Can Quantum Lattice Fluctuations Destroy the Peierls Broken Symmetry Ground State?

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Abstract

The study of bond alternation in one-dimensional electronic systems has had a long history. Theoretical work in the 1930s predicted the absence of bond alternation in the limit of infinitely long conjugated polymers; a result later contradicted by experimental investigations. When this issue was re-examined in the 1950s it was shown in the adiabatic limit that bond alternation occurs for any value of electron-phonon coupling. The question of whether this conclusion remains valid for quantized nuclear degrees of freedom was first addressed in the 1980s. Since then a series of numerical calculations on models with gapped, dispersionless phonons have suggested that bond alternation is destroyed by quantum fluctuations below a critical value of electron-phonon coupling. In this work we study a more realistic model with gapless, dispersive phonons. By solving this model with the DMRG method we show that bond alternation remains robust for any value of electron-phonon coupling.

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The effect of quantizing the nuclear degrees of freedom on the bond alternation was studied by Fradkin and Hirsch on models of noninteracting electrons. They used both renormalization group arguments and Monte Carlo simulations in their investigations. In a model with gapless, dispersive (or Debye) phonons they showed that for any value of the electron-phonon interaction the metallic state is unstable with respect to a lower symmetry insulating phase that exhibits bond alternation. This result confirms the adiabatic prediction. The transition from the metallic state to the insulating state is called the Peierls transition, with the ground state named the Peierls state. They also predicted that for the same model with spinless fermions the Peierls state is destroyed by quantum lattice fluctuations below a critical value of the electron-phonon interaction. Since a model of spinless fermions is equivalent to the XY quantum antiferromagnet on open chains, this result suggests that strong electronic interactions coupled to quantized phonons might destroy the Peierls state.

More recent numerical calculations on various models have also indicated that the Peierls state may be destroyed by quantized phonons below a critical value of the electron-phonon interaction. Using a finite size scaling analysis of the spin gap Caron and Moukouri showed that at a critical value of the electron-phonon interaction there is a Kosterlitz-Thouless transition in the XY spin-Peierls model with gapped, non-dispersive (or Einstein) phonons. Similar conclusions were made for the Heisenberg spin-Peierls model, again with Einstein phonons. The Holstein model with Einstein phonons for both spinless and spinful fermions have also be shown to exhibit a Peierls phase transition at a non-zero value of the electron-phonon interaction.

Of more direct relevance to the present work is the investigation by Sengupta et al. In this work the electronic degrees of freedom are modelled by a tight-binding model with onsite and nearest neighbour Coulomb interactions (namely, the extended Hubbard model). The nuclear degrees of freedom are described by Einstein bonds phonons. As in previous work with Einstein phonons, there is a critical value of the electron-phonon interaction below which lattice fluctuations destroy the Peierls state.

In this article we focus our attention on the role of quantized gapless, dispersive (or Debye) phonons on the Peierls state. The electronic degrees of freedom are modelled by the extended Hubbard model, with the electronic and nuclear degrees of freedom being coupled via linear distortions of the bond lengths. We study this model as function of the electron-
phonon interaction, the Coulomb interaction and the phonon frequency. In all cases we consider a half filled band. In the limit of large Coulomb interactions this model at half-filling maps onto the quantum Heisenberg antiferromagnet, thus establishing a connection with our previous work. Alternatively, in the limit of vanishing phonon frequency (namely, $M \to \infty$) the model maps onto the classical, adiabatic model, which has been extensively studied (see, for example and references therein).

