Metal-insulator transition in the one-dimensional Holstein model at half filling

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We study the one-dimensional Holstein model with spin-$\frac{1}{2}$ electrons at half filling. Ground-state properties are calculated for long chains with great accuracy using the density-matrix renormalization-group method and extrapolated to the thermodynamic limit. We show that for small electron-phonon coupling or large phonon frequency, the insulating Peierls ground state predicted by mean-field theory is destroyed by quantum lattice fluctuations and that the system remains in a metallic phase with a nondegenerate ground state and power-law electronic and phononic correlations. When the electron-phonon coupling becomes large or the phonon frequency small, the system undergoes a transition to an insulating Peierls phase with a twofold degenerate ground state, long-range charge-density-wave order, a dimerized lattice structure, and a gap in the electronic excitation spectrum. [S0163-1829(99)09035-9]

A long time ago, Peierls[1] suggested that a one-dimensional metal should exhibit an instability against a periodic lattice distortion of wave vector equal to twice the Fermi wave vector. Although this distortion increases the lattice elastic energy, it opens a gap in the electronic spectrum at the Fermi surface, lowering the electronic energy. Thus, the Peierls insulating state can be energetically favored over the metallic state. A wide range of quasi-one-dimensional materials, such as *MX* chains, charge-density-wave (CDW) compounds, conjugated polymers and charge-transfer salts,[2] have electronic properties that are dominated or at least affected by the Peierls instability. These systems are often modeled by the one-dimensional Holstein model,[3] the Su-Schrieffer-Heeger model,[4] or various spin-Peierls[5] models.

The Peierls instability is well understood in the static lattice (adiabatic) limit and within mean-field theory. An interesting and still controversial question is how the Peierls ground state is modified when quantum lattice fluctuations are taken into account. These quantum lattice fluctuations could have an important effect in most quasi-one-dimensional materials with a Peierls ground state because the lattice zero-point motion is often comparable to the amplitude of the Peierls distortion.[6] Thus, this question has motivated several studies of quantum lattice fluctuation effects in the Holstein,[7–14] Su-Schrieffer-Heeger,[15–19] and spin-Peierls[20–27] models. In spinless fermion models and spin-Peierls models these studies have shown that the transition to a Peierls state occurs only when the electron-phonon coupling exceeds a finite critical value or when the phonon frequency drops below some finite threshold value. Thus, in these systems quantum lattice fluctuations destroy the Peierls instability for small electron-phonon coupling or large phonon frequency. In more realistic models with spin-$\frac{1}{2}$ electrons, however, previous studies[7,9,16,17,19] have generally concluded that the ground state is a Peierls state for any finite electron-phonon coupling at finite phonon frequency, in qualitative agreement with mean-field theory.

Here, we consider the one-dimensional Holstein model with spin-$\frac{1}{2}$ electrons at half filling. This model describes electrons coupled to dispersionless phonons, represented by local oscillators. It has as Hamiltonian

$$H=\frac{1}{2M}\sum_i p_i^2+\frac{K}{2}\sum_i q_i^2-\alpha\sum_i q_i(n_i-1)$$

$$-t\sum_{i\sigma}(c_{i\sigma}^\dagger c_{i+1\sigma}+c_{i+1\sigma}^\dagger c_{i\sigma}), \tag{1}$$

where q_i and p_i are the position and momentum operators for a phonon mode at site i, $c_{i,\sigma}^\dagger$ and $c_{i,\sigma}$ are creation and annihilation operators for an electron of spin σ on site i, and $n_i=c_{i,\uparrow}^\dagger c_{i,\uparrow}+c_{i,\downarrow}^\dagger c_{i,\downarrow}$. The half-filled band case corresponds to a density of one electron per site. At first sight, there are four parameters in this model: the oscillator mass M and spring constant K, the electron-phonon coupling constant α, and the electron hopping integral t. However, if phonon creation and annihilation operators are denoted by $b_i^\dagger$ and b_i, respectively, the Holstein Hamiltonian can be written (up to a constant term)

$$H=\omega\sum_i b_i^\dagger b_i-\gamma\sum_i (b_i^\dagger+b_i)(n_i-1)$$

$$-t\sum_{i\sigma}(c_{i+1\sigma}^\dagger c_{i\sigma}+c_{i\sigma}^\dagger c_{i+1\sigma}), \tag{2}$$

where the phonon frequency is given by $\omega^2=K/M$ (we set $\hbar=1$) and a new electron-phonon constant is defined by $\gamma=\alpha a$ with the range of zero-point phonon position fluctuations given by $a^2=\omega/(2K)$. We can set the parameters t and a equal to 1 by redefining the overall energy scale and the units of phonon displacements. Thus, the properties of the Holstein Hamiltonian (2) depends only on the two interaction parameters ω and γ.

