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# Phase diagram of the Hubbard chain with two atoms per cell

M. E. Torio,[1] A. A. Aligia,[2] and H. A. Ceccatto[1]
[1]*Instituto de Física Rosario, Consejo Nacional de Investigaciones Científicas y Técnicas and Universidad Nacional de Rosario, Boulevard 27 de Febrero 210 bis, (2000) Rosario, Argentina*
[2]*Centro Atómico Bariloche and Instituto Balseiro, Comisión Nacional de Energía Atómica, 8400 Bariloche, Argentina*
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We obtain the quantum phase diagram of the Hubbard chain with alternating on-site energy at half filling. The model is relevant for the ferroelectric perovskites and organic mixed-stack donor-acceptor crystals. For any values of the parameters, the band insulator is separated from the Mott insulator by a dimer phase. The boundaries are determined accurately by crossing of excited levels with particular discrete symmetries. We show that these crossings coincide with jumps of charge and spin Berry phases with a clear geometrical meaning.

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The transition between a band insulator and a Mott insulator in a one-dimensional (1D) model for ferroelectric perovskites[1] has been a subject of great interest in recent years.[1–9] The model describing this transition, originally proposed[10] for the neutral-ionic transition in mixed-stack donor-acceptor organic crystals,[11,12] is

$$H=-t\sum_{i\sigma}\ (c^{\dagger}_{i+1\sigma}c_{i\sigma}+\text{H.c.})$$

$$+\Delta\sum_{i\sigma}\ (-1)^{i}n_{i\sigma}+U\sum_{i}\ n_{i\uparrow}n_{i\downarrow}\,. \qquad (1)$$

At a fixed value of $\Delta$, exact-diagonalization studies on rings of up to 12 sites[2,6] and Hartree-Fock calculations[3] found evidence of a transition with increasing $U$ from a band insulating (BI) ionic phase to a Mott insulating (MI) quasineutral phase, which could be expected on general grounds. Furthermore, the transition point was characterized[4] as a metallic point, with divergent delocalization. On the other hand, a field theoretical approach,[5] valid in the weak coupling limit $(\Delta,U)\ll t$, concluded that a spontaneously dimerized insulating (SDI) phase (also called bond-ordered wave) intervenes between the BI and MI phases. However, due to the limitations of this technique the precise extension of this phase remained unknown. Very recently, density matrix renormalization group (DMRG) investigations[7,8] and a quantum Monte Carlo (QMC) approach[9] found contradictory evidence: the two DMRG calculations reached opposite conclusions regarding the existence of the SDI phase, while in the QMC results the SDI-MI phase transition was not observed. Thus, the existence of all these conflicting results calls for a further investigation of this model.

In this Rapid Communication we clarify this controversy and accurately determine the whole ground-state phase diagram of Hamiltonian Eq. (1). This is accomplished by the combined use of the method of topological transitions (MTT) (jumps in charge and spin Berry phases)[13–15] and the method of crossing excitation levels (MCEL) based on the conformal field theory with renormalization group analysis.[16,17] These methods, briefly explained below, are somehow complementary in the sense that while the geometrical content of the MTT is more clearly displayed in the strong coupling limit, the MCEL is based on a weak-coupling approach. A nice feature here is that they turn out to be equivalent for this problem, so that the results obtained are expected to be valid for all parameter values. State of the art diagonalization of rings with up to 16 sites are performed to determine the phase boundaries with errors estimated in a few percent of $t$.

The Berry phases are calculated numerically from the ground state $|g(\Phi_{\uparrow},\Phi_{\downarrow})\rangle$ of $\tilde{H}(\Phi_{\uparrow},\Phi_{\downarrow})$ in rings of even number of sites $L$ threaded by fluxes $\Phi_{\sigma}$ for spin $\sigma$. The Hamiltonian $\tilde{H}$ differs from $H$ in that the hopping term has the form $-t\Sigma_{i\sigma}(\tilde{c}^{\dagger}_{i+1\sigma}\tilde{c}_{i\sigma}e^{i\phi_{\sigma}/L}+\text{H.c.})$. One can map $\tilde{H}$ with periodic boundary conditions (BC) into $H$ with twisted BC ($c^{\dagger}_{i+L\sigma}=e^{i\phi_{\sigma}}c_{i\sigma}$) using the canonical transformation $c_{j\sigma}=e^{ij\phi_{\sigma}/L}\tilde{c}_{j\sigma}$. The charge (spin) Berry phase $\gamma_c$ ($\gamma_s$) is the phase captured by the ground state when it is followed adiabatically in the cycle $0\leqslant\Phi\leqslant 2\pi$, keeping $\Phi_{\uparrow}=\Phi_{\downarrow}=\Phi$ ($\Phi_{\uparrow}=-\Phi_{\downarrow}=\Phi$). Discretizing the interval $0\leqslant\Phi\leqslant 2\pi$ into $N+1$ points $\Phi_r=2\pi r/N$ ($r=0,N$), the Berry phases are calculated using[13]

