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The Peierls–Hubbard model at weak coupling

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Abstract

We investigate the Peierls transition in the one-dimensional Peierls–Hubbard model at half-filling in the adiabatic approximation for the lattice. Depending on the value of the electron–lattice coupling constant g the equilibrium dimerization can be either enhanced or suppressed by the Hubbard interaction U. Applying second-order perturbation theory we determine the critical value $g_c = 0.689\,348$ below which the Hubbard interaction enhances the dimerization.

1. Introduction

The coupling of a one-dimensional metal to an elastic lattice results in an instability towards a lattice distortion known as the Peierls transition [1]. This phenomenon can be observed in various quasi-one-dimensional materials, e.g. conjugated polymers [2] like polyacetylene, charge-transfer salts [3], and spin–Peierls compounds like $CuGeO_3$.

From a theoretical point of view, a first step towards a quantitative description of the Peierls transition has been made by Su, Schrieffer and Heeger (SSH) [4]. However, in their model neither the dynamics of the lattice nor the electron–electron interaction has been taken into account. Subsequently there has been made some effort to include phonons beyond the adiabatic approximation. While in the approach of SSH the Peierls transition occurs for any nonzero value of the electron–phonon (el–ph) coupling, a minimum strength of the el–ph coupling is required for the transition if quantum phonons are included [5].

In this paper we consider the limit of a static lattice and focus on the role of the electron–electron interaction. Correlation effects on the Peierls transition have been studied using a variety of methods including variational wavefunctions [6, 7], Hartree–Fock plus perturbation theory [8], quantum Monte Carlo [9], numerical diagonalization of small systems [10–13], bosonization [14, 15], and incremental expansion [16, 17]. It is now generally accepted that for small values of the el–ph coupling constant $g < g_c$ the dimerization is enhanced when the Hubbard interaction U is switched on while for $g > g_c$ it is suppressed. Estimates for the critical el–ph coupling that have been obtained in the literature are $g_c \approx 0.75$ in [7], $g_c \approx 0.76$

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in [12] and $g_c \approx 0.69$ in [16, 17]. For g not too close to g_c the dimerization reaches a maximum at U of the order of the bandwidth and goes to zero for $U \to \infty$.

Apart from this qualitative agreement there is still a lack of rigorous results, in particular in the limit of weak el–ph coupling $g \ll g_c$ which is difficult to address in the aforementioned approaches. In order to remove the uncertainties we study the Peierls–Hubbard model in the weak coupling regime using second-order perturbation theory with respect to the Hubbard interaction. This allows use to derive rigorous results in the limit $U \to 0$ for all values of the el–ph coupling.

The paper is organized as follows. In section 2 we introduce the Peierls–Hubbard model and discuss the validity of the perturbative approach. The main results concerning the Peierls transition are presented in section 3. In section 4 we discuss our results and compare them with different approaches.

2. Model and perturbation theory

We consider the one-dimensional Peierls–Hubbard model

$$H = -t \sum_{i,\sigma} (1 - \alpha(u_{i+1} - u_i))(c_{i\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{K}{2} \sum_i (u_i - u_{i+1})^2 \tag{1}$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) an electron with spin σ ($= \uparrow, \downarrow$) on a lattice of N sites, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, and u_i is the deviation of the ith atom from its equilibrium position in units of the lattice constant a. U and K are the on-site Hubbard interaction and the elastic constant of the lattice, respectively, and t is the hopping parameter. In (1) the phonons are treated in the adiabatic limit which is formally obtained by letting the mass of the atoms go to infinity. Since the lattice distortion is assumed small compared to the lattice constant, the modification of the hopping amplitude can be treated in linear order via the parameter α. In the following we restrict ourselves to half-filling where due to $2k_F = \pi/a$ the Peierls instability leads to an alternating lattice distortion

$$u_i = (-1)^i u. \tag{2}$$

It is convenient to express the el–ph coupling and the dimerization amplitude via the dimensionless parameters g and δ, respectively, which are defined by

$$g = \alpha \sqrt{\frac{t}{K}} \tag{3}$$

$$\delta = 2\alpha u. \tag{4}$$

In terms of these parameters Hamiltonian (1) reads

$$H = -t \sum_{i,\sigma} (1 + (-1)^i \delta)(c_{i\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{Nt\delta^2}{2g^2}. \tag{5}$$