Mean-field theory predicts that the ground state of this model is a Peierls state for any nonzero electron-phonon coupling and $\omega<\infty$. Early works based on strong-coupling perturbation theory and quantum Monte-Carlo simulations,[7] as well as variational calculations[9] seemed to support this point of view. However, the quantum Monte-Carlo results were

limited to small systems (up to 16 sites) and their interpretation relied on a questionable finite-size-scaling analysis. The strong-coupling perturbation theory is based on the formation of small bipolarons in the $\gamma/\omega \to \infty$ limit, but it has been argued that, as the coupling γ decreases, the bipolaron size becomes large and the strong-coupling picture breaks down.[28] On the other hand, a functional integral calculation suggests that the transition occurs at finite electron-phonon coupling,[10] but the accuracy of this approach is hard to estimate. Moreover, the static and dynamical properties of small clusters (up to six sites) show that there is a sharp crossover at a finite electron-phonon coupling from a quasifree electron ground state to an ordered bipolaronic ground state, which can be seen as a precursor to the Peierls ground state of the infinite system.[29–31] A similar crossover is observed in an approximate solution of the Hamiltonian (2), where only a single-phonon mode $b_\pi \sim \Sigma_i (-1)^i b_i$ is explicitly taken into account.[32]

In this paper, we discuss the ground-state properties of the Holstein model of spin-$\frac{1}{2}$ electrons in the thermodynamic limit. We demonstrate that quantum lattice fluctuations suppress the Peierls instability for small electron-phonon coupling or large phonon frequency. In this regime, the ground state is unique, gapless, and shows only power-law correlations between electron position and between phonon displacements. This ground state is similar to the ground state of the noninteracting system ($\gamma = 0$). When the electron-phonon coupling becomes large or the phonon frequency becomes small the system undergoes a transition to an insulating Peierls phase, which is qualitatively described by mean-field theory. In this regime the ground state is doubly degenerate, and there is a gap in the electronic spectrum, long-range CDW order and a dimerized lattice structure.

Our results are based on density-matrix renormalization-group (DMRG) calculations.[33] DMRG is as accurate as exact diagonalization on small systems but can be applied to much larger systems while maintaining very good precision. It has already been applied successfully to the study of the Peierls instability in quantum lattices with spinless fermion or spin degrees of freedom.[20,12,25] There have not been any applications of DMRG to models of spin-$\frac{1}{2}$ electrons coupled to phonons yet, because these systems are significantly harder to deal with due to the additional degrees of freedom and the larger amplitude of phonon displacements. For this paper, we have used an improved DMRG method for systems with boson degrees of freedom, which has been described in a previous work.[34] With this approach both the error due to the necessary truncation of the phonon Hilbert space and the DMRG truncation error can be kept negligible. The accuracy of this DMRG technique has been demonstrated by comparison with many numerical and analytical methods for the polaron problem (a single electron) in the one-dimensional Holstein model.[34–36] The maximum number of density-matrix eigenstates m used in our calculations is 800, giving truncation errors from 10^{-7} to 10^{-11} depending on the system size and parameters. The error in the ground-state energy is estimated to be smaller than $10^{-5}t$. The actual number of phonon states kept for each local oscillator ranges from 8 to 32 depending on the electron-phonon coupling strength. We have studied open chains with an even number N of sites (up to 100) and extrapolate results to the thermodynamic limit. Open boundary conditions are used because the DMRG method usually performs much better in this case than for periodic boundary conditions.