The Hubbard-Peierls model with dispersive, gapless phonons is defined by,

$$H = H_1 + H_2$$

where

$$H_1 = -\sum_{\ell=1,\sigma}^{N-1} \left(t + \alpha(u_\ell - u_{\ell+1})\right) (c_{\ell\sigma}^c c_{\ell+1\sigma} + c_{\ell+1\sigma}^c c_{\ell\sigma}) + U \sum_{\ell=1}^{N} \left(N_{\ell\uparrow} - \frac{1}{2}\right) \left(N_{\ell\downarrow} - \frac{1}{2}\right) + \frac{1}{2} \sum_{\ell} V(N_\ell - 1)(N_{\ell+1} - 1).$$

and

$$H_2 = \sum_\ell \left(\frac{P_\ell^2}{2M} + \frac{K}{2}(u_\ell - u_{\ell+1})^2\right).$$

$u_\ell$ and $P_\ell$ are the conjugate displacement and momentum operators for the $\ell$th site. $c_{\ell\sigma}^c$ creates an electron with spin $\sigma$ on site $\ell$. $t$ is the electronic hybridization integral, $U$ and $V$ are the onsite and nearest neighbour Coulomb interactions, respectively, $\alpha$ is the electron-phonon coupling constant, $M$ is the nuclear mass, and $K$ is the elastic spring constant.

In the adiabatic limit (defined by $M \to \infty$) and the noninteracting limit (defined by $U = V = 0$) the bond alternation, defined by

$$\delta_0 = \frac{1}{N} \sum_\ell \frac{(u_{\ell+1} - u_\ell)}{a} (-1)^\ell$$

(where $a$ is the average bond length), satisfies

$$\delta_0 = 4 \exp \left(-\left[1 + \frac{1}{2\lambda}\right]\right)$$

for $\lambda \ll 1$. $\lambda$ is the usual definition of the electron-phonon coupling parameter, defined as $\lambda = 2\alpha^2/\pi Kt$. A non-zero value of the electron-phonon interaction, $\lambda$, therefore implies a non-zero value for the bond alternation. The purpose of this work is to address the role of quantized phonons on the bond alternation, and in particular to investigate whether there
is a non-zero value of $\lambda$ for the Peierls transition. We find that although quantized phonons reduce the amplitude of the broken symmetry order parameter, in contrast to the previous investigations using Einstein phonons, there is no evidence that the Peierls state is destroyed at a finite value of the electron-phonon interaction.

I. METHODS

The lattice degrees of freedom are quantized for dispersive phonons by introducing the phonon creation and annihilation operators,

$$b^\dagger_\ell = \sqrt{\frac{K}{\hbar \omega}} u_\ell - i \sqrt{\frac{\omega}{4K\hbar}} P_\ell$$

and

$$b_\ell = \sqrt{\frac{K}{\hbar \omega}} u_\ell + i \sqrt{\frac{\omega}{4K\hbar}} P_\ell,$$

respectively, where $\omega = \sqrt{2K/M}$.

Eq. (1) is solved by the density matrix renormalization group (DMRG) method for chains of up to 136 sites. The DMRG method is an efficient truncation procedure for solving quantum lattice Hamiltonians, especially in one-dimension. Solving electron-phonon models, however, poses special problems as the number of phonons is not conserved. Thus it is necessary to retain enough oscillator levels per site ($M_p$) to ensure convergence of the key quantities. The number of electron-phonon states per site ($4 \times M_p$) is usually too many to augment with the system block, thus it is necessary to truncate this single site basis. There are therefore four convergence parameters to tune for this model: the number of oscillator levels per site, the number of optimized electron-phonon states per site, the number of states per system block, and the overall number of superblock states.

We first establish convergence with respect to the number of optimized electron-phonon states per site. Table I shows that both the ground state energy and the phonon order parameter (defined by Eq. (9)) have converged to better than 0.2% for 14 states per site. Next, we consider convergence with respect to the number of system and superblock states. Table II shows excellent convergence when the number of system block states is 250 and the eigenvalue product cutoff $\epsilon = 10^{-14}$. Finally, we consider convergence with respect to the number of bare oscillator levels per site. Table III and Table IV show excellent convergence at 6 levels per site for both the ground state energy and the phonon order parameter.
TABLE I: The ground state energy, $E$, (in units of $t$) and the phonon order parameter, $Nm$, (defined by Eq. (9)) of the Hubbard-Peierls model as a function of the number of electron-phonon states per site, $M$, for a 40-site chain with 6 oscillator levels per site. $\omega = t$, $U = 2.5t$, $V = U/4$, and $g = 0.1$.

