

Incremental expansions for Hubbard–Peierls systems

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The ground state energies of infinite half-filled Hubbard–Peierls chains are investigated by combining an incremental expansion with exact diagonalization of finite chain segments. The ground-state energy of equidistant infinite Hubbard (Heisenberg) chains is calculated with a relative error of less than 3×10^{-3} for all values of U using diagonalizations of 12-site (20-site) chain segments. For dimerized chains the dimerization order parameter d as a function of the on-site repulsion interaction U has a maximum at nonzero values of U , if the electron–phonon coupling g is lower than a critical value g_c . The critical value g_c is found with high accuracy to be $g_c = 0.69$. For smaller values of g the position of the maximum of $d(U)$ is approximately $3t$, and rapidly tends to zero as g approaches g_c from below. We show how our method can be applied to calculate breathers for the problem of phonon dynamics in Hubbard–Peierls systems. © 1998 American Institute of Physics. [S0021-3640(98)00812-3]

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The effect of correlations on the Peierls transition has been one of challenging problems in the theory of quasi-one-dimensional compounds. One of the most important theoretical treatments of the Peierls transition goes back to the solution of the exactly solvable model of noninteracting fermions proposed by Su, Schrieffer, and Heeger (SSH).¹ Although being successful in explaining a number of properties of real quasi-one-dimensional systems, the SSH model is in a clear disagreement with such experimental results as the emergence of negative spin magnetization densities for neutral solitons.² One is faced with the necessity of treating the Coulomb interaction in the electron subsystem. This interaction should be accounted for by including a positive Hubbard on-site interaction term in the SSH model. We refer to this extended model as the Peierls–Hubbard (PH) model. Due to strong one-dimensional quantum fluctuations a mean field theory calculation of the PH model gives qualitatively wrong results, predicting a constant dimerization for small U and the abrupt disappearance of a bond order wave state as U increases above a certain threshold at half filling.³ Including many-body effects it has been shown by many authors (see Ref. 4 and citations therein) that the dimerization d first increases up to a maximum and then decreases with further increase of U .

It is very difficult to perform an accurate exact-diagonalization investigation of the Peierls transition in the correlated regime. In the framework of a standard exact-

diagonalization approach the required cluster sizes are found to be far outreaching the capabilities of modern computer systems. Calculations which have been performed using available cluster sizes are drastically dependent on the boundary conditions (see Ref. 5, for instance), and the final conclusions have had to be based on extrapolations. The basic questions about the value of g_c , the behavior of the system near the critical point, and the position and value of the dimerization maximum U_{\max} as a function of the electron phonon coupling have remained unanswered. The lack of accurate numerical results has made it hard to identify the values of model parameters for real systems. We will show that by combining an incremental expansion technique (IET) with numerically exact diagonalizations, one can overcome the above-mentioned difficulties and perform a reliable numerical calculation of correlated one-dimensional Peierls systems in both the strong and weak correlation regimes.

The quantum chemical method of increments has recently found a wide range of application in condensed matter (see Ref. 6 and references therein). The IET starts with the splitting of a given Hamiltonian operator H into an unperturbed part H_0 and a number of perturbations $H_1 + H_2 + \dots$, so that $H = H_0 + \sum H_i$. The hierarchy of increments is defined in the following way. The first order increment $I_k^{(1)}$ is found by taking the ground-state energy \mathcal{E}_k of the Hamiltonian $H_0 + H_k$ and subtracting from it the ground-state energy \mathcal{E}_0 of H_0 , $I_k^{(1)} = \mathcal{E}_k - \mathcal{E}_0$. Phenomenologically this increment represents the action of the perturbation H_k separately from all other perturbations H_i . The total change of the unperturbed ground-state energy in first incremental order is then given by $\sum_i I_i^{(1)}$. The second order increment $I_{k,l}^{(2)}$ is found by taking the ground-state energy $\mathcal{E}_{k,l}$ of the Hamiltonian $H_0 + H_k + H_l$ and subtracting from it \mathcal{E}_0 and the first order increments $I_k^{(1)}$ and $I_l^{(1)}$, $I_{k,l}^{(2)} = \mathcal{E}_{k,l} - I_k^{(1)} - I_l^{(1)} - \mathcal{E}_0$. The increments $I_{k,l}^{(2)}$ represent the difference between the combined action of a pair H_i, H_k and the sum of the uncorrelated actions of both perturbations. In a similar manner higher-order increments are found. The change of the unperturbed ground-state energy of the full system is given exactly by the sum over all increments (all orders!). Since the increments are usually calculated numerically, the incremental expansion can be performed up to some given order. This expansion is nonperturbative since the increments are not related to some small parameter of a perturbation theory. The idea of the incremental expansion is similar to Faddeev's treatment of the 3-body problem wherein the unknown 3-body scattering matrix is expressed in terms of the exactly known 2-body scattering matrices. The discussion of the interrelation of increments and Faddeev equations and also the derivation of the incremental expansion by a resummation of the perturbation theory is given in Ref. 7.