In previous studies of the Peierls instability in the Holstein model the ground-state symmetry was explicitly broken as in the mean-field and adiabatic approximations.[7,9,10] Thus, the Peierls ground state was revealed by a lattice distortion (dimerization)

$$\langle q_i \rangle = (-1)^i m_p \tag{3}$$

and a CDW

$$\langle n_i \rangle = 1 + (-1)^i m_e , \tag{4}$$

with $m_e, m_p \neq 0$, where $\langle \hat{O} \rangle$ means the ground-state expectation value of operator $\hat{O}$, and m_p and m_e are the phonon and electronic order parameter, respectively.[7] For $m_e, m_p \neq 0$, the ground state was twofold degenerate [this degeneracy corresponds to the two possible phases of the oscillations (3) and (4)]. Note that, as all eigenstates of the Holstein Hamiltonian satisfy

$$\langle q_i \rangle = \frac{\alpha}{K} (\langle n_i \rangle - 1), \tag{5}$$

the order parameters are related by

$$m_p = \frac{\alpha}{K} m_e . \tag{6}$$

Our DMRG method gives an excellent approximation to the exact ground state of the Holstein model on a lattice of finite size. It is known exactly that the ground state of the half-filled Holstein model on a finite lattice is unique for $\omega \neq 0$, implying that there is no degenerate broken symmetry ground state at any finite electron-phonon coupling or nonzero phonon frequency.[37] Instead, there is a quasidegeneracy of the ground state when the electron-phonon coupling exceeds a finite critical value[31] (this point will discussed in more detail later). Therefore, we always find $\langle q_i \rangle = 0$ and $\langle n_i \rangle = 1$ in our calculations. This property follows directly from the uniqueness of the ground state and the electron-hole symmetry, i.e., the invariance of the Hamiltonian (1) under the transformation

$$c_{i\sigma}^\dagger \to (-1)^i c_{i\sigma}, \quad q_i \to -q_i . \tag{7}$$

To observe the consequences of the Peierls instability we have to look at correlation functions. The most important ones for a Peierls state are the staggered charge-density correlation function

$$C_n(m) = (-1)^m (\langle n_i n_{i+m} \rangle - 1) \tag{8}$$

and the staggered phonon displacement correlation function

$$C_q(m) = (-1)^m \langle q_i q_{i+m} \rangle . \tag{9}$$

We have found that, for small electron-phonon coupling γ or large phonon frequency ω, both correlation functions decrease as a power-law $m^{-\beta}$ with $2 \geqslant \beta > 0$ as a function of the distance m. An example is shown in Fig. 1(a). As the electron-phonon coupling increases or the phonon frequency decreases, the exponent β becomes smaller. For sufficiently

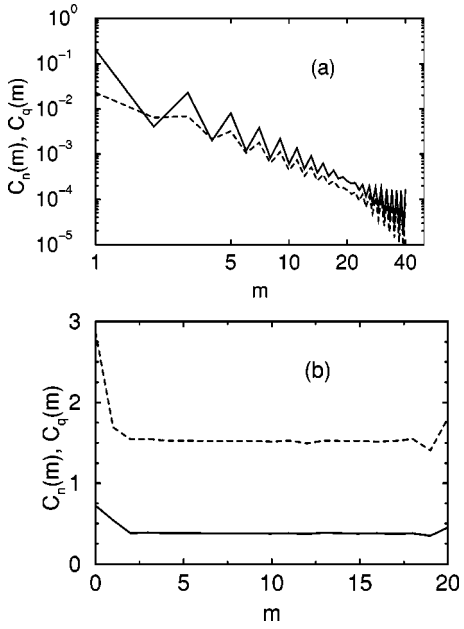

FIG. 1. Staggered charge-density correlation function $C_n(m)$ (solid line) and staggered phonon displacement correlation function $C_q(m)$ (dashed line) in the metallic phase for $\gamma=0.4$ (a) and in the Peierls phase for $\gamma=1$ (b). The distance m is calculated from the middle of an open chain of 80 sites (a) and 40 sites (b), respectively. In both cases $\omega=1$.

large electron-phonon coupling or small phonon frequency the behavior of both correlation functions is completely different. As seen in Fig. 1(b), in this case both functions tend to finite values at large distances, showing the existence of long-range order.

It is not always possible to determine the presence or absence of long-range order in the thermodynamic limit from the correlation functions of a finite chain. A better approach is to compute the electronic and phononic static staggered susceptibilities defined as

$$\chi_e=\frac{1}{N}\sum_m C_n(m) \tag{10}$$

and

$$\chi_p=\frac{1}{N}\sum_m C_q(m), \tag{11}$$

respectively. It is clear that both χ_e and χ_p vanish in the thermodynamic limit if there is no long-range order. For instance, both susceptibilities vanish as $1/N$ in the noninteracting limit ($\gamma=0$). In Fig. 2(a) we show both χ_e and χ_p as a function of the inverse chain length for a weak electron-phonon coupling. Both quantities clearly tend to zero in an infinite chain. Thus, we conclude that there is no long-range CDW order nor lattice distortion in the ground state of the Holstein model for the parameters ($\gamma=0.4,\omega=1$) used in this example. On the other hand, it is clear that χ_e and χ_p remain finite for $N\to\infty$ if there is long-range CDW order or a lattice dimerization, respectively. For instance, in the mean-field approximation, one finds