| $M$  | $E$   | $Nm$  |
|------|-------|-------|
| 6    | -58.716 | 0.663 |
| 10   | -59.969 | 0.629 |
| 14   | -60.220 | 0.628 |
| 18   | -60.275 | 0.629 |

TABLE II: The ground state energy, $E$, (in units of $t$) and the phonon order parameter, $Nm$, of the Hubbard-Peierls model as a function of the density matrix eigenvalue product cutoff, $\epsilon$, the number of system block states, $M$, and the superblock Hilbert space size, SBHSS, for a 40-site chain with 6 oscillator levels per site. $\omega = t$, $U = 2.5t$, $V = U/4$, and $g = 0.1$.

| $\epsilon$ | $M$  | SBHSS   | $E$   | $Nm$  |
|-------------|------|----------|-------|-------|
| $10^{-12}$  | 238  | 141400   | -60.218 | 0.641 |
| $10^{-13}$  | 234  | 232360   | -60.219 | 0.633 |
| $10^{-14}$  | 192  | 285418   | -60.219 | 0.637 |
| $10^{-14}$  | 246  | 359782   | -60.220 | 0.629 |
| $10^{-14}$  | 308  | 415394   | -60.220 | 0.629 |
| $10^{-15}$  | 250  | 506814   | -60.220 | 0.628 |
| $10^{-16}$  | 250  | 652632   | -60.220 | 0.629 |

TABLE III: The ground state energy (in units of $t$) of the Hubbard-Peierls model as a function of the number of sites, $N$. $\omega = t$, $U = 2.5t$, $V = U/4$, and $g = 0.1$.

| Number of oscillator levels per site | 1  | 2  | 3  | 4  | 5  | 6  | 7  |
|-------------------------------------|----|----|----|----|----|----|----|
| 16                                 | -23.072 | -23.506 | -23.635 | -23.668 | -23.684 | -23.685 | -23.685 |
| 24                                 | -34.859 | -35.559 | -35.775 | -35.830 | -35.860 | -35.862 | -35.862 |
| 40                                 | -58.440 | -59.671 | -60.058 | -60.162 | -60.215 | -60.220 | -60.221 |
TABLE IV: The phonon order parameter, $N_m$, of the Hubbard-Peierls model as a function of the number of sites, $N$. $\omega = t$, $U = 2.5t$, $V = U/4$, and $g = 0.1$.

| Number of oscillator levels per site | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|-------------------------------------|---|---|---|---|---|---|---|
| $N$                                 | 16 | 0 | 0.321 | 0.367 | 0.367 | 0.384 | 0.385 | 0.385 |
|                                     | 24 | 0 | 0.398 | 0.455 | 0.455 | 0.477 | 0.479 | 0.479 |
|                                     | 40 | 0 | 0.518 | 0.593 | 0.595 | 0.625 | 0.628 | 0.629 |

Typically, we use 6 oscillator levels per site, with 14 optimized single site states, 250 block states, and 500,000 superblock states. One finite lattice sweep is performed at the target chain size. In addition, in situ optimization of the single site basis is performed for each site at the target chain size. In all cases we investigate linear chains with open boundary conditions. We maintain constant chains lengths by fixing the position of the end sites.

The Hubbard-Peierls model in the classical limit (defined by Eq. (1)) is solved using the Hellman-Feynmann theorem which implies that,

\[
(u_{\ell+1} - u_\ell) = -\frac{\pi t \lambda}{\alpha} \left( \sum_\sigma \langle c_{\ell\sigma}^\dagger c_{\ell+1\sigma} + c_{\ell+1\sigma}^\dagger c_{\ell\sigma} \rangle - \Gamma \right),
\]

where $\langle \cdots \rangle$ means the expectation value in the ground state. The ground state bond alternation is found by iterating Eq. (8) until there is convergence.