We consider t, U, and g as given model parameters while the dimerization δ is free to adjust itself such that the total energy is minimal. In the following we measure all energies in units of the hopping amplitude t (i.e. we set $t = 1$). The ground state energy of the Hamiltonian (5) can only be calculated analytically in the limiting cases $\delta = 0$ and 1. $\delta = 0$ corresponds to the ordinary Hubbard model which has been solved using the Bethe ansatz [18] and for $\delta = 1$ the system is completely dimerized. For other values of δ one has to resort to approximations or to numerical methods. Since we are only interested in the weak coupling regime we use second-order perturbation theory with respect to the Hubbard interaction. First of all we want to justify the assertion that perturbation theory can indeed be applied for the model (5). In the case $\delta = 0$ the exact ground state energy known from the Bethe ansatz solution [18] can be expressed as an integral over Bessel functions. As pointed out by Economou and Poulopoulos [19] this integral can be converted into an asymptotic series in U. Metzner and Vollhardt [20] showed that the exact second-order term of this asymptotic expansion can be calculated using perturbation theory. Furthermore, they conjectured that this is true not only for the second-order term but for all coefficients of the expansion. For $\delta > 0$ the conditions for applying perturbation theory are more favourable than for $\delta = 0$ since the unperturbed ground state energy E_0 is separated from all excited states by an energy gap $\Delta = 4\delta$ which avoids divergent contributions from small denominators. We expect therefore that the ground state energy of the Peierls–Hubbard model can be expanded in a series with a finite radius of convergence, $U_0(\delta)$, for all $\delta > 0$ and that the coefficients of this expansion can be obtained from perturbation theory. Krivnov and Ovchinnikov [21] have pointed out that within the parquet approximation for a continuum version of the model (5) the leading nth-order contribution to the ground state energy is $\propto \delta^2 U^n \ln^{n+1} \delta$. Similar conclusions were obtained by Horovitz and Solyom [22] using a scaling approach and by Kivelson *et al* [23] by comparison of exact results on the massive Thirring model with the perturbation theory for a model of spinless fermions. Fermions with spin were considered in [24] and again a perturbation expansion in powers of $U \ln \delta$ was obtained. Thus the radius of convergence behaves as $U_0(\delta) \propto 1/|\ln \delta|$ and even for exponentially small dimerization δ perturbation theory can be applied over some finite range of U. Writing $\epsilon(\delta, U) = E(\delta, U)/N$, the ground state energy per site of the electronic part of (5), the expansion of ϵ in powers of U takes the form

$$\epsilon(\delta, U) - \frac{U}{4} = \epsilon_0(\delta) + \epsilon_2(\delta)U^2 + \epsilon_4(\delta)U^4 + \cdots \tag{6}$$

where we have used the fact that due to particle–hole symmetry $\epsilon(\delta, U) - U/4$ is an even function of U. In particular, in the case of complete dimerization, $\delta = 1$, it is straightforward to calculate the exact ground state energy and expand it in a series which converges for $U < 8$:

$$\epsilon(1, U) - \frac{U}{4} = -2\sqrt{1 + \frac{U^2}{64}} = -2 - \frac{U^2}{64} + \frac{U^4}{16\,384} + \cdots. \tag{7}$$

3. Equilibrium dimerization

In order to determine the equilibrium dimerization we minimize the ground state energy of the Hamiltonian (5), including the lattice contribution, with respect to δ and obtain the condition

$$\epsilon_0'(\delta) + \epsilon_2'(\delta)U^2 + \epsilon_4'(\delta)U^4 + \cdots + \frac{\delta}{g^2} = 0. \tag{8}$$