$$\chi_e=m_e^2, \quad \chi_p=m_p^2. \tag{12}$$

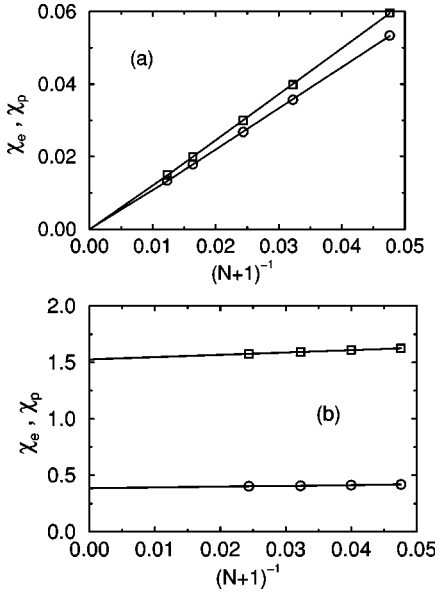

FIG. 2. Electronic (circle) and phononic (square) staggered static susceptibilities as a function of the inverse chain length in the metallic phase for $\gamma=0.4$ (a) and in the Peierls phase for $\gamma=1$ (b). In both cases $\omega=1$. Solid lines are linear fits.

Figure 2(b) shows χ_e and χ_p as a function of the inverse system size for a relatively strong electron-phonon coupling. In this case, both susceptibilities remain finite for $N\to\infty$ and thus, reveals the presence of a Peierls state with long-range CDW order and lattice dimerization for the parameters considered in this example ($\gamma=1,\omega=1$).

Using Eqs. (6) and (12), one sees that

$$\sqrt{\chi_p}=\frac{\alpha}{K}\sqrt{\chi_e} \tag{13}$$

in the mean-field approximation. It is possible to demonstrate that this relation holds for the exact ground state in several special cases, such as the adiabatic limit ($\omega\to0$) and the anti-adiabatic limit ($\omega\to\infty$). Although we can not prove the validity of Eq. (13) for the general case, our numerical results show that it is always satisfied (within numerical errors) in an infinite system. This simply means that lattice dimerization and CDW are two inseparable features of the Peierls ground state. Therefore, we define a unique order parameter Δ as

$$\Delta=\alpha\sqrt{\chi_p}\approx\frac{\alpha^2}{K}\sqrt{\chi_e}, \tag{14}$$

where χ_p and χ_e are the infinite system extrapolation of the ground-state susceptibilities (10) and (11) calculated from DMRG simulations. If the ground state of the Holstein model is a Peierls state, one has $\Delta>0$, and otherwise $\Delta=0$. Obviously, this definition of Δ is just a generalization of the usual gap parameter of mean-field theory Δ_{MF}, which is related to the other mean-field order parameters m_e and m_p by

$$\Delta_{MF}=\alpha|m_p|=\frac{\alpha^2}{K}|m_e|. \tag{15}$$

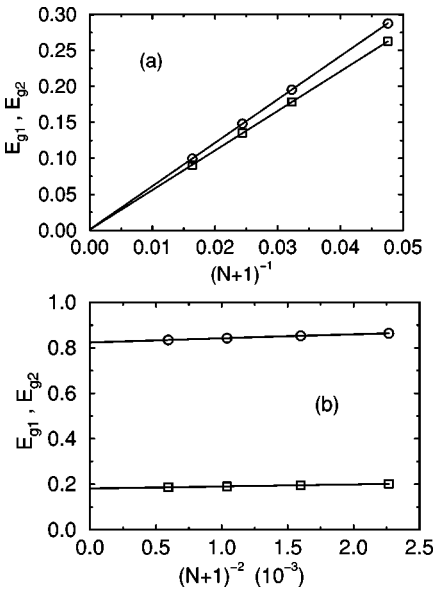

FIG. 3. Gaps E_{g1} (circle) and E_{g2} (square) vs the inverse chain length in the metallic phase for $\gamma=0.4$ (a) and vs the square of the inverse chain length in the Peierls phase for $\gamma=1$ (b). In both cases $\omega=1$. Solid lines are linear fits.