$$\gamma_{c,s}=-\lim_{N\to\infty}\text{Im}\left\{\ln\left[\prod_{r=0}^{N-2}\langle g(\Phi_r,\pm\Phi_r)|g(\Phi_{r+1},\pm\Phi_{r+1})\rangle\right.\right.$$

$$\left.\left.\times\langle g(\Phi_{N-1},\pm\Phi_{N-1})|g(2\pi,\pm 2\pi)\rangle\right]\right\}, \qquad (2)$$

where $|g(2\pi,\pm 2\pi)\rangle=\exp[i2\pi/L\Sigma_j j(n_{j\uparrow}\pm n_{j\downarrow})]|g(0,0)\rangle$.

An important property of $\gamma_c$ is that if the system is modified by some perturbation, the change in the polarization $P_{\uparrow}+P_{\downarrow}$ is proportional to the corresponding change in $\gamma_c$.[3] Here $P_{\sigma}$ is the contribution of electrons with spin $\sigma$ to the polarization of the system. Similarly, changes in $\gamma_s$ are related to changes in the difference $P_{\uparrow}-P_{\downarrow}$ between the electric polarizabilities for spins up and down:[14] $\Delta P_{\uparrow}\pm\Delta P_{\downarrow}=e\Delta\gamma_{c,s}/2\pi[\text{mod}(e)]$. A more crucial property is that in systems with inversion symmetry $\gamma_c$ and $\gamma_s$ can only be either 0 or $\pi$, which has led to the idea that $\underline{\gamma}=(\gamma_c,\gamma_s)$ can be used as a topological vector to characterize different

 

phases.[13] Such a possibility is clear in the strong-coupling limit $t\to 0$, where (usually) all particles are localized: one can choose a gauge in which all scalar products in Eq. (2) except the last one are equal to 1, so that $\gamma_c$ is determined by the sum $i2\pi/L\Sigma_{j=0}^{L-1} j(n_{j\uparrow}+n_{j\downarrow})$. For example, if there is one particle per site ($U\to\infty$), it gives $i\pi(L-1) \equiv i\pi[\mathrm{mod}(2\pi i)]$ for $L$ even, and then $\gamma_c=\pi$. Similarly, for a Néel state it is easy to see that $\gamma_s=\pi$, and for a charge density wave (CDW) with maximum order parameter ($\Delta\to\infty$) $\overline{\gamma}=(0,0)$. These values are consistent with the changes in $P_\uparrow \pm P_\downarrow$ originated by the charge transport of all electrons with a given spin to nearest-neighbor sites, required to change the extreme BI state with $\overline{\gamma}=(0,0)$ to the Néel state with $\overline{\gamma}=(\pi,\pi)$. For the extreme MI state ($U\to\infty$), which is a spin-density wave (SDW), we also have $\overline{\gamma}=(\pi,\pi)$.[13,15] By continuity, one might expect that these values of $\overline{\gamma}$ characterize also the BI and MI phases in weak coupling. As explained below, this is confirmed by an analysis based on the MCEL. This change in topological parameters (which is sharp even in finite systems) indicates nontrivial changes in $P_\uparrow \pm P_\downarrow$ characteristic of a phase transition.