Equation (8) defines the function $\delta(U)$ which can also be expanded in a series containing only even powers of U

$$\delta(U) = \delta_0 + \delta_2 U^2 + \delta_4 U^4 + \cdots. \tag{9}$$

Reinserting equation (9) into (8) and comparing order by order in U yields

$$\delta_0 = -g^2 \epsilon_0'(\delta_0) \tag{10}$$

$$\delta_2 = -\frac{\epsilon_2'(\delta_0)}{g^{-2} + \epsilon_0''(\delta_0)} \tag{11}$$

$$\delta_4 = -\frac{\frac{1}{2}\delta_2^2 \epsilon_0'''(\delta_0) + \delta_2 \epsilon_2''(\delta_0) + \epsilon_4'(\delta_0)}{g^{-2} + \epsilon_0''(\delta_0)}. \tag{12}$$

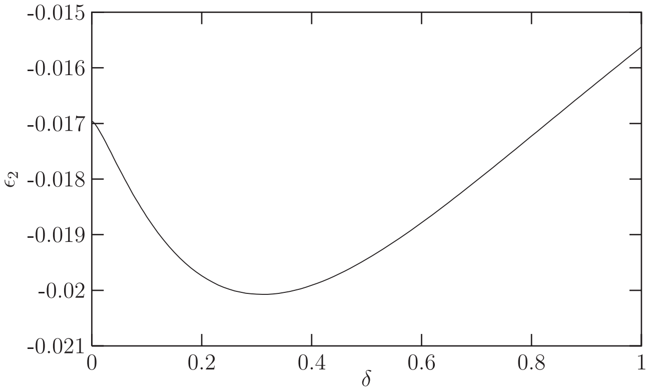

Figure 1. Second-order contribution to the ground state energy per site, $\epsilon = \epsilon_0 + \epsilon_2 U^2 + \epsilon_4 U^4 + \cdots$, as a function of the dimerization parameter δ. The minimum occurs at $\delta_c = 0.310\,523$.

The zeroth-order dimerization has been calculated in [4]. In the limit $g \ll 1$ it is given by

$$\delta_0 = 4\exp\left(-\frac{\pi}{4g^2} - 1\right). \tag{13}$$

Now we turn to the second-order contribution $\propto U^2$ of the ground state energy. Considering the Hubbard interaction in equation (5) as a perturbation, the second-order coefficient of the series (6) reads

$$\epsilon_2(\delta) = -\frac{1}{N}\sum_{n\neq 0}\frac{|\langle n|D|0\rangle|^2}{E_n - E_0} \tag{14}$$

where E_n is the energy of the eigenstate $|n\rangle$ of the noninteracting Hamiltonian H_0, and $D = \sum_i n_{i\uparrow}n_{i\downarrow}$. Representing $|n\rangle$ in the one-particle basis of H_0, equation (14) can be converted into

$$\epsilon_2(\delta) = -\frac{1}{32}\int_{-\pi}^{\pi}\frac{\mathrm{d}k}{2\pi}\int_{-\pi}^{\pi}\frac{\mathrm{d}k'}{2\pi}\int_{-\pi}^{\pi}\frac{\mathrm{d}q}{2\pi}\,\frac{\left|1 + \mathrm{e}^{\mathrm{i}(\varphi_{k+q} - \varphi_k + \varphi_{k'-q} - \varphi_{k'})}\right|^2}{\varepsilon_{k+q} + \varepsilon_k + \varepsilon_{k'-q} + \varepsilon_{k'}} \tag{15}$$

where

$$\varepsilon_k = 2\sqrt{\cos^2 k + \delta^2 \sin^2 k} \tag{16}$$

$$\mathrm{e}^{\mathrm{i}\varphi_k} = \frac{1 + \mathrm{e}^{-2\mathrm{i}k} + \delta(1 - \mathrm{e}^{-2\mathrm{i}k})}{|1 + \mathrm{e}^{-2\mathrm{i}k} + \delta(1 - \mathrm{e}^{-2\mathrm{i}k})|}. \tag{17}$$