II. RESULTS AND DISCUSSION

We first investigate the Hubbard-Peierls model for arbitrary electron-phonon interactions in the noninteracting limit ($U = V = 0$). Following Fradkin and Hirsch, we use the dimensionless electron-phonon interaction, $g = \sqrt{\alpha^2/Kt} \equiv \sqrt{\lambda \pi/2}$.

The Peierls broken-symmetry ground state is characterized by a non-zero value of the staggered phonon order parameter, defined by

\[
m(N) = \frac{1}{N} \sum_\ell \langle B_{\ell+1} - B_\ell \rangle (-1)^{\ell},
\]

where $B_\ell = (b_{\ell}^\dagger + b_\ell)/2$ is the dimensionless displacement of the $\ell$th site and $N$ is the number of sites. Notice from Eq. (6) and Eq. (7) that the bond alternation, $\delta_0$, is proportional to
FIG. 1: The phonon order parameter versus the electron-phonon interaction for the noninteracting Hubbard-Peierls model. $\omega = t$. The inset shows a linear extrapolation of $Nm$ versus $g$ to the origin. (The crosses indicate the evaluated points.)

$\sqrt{\omega m(N)}$. To determine whether this order parameter vanishes as a function of the electron-phonon interaction in the asymptotic limit it is necessary to perform a finite size scaling analysis. Fradkin and Hirsch suggested that the scaling relation

$$m(N) = \frac{1}{Ng} F(Nm(\infty))$$

should apply. Thus, curves of $Nm(N)$ versus $g$ are expected to coincide at the critical value of $g$ at which $m(\infty)$ vanishes.

Fig. 1 shows $Nm$ versus $g$ for values of $\omega = t$ and $U = V = 0$. These results were obtained using the density matrix renormalization group method, as described in the Methods section. It is clear that for small values of $g$ $m$ is linearly proportional to $g$ for all chain lengths. Furthermore, the curves extrapolate linearly to the origin indicating a zero value for the critical $g$. This confirms Fradkin and Hirsch's original prediction for the noninteracting limit of this model, and accords with the adiabatic prediction. Notice that since the distortion of the $\ell$th bond from its uniform value, $(u_{\ell+1} - u_{\ell+1})$, is proportional to $\sqrt{\omega g \langle B_{\ell+1} - B_\ell \rangle}$, the bond alternation is $\propto g^2$ or $\propto \lambda$ for $g \ll 1$.

We next consider the role of Coulomb interactions on the value of the bond alternation. It
is known that in the adiabatic limit the bond alternation initially increases as the Coulomb repulsion increases. This is because electronic interactions suppress the quantum fluctuations between the two degenerate bond alternation phases. The bond alternation is maximized when the electronic kinetic energy roughly equals its potential energy, namely when $U \sim 4t$. As the Coulomb interaction increases further the bond alternation decreases, eventually scaling as $\sim t/(U - V)$.

Fig. (2) shows $N_m$ versus $g$ for values of $\omega = t$, $U = 2.5t$, and $V = U/4$. These Coulomb parameters were chosen to coincide with those used by Sengupta et al., who studied a similar model to Eq. (1), but with Einstein bond phonons. As already stated, they reported that quantized phonons destroy the Peierls ground state below a critical value of the electron-phonon interaction. In contrast to that work, however, we see that for our model with Debye phonons the predictions are qualitatively similar to the noninteracting limit, namely $N_m$ decreases as a linear function of $g$ as $g \to 0$. We note, however, that the phonon order parameter for a given value of $g$ is larger for this value of $U$ than for the noninteracting limit.
The phonon order parameter, $m$, as a function of the Coulomb interaction $U$ is illustrated in Fig. (3) for 72-site chains. $g = 0.01$, and thus the results lie in the linear regime where $m \propto g$. As for the adiabatic limit, $m$ initially increases with $U$ before asymptotically decreasing as $U \to \infty$. We might therefore expect that in the strong coupling limit ($U \to \infty$) quantum fluctuations have a better chance to destroy the Peierls state below a critical electron-phonon interaction. That this is not the case was demonstrated by the present authors in an investigation of the Heisenberg spin-Peierls model. This model is the Hubbard-Peierls model in the strong coupling limit at half-filling. The Heisenberg spin-Peierls model is parameterized by $J \equiv 4t^2/(U - V)$, $\omega$ and $g$. Ref showed that as for the Hubbard-Peierls model, $Nm$ also decreases as a linear function of $g$ as $g \to 0$. We have therefore shown that for all electronic interactions the Peierls state is robust to quantized lattice fluctuations.