Now we apply the outlined ideas to the PH Hamiltonian. This Hamiltonian is given by a sum of electronic and lattice parts $H = H_{\text{el}} + H_{\text{lat}}$. The electronic part in fermionic second quantization form is given by

$$H_{\text{el}} = \sum_{i,\sigma} t_i (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.}) + U \sum_i (n_{i,\uparrow} n_{i,\downarrow}). \quad (1)$$

Here U is an on-site Hubbard repulsion matrix element and t_i is the hopping matrix element between the i th and $(i+1)$ th sites. We consider the case of one electron per site (half filling). In the harmonic approximation the lattice part is given as $H_{\text{lat}} = 1/2K \sum_i v_i^2$. Here v_i is a bond-length change (see, e.g., Ref. 4) and K is the spring constant. The electron-lattice interaction is assumed to be of the form $t_i = -(t - \gamma v_i)$.

The strength of the electron–phonon interaction is measured by the dimensionless coupling $g = \gamma/\sqrt{Kt}$. Solving the PH model amounts to finding a minimum of the total energy of the system considered as a functional of the bond length changes v_i . A remarkable proof of Lieb and Nachtergaele⁸ tells us that the minimum configuration has to be a dimerized state with alternating bond lengths $v_i = (-1)^i v_0$. In the following we will use the dimensionless dimerization $d = v_0\sqrt{K}/t$ (see Refs. 5 and 4).

Let us now formulate the incremental expansion of the PH model. A dimerized state represents a sequence of alternating weak and strong bonds formed by a modulation of the transfer integral t_i . It is natural to cut all the weak bonds and to consider the remaining set of noninteracting 2-site dimers as an unperturbed Hamiltonian H_0 . The weak bonds are considered as a perturbation. The unperturbed Hamiltonian H_0 is written as

$$H_0 = \sum_{k=-\infty}^{\infty} t_{2k} (c_{2k,\sigma}^+ c_{2k+1,\sigma} + \text{h. c.}) + U \sum_{i=-\infty,\sigma}^{\infty} n_{i,\uparrow} n_{i,\downarrow}. \quad (2)$$

The ground state of the Hamiltonian operator H_0 is known exactly and is a nondegenerate spin-singlet state $S=0$ formed by a set of noninteracting dimers having two electrons per dimer. The PH Hamiltonian H is a sum of H_0 and a number of perturbations, formed by the (weak) bonds linking neighboring dimers,

$$H = H_0 + \sum_k V_k, \quad V_k = \sum_{\sigma} t_{2k-1} (c_{2k-1,\sigma}^+ c_{2k,\sigma} + \text{h. c.}).$$