We find another phase with $\overline{\gamma}=(\pi,0)$. From field theory[5] we know that this corresponds to the SDI phase with order parameter $D=\Sigma_{j\sigma}(-1)^j(c^\dagger_{j+1\sigma}c_{j\sigma}+\mathrm{H.c.})$. If we consider the more general Hamiltonian

$$H'=H-(t_{AB}-t)\sum_{i\sigma}(c^\dagger_{i+1\sigma}c_{i\sigma}+\mathrm{H.c.})(n_{i\bar{\sigma}}-n_{i+1\bar{\sigma}})^2$$

$$+V\sum_{i\sigma\sigma'} n_{i\sigma}n_{i+1\sigma'}, \qquad (3)$$

we confirm that the SDI phase of $H'$, well established in previous studies,[15,17–20] is smoothly connected with that of $H$ for $t_{AB}\to\infty$. Furthermore, the model of Eq. (3) with $\Delta=0$ and $(V,t_{AB}-t)>0$ contains essentially the same phases as $H$, and allows a more detailed study of the relation between the MTT and MCEL. For $V=0$, while DMRG results in chains of 40 sites are unable to detect the opening of an exponentially small gap,[15] the MTT predictions with $L$ up to 12 (Ref. 15) practically coincide with those of field theory for $t_{AB}\sim 1$ (Refs. 18 and 19) and with exact results for $t_{AB}\to 0$.[21]

The MCEL is based on the fact that in a conformal field theory (which ultimately describes the low-energy physics of 1D systems in the charge and spin sectors if they are gapless) the exponent $\nu$ of the long-distance power-law decay of correlation functions $\langle O(x)O(x+d)\rangle \sim d^{-\nu}$ is given in terms of excitation energies related to the operator $O(x)$ in the finite ring. A crossing of appropriately chosen excitation energies for different operators indicates a change in the character of the dominant correlations at large distance (a phase transition).[16,17] The relevant excitation energies for $H'$ with $\Delta=0$ have been studied by Nakamura.[17] In particular, in the weak coupling limit it is known that there is a Gaussian transition from the CDW to the SDI in $H'(\Delta=0)$, with the charge gap vanishing only at the transition point.[17–19] This transition is determined by the crossing of the lowest states with opposite parity under inversion and the same total momentum $K=\pi/a$ ($a$ is the nearest-neighbor distance), calculated with periodic (antiperiodic) BC if $L=4n(4n+2)$.[17] We show that this crossing coincides with the jump in $\gamma_c$. In Fig. 1 we represent $E(\Phi)=\langle g(\Phi,\Phi)|\tilde{H}'|g(\Phi,\Phi)\rangle$ for the simplest case with $L$ multiple of four. Minimizing $E(\Phi)$ with respect to $\Phi$ and $\tilde{K}$ leads to $\Phi=\pi$, $\tilde{K}=\pi/a$, and the Berry phases are obtained adiabatically following this state. Using $c_{j\sigma}=e^{ij\phi_\sigma/L}\tilde{c}_{j\sigma}$, one sees that while the total wave vector $\tilde{K}$ of $\tilde{H}'$ remains constant as $\Phi$ is changed, in general $K=\tilde{K}+(N_\uparrow\Phi_\uparrow+N_\downarrow\Phi_\downarrow)/(L\,a)$, where $N_\sigma$ is the number of particles with spin $\sigma$. The conditions leading to the minimum energy ($\Phi=\pi,\tilde{K}=\pi/a$) correspond to antiperiodic BC and $K=0$ in $H'$.