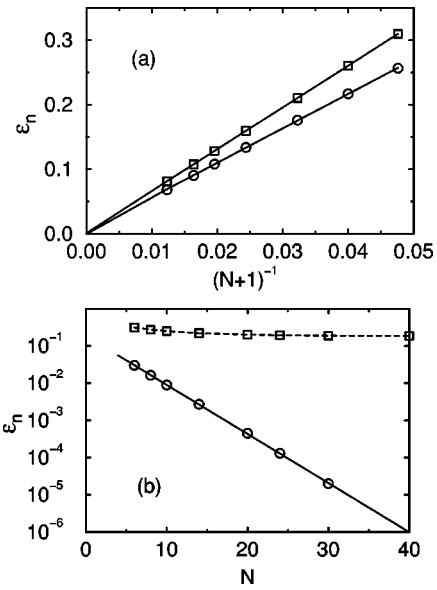

FIG. 4. Lowest excitation energy ε_1 (circle) and second lowest excitation energy ε_2 (square) as a function of the system size N in the metallic phase for $\gamma=0.4$ (a) and in the Peierls phase for $\gamma=1$ (b). In both cases $\omega=1$. Solid lines are linear fits.

In the mean-field approximation the Peierls distortion opens a gap $2\Delta_{MF}$ in the electronic spectrum. It is sometimes assumed that this relation between Peierls gap and order parameters remains valid when quantum lattice fluctuations are taken into account.[10] In such a case the exact Peierls gap would simply be given by 2Δ. However, it is likely that the Peierls gap is more reduced by the quantum lattice fluctuations than the dimerization or CDW amplitude[6] and becomes smaller than the value 2Δ obtained from Eq. (14). Unfortunately, calculating the optical gap of the Holstein model with a DMRG method is not possible yet.[38] To find how the appearance of the Peierls ground state correlates with a gap in the infinite system we have calculated the charge gaps

$$E_{g1}=2[E_0(1)-E_0(0)] \tag{16}$$

and

$$E_{g2}=E_0(2)-E_0(0), \tag{17}$$

where $E_0(x)$ is the DMRG ground-state energy with x electrons added to $(x>0)$ or removed from $(x<0)$ the half-filled band. In these definitions we implicitly use the electron-hole symmetry of the model at half filling, which implies that $E_0(-x)=E_0(x)$. It should be noted that with these definitions the charge gaps incorporate lattice relaxation effects occurring when the band filling is modified. Therefore, E_{g1} and E_{g2} are not always equal to the optical gap of the system. E_{g1} can be interpreted as the energy required to create a quasiparticle excitation made of an electron dressed by phonons. Similarly, $2E_{g2}$ represents the energy required to create a quasiparticle excitation, which is a bound pair of electrons dressed by phonons, when such electron binding occurs $(E_{g2}<E_{g1})$. Otherwise, one expects $E_{g2}\approx E_{g1}$. Figures 3(a) and 3(b) show both gaps for several system sizes. If there is no long-range order $(\Delta=0)$ we find that the gaps extrapolate to zero in the limit $N\to\infty$ [Fig. 3(a)]. Therefore, we think that in this regime the system is still a metal, as in the noninteracting case $(\gamma=0)$. However, if the ground state of the infinite system is a Peierls state $(\Delta>0)$, we find that both gaps extrapolate to a nonzero value in the thermodynamic limit [Fig. 3(b)]. For $\gamma=1$ and $\omega=1$, $E_{g1}=0.82$, and $E_{g2}=0.18$, which are much smaller than the value that one would anticipate from the amplitude of the Peierls distortion $2\Delta=2.5$. For comparison, the mean-field result for the same parameters is $2\Delta_{MF}=3.1$. This confirms that the quantum lattice fluctuations have a much stronger effect on the Peierls gap than on the amplitude of the Peierls distortion.[6] Nevertheless, we have never found that either E_{g1} or E_{g2} vanishes for $N\to\infty$ in the Peierls ground state. In small clusters, a sharp drop of the Drude weight occurs simultaneously with the crossover to the ordered bipolaronic ground state.[31] Therefore, the opening of the electronic gap always seems to accompany the appearance of long-range order in the ground state and we conclude that a Peierls ground state is always an insulator.