We now turn to discuss the phonon order parameter as a function of the phonon frequency, $\omega$. As $\omega \to 0$ (and more oscillator levels are occupied) the system approaches the classical limit. To make a direct comparison to the classical limit we also solve Eq. (1) in this limit. The classical Hamiltonian is defined by,

$$H = H_1 + \frac{K}{2} \sum_\ell (u_\ell - u_{\ell+1})^2 + \Gamma \sum_\ell (u_\ell - u_{\ell+1})$$  \hspace{1cm} (11)

(where $H_1$ is defined by Eq. (2)), and the bond variables are now classical variables. The
FIG. 4: The scaled bond alternation of the Hubbard-Peierls model for a 50-site chain. The adiabatic limit (using Eq. (11)) (diamonds); the quantum case (using Eq. (11)), $\omega = 0.1t$ (circles), and $\omega = t$ (triangles). $U = 2.5t$ and $V = U/4$.

role of the last term is to ensure constant chain lengths, where $\Gamma$ is self-consistently chosen so that $\sum_{\ell}(u_{\ell} - u_{\ell+1}) = 0$. The ground state bond alternation of the classical model is found iteratively using the Hellmann-Feynman procedure, as described in the Methods section.

Fig. (4) shows $\delta_0$ (scaled by $g$) of a 50-site chain versus $g$ for the two quantum cases, $\omega = 0.1t$ and $\omega = t$, as well as for the adiabatic limit. Evidently $\delta_0/g$ tends linearly $\to 0$ as $g \to 0$. Thus, $\delta_0 \propto g^2 \propto \lambda$. Moreover, as predicted, the phonon order parameter decreases as a function of $\omega$. As $g$ increases the deviation between the quantum and classical predictions increases.

Finally, we discuss the nature of the Peierls transition at $\lambda = 0$. In the noninteracting limit the classical transition is given by Eq. (5). No analytical expression exists in the interacting limit. However, Fig. (4) shows that the transition (at $g = 0$) is qualitatively similar in the classical and quantum cases, as $\delta_0$ is proportional to $g^2 \equiv \lambda$. Moreover, the behaviour of the bond alternation as a function of chain length is the same for small electron-phonon interactions in the classical and quantum cases. Fig. (5) shows the scaled bond alternation versus inverse chain length in the adiabatic and quantum cases. The close agreement of these predictions suggests that the transition at $g = 0$ is the same in the
FIG. 5: The scaled bond alternation versus inverse chain length in the adiabatic limit. Crosses are the quantum result with $\omega = t$, $g = 0.1$, $U = 2.5t$, and $V = U/4$.

quantum and classical cases in the limit of long chains.

III. CONCLUSIONS

In conclusion, we have used the DMRG method to investigate the role of gapless, dispersive quantized phonons on the Peierls transition in the Hubbard-Peierls model. We showed that the staggered phonon order scales as $g$ (and the bond alternation scales as $g^2$, and thus $\propto \lambda$) as $g \rightarrow 0$ for all values of the Coulomb interaction and phonon frequency considered here. In the strong coupling limit the Hubbard-Peierls model maps onto the Heisenberg spin-Peierls model, which also exhibits a Peierls transition at $g = 0$. Thus, we conclude that the Peierls transition occurs at $g = 0$ for all values of the Coulomb interaction. Moreover, we showed that the quantum predictions for the bond order follow the classical prediction as a function of $1/N$ for small $g$. We therefore conclude that the zero $g$ phase transition is of the mean-field type.
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