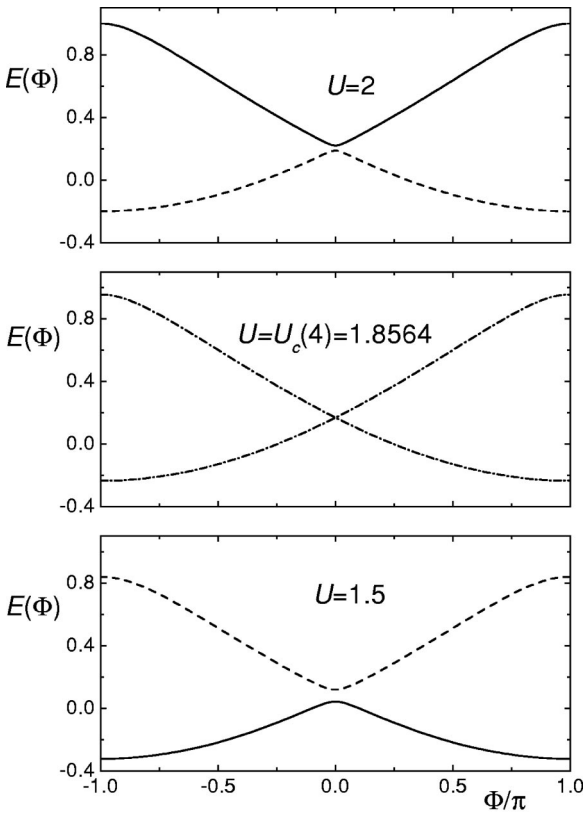


FIG. 1. Energy per site as a function of flux $\Phi_\uparrow=\Phi_\downarrow=\Phi$ for the two lowest lying eigenstates within the subspace of $\tilde{K}=\pi/a$, $S=0$. Parameters are $L=4$, $\Delta=0$, $t_{AB}=t=1$, $V=2$ and three different values of $U$ as indicated. Full (dashed) line correspond to states with $\gamma_c=0$ ($\gamma_c=\pi$). For $U=U_c(L)$ $\gamma_c$ is undefined due to the degeneracy at $\Phi=0$.

It is easy to see that the inversion $I\,c^\dagger_{j\sigma}I^\dagger=c^\dagger_{-j\sigma}$ $\equiv e^{-i\Phi_\sigma}c^\dagger_{L-j\sigma}$ is a symmetry of $H'(\Phi_\uparrow,\Phi_\downarrow)$ only if both $\Phi_\sigma$ are either 0 or $\pi$ (corresponding to periodic or antiperiodic BC). At $U=U_c(L)$ and $\Phi=0$ there is a crossing of the lowest levels with $\tilde{K}=\pi/a$ and total spin $S=0$. This crossing is possible because the corresponding wave functions have opposite parity, and therefore they do not mix at $\Phi=0$. For $\Phi\to 0$ one can use perturbation theory in $\Phi$, and for $U$ near $U_c(L)$ the state $|g(\Phi)\rangle$ is determined by a $2\times 2$ matrix involving the above mentioned two states for $\Phi=0$ with off-

diagonal matrix elements linear in $\Phi$. From the trivial solution to this problem one realizes that the product in Eq. (2) for $U \to U_c(L) - 0^+$ differs from that for $U \to U_c(L) + 0^+$ in sign. Hence, $\gamma_c$ jumps at the same place where the transitions occurs according to the MCEL. While for the $t-U-V$ model ($H'$ with $\Delta = 0 = t_{AB} - t$) in weak coupling the transition is second order and the charge gap vanishes at the transition, for $(U,V) \gg t$ the transition is first order, from a fully gapped CDW to a charge gapped SDW.[17,20,22] As a consequence, the MCEL loses its support from the conformal invariant (massless) theory. However, in this limit the geometrical meaning of the jump in $\gamma_c$ is very clear, as explained earlier, and justifies the method.

In the MCEL, the Kosterlitz-Thouless transition, which corresponds to the opening of a spin gap, is detected through the crossing of a singlet even under inversion with an odd triplet, with $K=0$ and periodic BC (for $L=4n$).[17] At $\Phi=0$ or $\Phi=\pi$, $H'(\Phi,-\Phi)$ has SU(2) and inversion symmetries, which are lost for other values of $\Phi$. Therefore, a similar analysis as above shows that $\gamma_s$ jumps at this point.[14] If $L=4n+2$, periodic and antiperiodic BC are interchanged. When $\Delta \neq 0$ the symmetry under translations in one lattice spacing $a$ is lost, $K=\pi/a$ becomes equivalent to $K=0$, and the CDW order parameter is different from zero also in the SDI and MI phases. The field theory results for $H$ show that for $(\Delta,U) \ll t$ the spin transition retains the same features.[5] The charge transition, which for $\Delta=0$ is described by the sine Gordon model, for $\Delta \neq 0$ is determined by the double sine Gordon model, and the universality class changes from Gaussian to Ising. However, the transition remains second order and the charge gap vanishes at the transition.[5] Then, at this point and sufficiently low energies the charge sector is described by a conformal invariant theory, justifying the MCEL.