Equation (15) is equivalent to equation (C5) in [8] in the limit of zero staggered magnetization. The integral (15) can be calculated numerically with very high precision. The result shown in figure 1 agrees with the analytical values $\epsilon_2(0) = -(7/16\pi^3)\zeta(3) = -0.016\,961$ and $\epsilon_2(1) = -1/64 = -0.015\,625$. More importantly, $\epsilon_2(\delta)$ has a minimum at $\delta_c = 0.310\,523$ which means that according to equation (11) the sign of the coefficient δ_2 changes from plus to minus. According to equation (10) the critical dimerization δ_c corresponds to a critical el–ph coupling constant

$$g_c = \sqrt{\frac{\delta_c}{|\epsilon_0'(\delta_c)|}} = 0.689\,348. \tag{18}$$

Therefore for $g < g_c$ the dimerization is enhanced by the Hubbard interaction while for $g > g_c$ it is suppressed. The second-order coefficient δ_2 of equation (9) which is displayed in figure 2

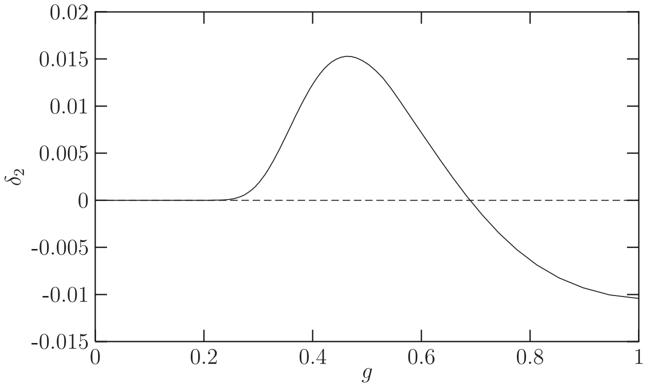

Figure 2. Second-order coefficient δ_2 of the equilibrium dimerization $\delta(U) = \delta_0+\delta_2 U^2+\delta_4 U^4+\cdots$ as a function of the el–ph coupling constant g. Note that δ_2 changes sign at $g_c = 0.689\,348$ which is related to $\delta_c = 0.310\,523$ via equation (18).

has a maximum at $g \approx 0.464$. In the limit of small el–ph coupling, $g \ll 1$, equation (11) simplifies to

$$\delta_2 = -\frac{\pi}{4}\epsilon_2'(\delta_0). \tag{19}$$

From a careful analysis of the numerical data for small values of δ we conjecture that

$$\epsilon_2(\delta) - \epsilon_2(0) \propto \delta^2\left(\ln\frac{c}{\delta}\right)^3 \tag{20}$$

with $c \approx 1.5$, in agreement with the result of the parquet summation [21]. Inserting this expression into equation (19) and using the asymptotic formula for $\delta_0(g)$ given in equation (13) we obtain the result

$$\frac{\delta_2}{\delta_0} \propto g^{-6}, \tag{21}$$

i.e. the relative weight of the second-order term in the expansion of the dimerization $\delta(U) = \delta_0 + \delta_2 U^2 + \delta_4 U^4 + \cdots$ increases strongly for $g \to 0$, although both δ_0 and δ_2 are exponentially small in this limit.

Unfortunately it becomes rather complicated to calculate the fourth-order term $\epsilon_4(\delta)$ using perturbation theory. We have therefore chosen a different approach based on the exact numerical diagonalization of small systems (up to $L = 14$ lattice sites) using the Lanczos algorithm which allows us to calculate the ground state energy with a relative precision of better than 10^{-14}. In order to avoid even–odd oscillations we have implemented antiperiodic boundary conditions for $L = 4n$ and periodic boundary conditions for $L = 4n+2$. This guarantees that the ground state is non-degenerate. Since we know the exact second-order term $\epsilon_2(\delta, L)$ (for given system size L) it is possible to extract $\epsilon_4(\delta, L)$ with very high precision. However, one is left with the problem of extrapolating these values to $L = \infty$. We have tried various extrapolation procedures. For $\delta \geqslant 0.2$ the ansatz $\epsilon_4(\delta, L) = \epsilon_4(\delta, \infty) + a\exp(-bL + c/L)$, which is motivated by the existence of a gap in the excitation spectrum, yields very stable results for $\epsilon_4(\delta, \infty)$. In particular, the asymptotic behaviour close to the fully dimerized limit, $\epsilon_4(\delta) = 2^{-14}(1 + 3(1 - \delta)/2 + \cdots)$, for $\delta \to 1$ is correctly recovered (see figure 3). However, for $\delta < 0.2$ we could not perform a reliable finite-size scaling of our data. The reason is that the correlation length, which is inversely proportional to the gap, is getting much larger than the size of the systems that