We have also analyzed the scaling of the lowest excitation energies $\varepsilon_n=E_n-E_0$ with the system size, where E_n is the energy of the nth lowest eigenstate of the Hamiltonian (2) at half filling. In the phase without long-range order we have found that the ε_n decrease as a power-law for increasing system size and vanish in the thermodynamic limit, as seen in Fig. 4(a). These results confirm that in this case the infinite system has a unique ground state but is gapless; there is a continuous band of excitations starting from the ground state, as expected for a metal. In the Peierls phase, the energy difference ε_1 between the ground state and the first excited state is very small even in small chains and the other excited states have a much higher energy. Thus, the ground state appears almost degenerate in finite systems. Moreover, we observe completely different scalings for the ε_n. Figure 4(b) shows that ε_1 decreases exponentially with increasing system size, while the energy differences between the two lowest eigenstates and the higher excited states remain finite in

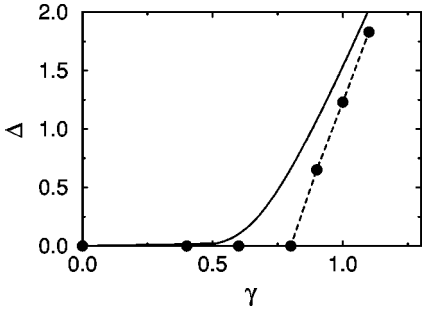

FIG. 5. Order parameter Δ (circle) as a function of the electron-phonon coupling γ for $\omega=1$. The solid line is the mean-field result Δ_{MF}.

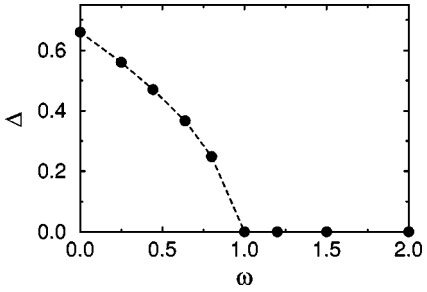

FIG. 6. Order parameter Δ as a function of the phonon frequency ω for $\lambda=\gamma^2/\omega=0.64$. For $\omega=0$ we show the exact adiabatic result.

the thermodynamic limit. This shows that the ground state of the Peierls phase is twofold degenerate in the thermodynamic limit. We have also checked that the order parameter Δ calculated for the first excited state tends to the same finite value as for the ground state in the thermodynamic limit. Therefore, both states are Peierls states with long-range CDW order and lattice dimerization, in qualitative agreement with mean-field predictions. The gap between the degenerate ground state and the other eigenstates also confirms the insulating nature of the system in the Peierls phase.

Our results demonstrate that the ground state of the one-dimensional Holstein model for spin-$\frac{1}{2}$ electrons at half filling can be either a metallic state or an insulating Peierls state depending on the interaction parameters γ and ω. The system undergoes a quantum phase transition between the metallic phase and the Peierls insulating phase at finite critical values γ_c and ω_c. In this aspect, the Holstein model for spin-$\frac{1}{2}$ electrons is similar to spin-Peierls and spinless fermion models. Unfortunately, DMRG simulations become less accurate and harder to carry out in the vicinity of the transition while, at the same time, the finite-size-scaling analysis requires more accurate results and larger system sizes. Therefore, determining the critical values γ_c and ω_c for which this metal-insulator transition occurs demands a substantial amount of computer time and we have not attempted to draw a phase diagram. Nevertheless, we can show the evolution of the order parameter Δ as a function of the electron-phonon γ for $\omega=1$ in Fig. 5. We see that the transition to the Peierls state occurs around $\gamma=0.8$. This is in good agreement with calculations based on a functional integral approach,[10] which predicts $\gamma_c\approx 1$ for a slightly larger phonon frequency $\omega=1.1$. As the adiabatic and anti-adiabatic limits are usually investigated for finite values of the electron-phonon coupling constant $\lambda=\alpha^2/(2K)$ $(=\gamma^2/\omega$ with our choice of units), we show Δ as a function of the phonon frequency ω for a fixed value $\lambda=0.64$ in Fig. 6. One can see that our results converge to the exact adiabatic result for small ω and that the transition from the Peierls phase to the metallic phase occurs around $\omega=1$.

In summary, we have studied the ground-state properties of the one-dimensional Holstein model for spin-$\frac{1}{2}$ electrons at half filling using DMRG. We have shown that this system undergoes a transition from a metallic phase to an insulating Peierls phase at finite values of the electron-phonon coupling and of the phonon frequency.

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