In spite of the breaking of translational symmetry, fortunately the relevant crossings for $H$ can still be identified looking for the ground-state energy in subspaces with $K=0$, total spin projection $S_z=0$, and a definite parity under inversion and time reversal. The latter allows us to separate states with even and odd $S$. If the more general model $H'$ with $\Delta \neq 0$ is considered, there are some regions of parameters in which the charge transition corresponds to a crossing of first excited states within the above mentioned subspaces, but we restrict ourselves here to the phase diagram of $H$. For this model, the connection between the jump in $\gamma_c$ and a symmetry switch of the ground state for appropriate BC has been noted earlier,[2,3,6] but the relation with the MCEL has not been discussed. Moreover, neither results for $\gamma_s$ nor numerical investigation of the SDI-MI transition has been reported so far. The calculation of $\gamma_s$ in $H$ presents technical difficulties due to additional crossing of levels (not related with phase transitions) which take place for $\tilde{K}=0$. We have verified numerically that the jumps in $\gamma_c$ and $\gamma_s$ correspond to the above mentioned level crossings.

For given $\Delta$, we have calculated the critical on-site repulsion $U_c$ ($U_s$) at which the charge (spin) transition takes place. In addition, for small $U$ and $\Delta$ we have fixed $U$ and determined the critical values $\Delta_c$ and $\Delta_s$. This was done by

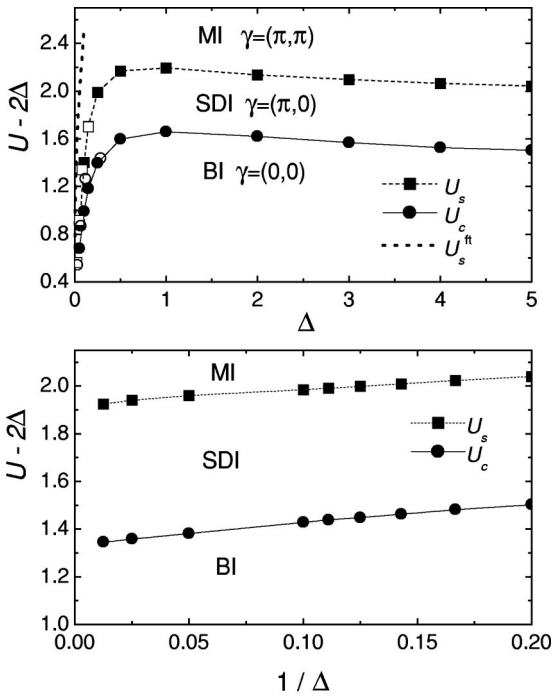


FIG. 2. Ground-state phase diagram of $H$ at half filling. The dashed line corresponds to the field theory result $\Delta_s^{ft}$ (see main text). The open (full) symbols were obtained keeping $U(\Delta)$ constant.

fitting a quadratic polynomial in $1/L^2$ to the results for $L=10$, 12, 14 and 16, followed by an extrapolation to $L=\infty$. This fit works very well for $\Delta \geqslant 0.25$ (we set $t=1$ as the unit of energy unless otherwise stated), and improves with increasing $\Delta$. The difference between $U_s(L)$ and $U_s(L+2)$ rapidly decreases with $L$ if $\Delta$ is not too small. Instead, for small values of $\Delta$ the finite size effects increase and, as a consequence, the error in the extrapolation becomes larger. To estimate this error we have repeated the fits using $L=8$, 10, 12 and 14; for $\Delta=0.05$ this gives a new estimation of $U_c$ ($U_s$) that differs from the previous one in 0.12 (0.07). For $\Delta<0.05$ the relative error in $U_c$ and $U_s$ becomes very large, and we do not present results since they lose quantitative validity (except at $\Delta=0$, where $U_c=U_s=0$ for all $L$). Instead, for $\Delta \geqslant 0.25$ the estimated error in $U_c, U_s$ is less than 0.06, and less than 0.03 for $\Delta \geqslant 0.5$.