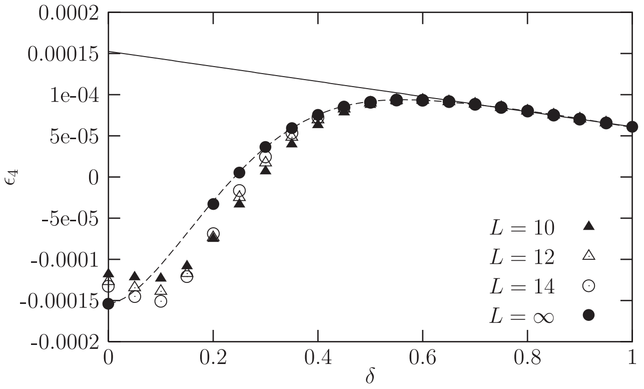

Figure 3. Fourth-order contribution of the ground state energy per site, $\epsilon(L) = \epsilon_0(L) + \epsilon_2(L)U^2 + \epsilon_4(L)U^4 + \cdots$, as a function of the dimerization parameter δ for $L = 10, 12, 14$, and ∞. The dashed curve is meant as a guide to the eye, only. The solid line is the asymptotic result $\epsilon_4(\delta) = 2^{-14}(1 + 3(1 - \delta)/2)$ valid in the limit $\delta \to 1$.

can be diagonalized numerically. On the other hand, for $\delta = 0$ where there is no gap, an unbiased polynomial fit yields $\epsilon_4(0, \infty) = -1.547 \times 10^{-4}$ which is quite close to the exact value [19] $\epsilon_4(0) = -(93/2048\pi^5)\zeta(5) = -1.538 \times 10^{-4}$. In figure 3 we plot $\epsilon_4(0, L)$ for $L = 10, 12, 14$ together with the extrapolated value $\epsilon_4(0, \infty)$ (whenever available) as a function of δ. Comparing with the corresponding results for ϵ_2 (see figure 1) we see that ϵ_4 is typically two orders of magnitude smaller than ϵ_2, which indicates that the weak coupling approach should be quite accurate in the region $U \lesssim 1$.

For $g < g_c$ the dimerization $\delta(U)$ reaches a maximum at $U = U_{\max}$ which is given by

$$U_{\max} = \sqrt{-\frac{\delta_2}{2\delta_4}} \tag{22}$$

when we neglect the terms of order $\sim U^6$ and higher in equation (9). Expanding $U_{\max}^2$ in powers of $g_c - g$ we obtain for g close to g_c

$$U_{\max}(g) \simeq \kappa (g_c - g)^{1/2} \tag{23}$$

with

$$\kappa = \frac{\delta_c \epsilon_2''(\delta_c)}{g_c \epsilon_4'(\delta_c)(1 + g_c^2 \epsilon_0''(\delta_c))} \approx 8.7 \tag{24}$$

to be compared with the value $\kappa = 8.25$ obtained in [16] using the incremental expansion. Note that the error in the determination of κ is only due to the limited precision of ϵ_4. Nevertheless, the fair agreement with the result of [16] indicates that the finite-size scaling of our Lanczos data yields reasonable results for ϵ_4.

In figure 4 the equilibrium dimerization δ of the Peierls–Hubbard model is displayed as a function of U for several values of the el–ph coupling g. The circles represent the dimerization including the fourth-order term in U while the solid curves correspond to the second-order approximation. For small values of g the maximum of δ is more pronounced and occurs around $U \approx 2$. This is somewhat smaller than the value $U \approx 3$ obtained using the incremental expansion [16]. Furthermore the maximum of δ is expected to shift to larger values of U with decreasing g but of course the precise position of the maximum depends on the terms of order $\propto U^6$ and higher which have been omitted in our weak coupling approach.

