c_i^{\dagger} c_{i+1\sigma} + \text{h.c}) $$

(11)

Figure 9(a) shows the chain length dependence of the dimerization operator for different $U$. It is clear that for $U = 2.21t$, when $L \to \infty$, $D$ approaches zero. At $U = 2.29t$, $D$ just starts to fall at the largest chain length we studied; it is expected that it will approach zero as the chain length is long enough. For $U = 2.25t$, which is between the two critical points, it seems that $D$ will diverge to a nonzero constant. For a large range of chain lengths, the results can be well fitted by a straight line shown in Fig. 9(a). The dependence of the finite chain dimerization $D(L)$ on $U$ is shown in Fig. 9(b) for $L=200$, 300, 400, and 500. These results indicate that in the thermodynamic limit, the ground states are dimerized when $U_c < U < U_s$.

The dimerization of the ground state for $U_c < U < U_s$ suggests that the exciton excitations are gapful in this region. So the physical picture on the exciton excitation is emerging: the exciton gap formed in the BI phase collapses at the critical point $U_c$; with further increasing $U$, the (small) exciton gap will first increase, reach a maximum and then decrease and collapse again at $U_s$; at $U > U_s$, the exciton excitations remain critical.

**Figure 10:** The ground-state phase diagram for Hamiltonian $\mathbf{1}$. The empty circles denote the DMRG results. The curves of $U_s$ and $U_c$ are shown with solid lines that are very close to each other. The curve of $U_e$ is shown by the dashed line which does not indicate a phase transition line, but rather denotes a serial of special points. The dotted line is $U = 2V$ which is the limit for $V \to \infty$.

When $U \ll V$, first order perturbation leads to

$$ \Delta_s(U) = \Delta_c(U) \approx V - cU $$

(12)
where \( c = V \int_0^\pi d k (\sqrt{2\pi \varepsilon_k})^{-1} \) is a constant determined by the single-particle energy dispersion \( \varepsilon_k = \sqrt{V^2 + 4\varepsilon^2 \cos^2 k} \). Since \( \Delta_s(U) \) drops almost linearly with \( U/t \) in the BI phase, we can estimate the value of \( U_s \) from Eq. (12) as \( U_s \approx V/c \). In the limit \( V \to 0 \), we have

\[
V/t \approx c_1 e^{-c_2 t/U_s}, \quad \text{or} \quad U_s/t \approx -\frac{c_2}{\log(V/c_1 t)}, \quad (13)
\]

where \( c_1 \) and \( c_2 \) are two constants of order one. Figure 10 shows the ground-state phase diagram for Hamiltonian 11. The curve for \( U_s \) and \( V < 1.0t \) is obtained from Eq. (13). The parameters \( c_1 \) and \( c_2 \) are fixed by the two \( U_s \) values for \( V = 0.3t \) and \( V = 1.0t \). When \( V \to 0 \), \( U_s \) goes to zero but the ratio \( U_s/V \) diverges. In the limit \( U/t \to \infty \), \( U_s \) is very close to \( 2V \). The difference between \( U_s \) and \( 2V \) is of order \( t: U_s - 2V \sim t \).

VII. SUMMARY

We have carried out systematic studies using the DMRG and TMRG methods to examine the critical behavior of a one-dimensional Hubbard model with an alternating site potential in the transition from band insulator to Mott insulator. Based on extensive numerical calculations and analytic analysis, we have clarified several important issues raised in recent works and have established the ground-state phase diagram. We have identified two critical points, \( U_e \) and \( U_s \), that separate the BI and MI phases. When \( U > U_s \), the system is in the MI phase where the charge excitations are massive but the spin excitations are critical. When \( U < U_e \), the system behaves like a classic band insulator: the charge and spin excitation gaps coincide and a charge-neutral spin-singlet exciton band forms below the band gap when \( U \) exceeds a special point \( U_c \). Between the two critical points, excitons condense and the ground state is dimerized. These results are consistent with the conclusions of a recent field theoretical study of the same model. The present work provides a detailed account for the critical behavior in the BI-to-MI transition in one dimension for correlated electron systems and establishes a good understanding for its ground-state phase diagram.

Acknowledgments

We thank Y. L. Liu, R. Noack, and M. Fabrizio for helpful discussions and M. Tsuchiizu for bringing to our attention Refs. 8 and 11. This work was supported in part by the Department of Energy at the University of Nevada, Las Vegas, the NSF of China and the Special Funds for Major State Basic research Projects of China.

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