The resulting phase diagram is presented in Fig. 2. In qualitative agreement with field theory results,[5] and for all values of $\Delta$, the transition from the BI phase to the MI phase with increasing $U$ takes place in two steps: first, a charge transition to the SDI phase at $U=U_c$ occurs, and then, for $U=U_s>U_c$, the spin gap closes. The behavior in the strong coupling limit is quite different from that of the $t-U-V$ model, for which a first order CDW-SDW transition occurs and is easily understood in terms of perturbation theory (PT).[17,20,22] Instead, $H$ remains nontrivial for $t \to 0$ as long as $U-2\Delta \sim t$, since charge fluctuations are still possible. As a consequence of this delocalization of charges, $\gamma_c$ inside the SDI phase cannot be calculated analytically just adding the position of the charges, as we explained before for $\Delta \to \infty$ or $U \to \infty$. For $t=0$ the SDI phase is absent, and PT in $t$ di-

verges at $U=2\Delta$ where the BI-MI transition takes place. For $t \ll |U-2\Delta| \ll U$ PT is valid, and can be used to calculate the energy of the BI and MI phases for negative and positive $U-2\Delta$, respectively. The MI phase in this limit is described by a Heisenberg model with exchange $J=2t^2/(U-2\Delta)$. The energies up to second order in $t$ are given by $E_{BI}=U-2\Delta+4t^2/(U-2\Delta)$ and $E_{MI}=-J\ln 2$. While the SDI phase cannot be described by PT in $t$, its boundaries are very accurately determined by our method for small $t$. The jumps in Berry phases have very little size dependence and show that $U_c \simeq 2\Delta+1.33t$ and $U_s \simeq 2\Delta+1.91t$ for $t \ll (\Delta, U)$. The fact that the SDI phase exists for positive values of $U-2\Delta$ was to be expected from the asymmetry of $E_{BI}$ and $E_{MI}$ under a change of sign of $U-2\Delta$.

The results for $(\Delta, U) \gg t$ can be extended qualitatively to $\Delta \sim t$. The SDI has a nearly constant width $\sim 0.6t$, and both $U_s$ and $U_c$ increase slightly with decreasing $\Delta$. For $\Delta<1$ the critical values $U_c$ and $U_s$ decrease abruptly, until they reach $U_c=U_s=0$ at $\Delta=0$. However, in the region $0<\Delta<0.25$ $(0<U\lesssim 2)$ the relative errors in $U_c$, $U_s$ become larger with decreasing $\Delta$; in particular, for $\Delta \lesssim 0.1$ our results are not quantitatively reliable. For $(\Delta, U) \ll t$, the spin transition can be estimated integrating out the charge degrees of freedom, assuming that they are described by a free massive boson. This leads to a renormalization of the effective interaction $g_{1\perp}$ responsible for the opening of a spin gap in the sine Gordon model which describes the spin sector at low energies.[5] From the vanishing of the renormalized $g_{1\perp}$ one obtains the approximate field theory result $\Delta_s^{ft} \sim E_g \sqrt{U/(8\pi t)}$, where $E_g$ is the gap for $\Delta=0$ and is known from the Bethe ansatz solution. For $U \ll t$, $E_g \cong (8/\pi)\sqrt{tU}\exp(-2\pi t/U)$, and the exponential dependence dominates the behavior of $\Delta_s^{ft}$. Due to the numerical uncertainties for $\Delta \lesssim 0.1$, we cannot establish where this exponential dependence deviates from the actual SDI-MI boundary. For small $\Delta$ and any value of $U$, an accurate field theory result for $\Delta_s$ might be obtained using a bosonization approach which starts from the exact solution for $\Delta=0$.[23]

The SDI order parameter $D$ couples directly with optical phonons with wave vector $K=0$ and, therefore, the latter should increase the extension of this phase. In principle, one can include these phonons in the numerical calculations using the adiabatic approximation. However, due to the breaking of inversion symmetry our method cannot be used to find the phase boundaries in this case. QMC calculations suggest that in the adiabatic approximation the whole MI phase disappears and the SDI takes its place.[9] This is not necessarily the case if the dynamics of the phonons is included.[5] We must emphasize that in the MI phase both dimer-dimer and spin-spin correlation functions have the same leading power-law decay at large distances. The dominance of spin-spin correlations due to logarithmic corrections characterizes the MI phase.[15,18,19] This renders it very difficult to determine the SDI-MI boundary by direct numerical evaluation of correlation functions.[15]

In summary, we have determined the quantum phase diagram of the Hubbard chain with alternating on-site energies at half filling using topological transitions. The method is justified from geometrical considerations in the strong coupling limit $(t \to 0)$ and by field theory arguments in the weak-coupling $(U, \Delta) \ll t$ region. We confirmed the existence of a spontaneously dimerized phase and determined its boundaries for the first time.

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