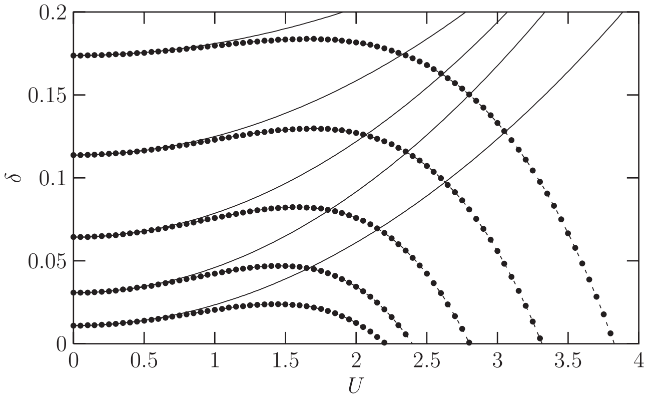

Figure 4. Dimerization δ as a function of U for $g = 0.4, 0.45, 0.5, 0.55, 0.6$ (from bottom to top). The full lines (circles) represent the second-(fourth-) order approximation of $\delta(u) = \delta_0 + \delta_2 U^2 + \delta_4 U^4 + \cdots$. The values of U where δ becomes negative indicate the breakdown of the weak coupling approximation.

4. Discussion

We have investigated the Peierls–Hubbard model in the weak coupling regime using second-order perturbation theory and exact diagonalization for the fourth-order contribution. The application of perturbation theory is justified by the existence of a gap in the excitation spectrum which removes the problem of small denominators. On the other hand, it is also due to this gap that finite-size scaling of the Lanczos data becomes problematic for small dimerization $\delta < 0.2$ where the correlation length exceeds the size of the systems that can be diagonalized numerically. The central result of this paper is the determination of the exact value of the el–ph coupling $g_c = 0.689\,348$ which separates the region where the Hubbard interaction enhances the dimerization ($g < g_c$) from the region where the dimerization is reduced ($g > g_c$). The corresponding dimerization parameter is found to be $\delta_c = 0.310\,523$. There have been many attempts to determine these parameters using different methods. Using the Gutzwiller variational wavefunction Baeriswyl and Maki [7] estimated $g_c \approx 0.75$. Exact diagonalization of small systems has been used to obtain $\delta_c \approx 0.4$ in [11] and $g_c \approx 0.76$ in [12], respectively. Finally, the most precise values up to now have been derived using the incremental expansion technique, which is based on the numerical diagonalization of finite chains. In [16, 17] $g_c = 0.69$ is obtained, which is very close to the exact value.

As mentioned before, all approaches that rely on finite-size extrapolation of small systems suffer from severe problems in the limit of small dimerization, $\delta < 0.1$, which corresponds to values of the el–ph coupling $g < 0.5$. In contrast, the perturbation theory approach can be applied for all values of g. In particular, it is possible to determine the asymptotic behaviour of $\epsilon_2(\delta)$ in the limit $\delta \to 0$ including logarithmic corrections. From there it can be inferred that the *relative* importance of the second-order term (compared to the leading term) in the expansion of the dimerization $\delta(U) = \delta_0 + \delta_2 U^2 + \delta_4 U^4 + \cdots$ goes as $\sim g^{-6}$ for $g \to 0$, although both δ_0 and δ_2 are exponentially small in this limit. On the other hand, considering *absolute* values, the correlation enhancement of the dimerization is less dramatic and essentially limited to the region $0.3 < g < g_c$ with the maximum occurring at $g = 0.464$. The parameters most frequently used for polyacetylene lie in the range between $g = 0.39$ [7] and $g = 0.57$ [4] which emphasizes the importance of correlation effects in real Peierls systems.

Acknowledgments

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