The incremental expansion is generated in the following way. The first order increment corresponds to a bond inserted between two neighboring dimers. By virtue of the general principles outlined above, it has the form $I^{(1)} = E_4 - 2E_2$, where E_{2n} , $n = 1, 2, \dots$ denotes the ground-state energy of a $2n$ -site segment cut out of the infinite chain. The second-order increment is defined for a triple of neighboring dimers and follows from inserting two bonds into H_0 . To find it one needs to subtract from the energy of three linked dimers the increments corresponding to 2 pairs of dimers and 3 single dimers in it, and hence the expression reads $I^{(2)} = E_6 - 2I^{(1)} - 3E_2 = E_6 - 2E_4 + E_2$. Note that in the incremental expansion only connected clusters of dimers yield nonzero increments, since the energy of a disconnected cluster is just the sum of the energies of its parts. The expressions for higher-order increments are found in similar fashion. Due to the choice of H_0 (see Eq. (2)) the increments do not depend on the site indices. One proves by induction that the expression for the n th order increment, $n > 2$, is

$$I^{(n)} = E_{2n+2} - 2E_{2n} + E_{2n-2}. \quad (3)$$

In order to find the ground-state energy of the infinite system one needs to count the number of increments of each order per dimer. In the infinite $1-d$ lattice which we are considering, there exists exactly one increment of each order per dimer (we make a one-to-one correspondence between dimers and increments of each order, assigning each increment to its left-most dimer). Therefore, taking into account that there are two sites per each dimer, we write the value of the ground-state energy of the infinite lattice per site as $\mathcal{E} = 1/2(E_2 + \sum_{n=1}^N I^{(n)})$. Here N is the number of increments taken into account.

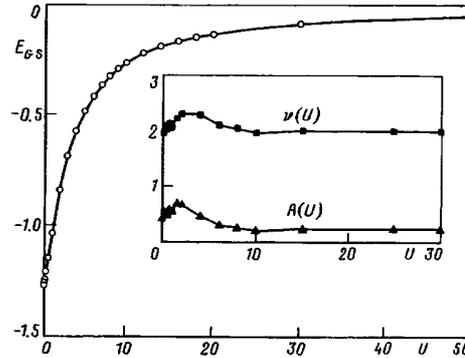


FIG. 1. Ground-state energy of the equidistant Hubbard model at half filling. Solid line — exact result,¹⁰ open circles — IET result for $N=5$ (see text). Inset: U dependence of prefactor A and exponent ν of the obtained functional dependence of the relative error on $(2N+2)$ (see text).

The feature that the number of increments of any given order per site is constant is an exclusive property of one-dimensional lattices. In higher dimensions the number of increments of a given order per site grows rapidly with the order of the increment. This special property of one dimension leads to the following result:

$$\mathcal{E}(N) = \frac{1}{2}(E_{2N+2} - E_{2N}). \quad (4)$$

Formula (4) is quite remarkable, since the calculation of the ground-state properties amounts to the exact diagonalization of two open chains whose length differs by two. Note that expressions of the type (4) have previously been used intuitively in quantum chemical calculations (see, for instance, Ref. 9).

To check our method we first performed a calculation of the ground-state energy of an equidistant Hubbard infinite chain at half filling, where the solution is known exactly.¹⁰ The equidistant case is the worst case for the method described above, since all the bonds have the same strength. The per site value of the ground-state energy \mathcal{E} was calculated using formula (4) with the incremental order $N=1, 2, 3, 4, 5$. The calculation was performed using a Lanczos algorithm. The results for $N=5$ are shown in Fig. 1, where the exact $\mathcal{E}(U)$ dependence for $t=1$ (solid line) is plotted against the results of Eq. (4) (open circles). The relative error R_E decays algebraically with increasing order of the increments $R_E = A(U)[2N+2]^{-\nu(U)}$. The exponent $\nu(U)$ and the prefactor $A(U)$ are plotted in the inset of Fig. 1. We find $\nu(U) \geq 2$ for all values of U . Note that $A(0)/A(\infty) \approx 2$, which implies that our results converge faster for large U . Note also that the errors are very small — typically below 0.1% for $N=6$. This has to be compared with a recent density matrix renormalization group (DMRG) calculation of the same system,¹¹ where system sizes up to 122 and extrapolations had to be used to achieve comparable precision.

Next we show the results of calculations of the dimensionless dimerization in the PH model as a function of U and g (Fig. 2). For $U=0$ the value of $d(g)$ is known exactly¹ (see the filled symbols for $U=0$ in Fig. 2). An analysis of the relative error R_d of determining d with the help of (4) yields exponential convergence $R_d \approx e^{-\lambda(g)(2N+2)}$. The

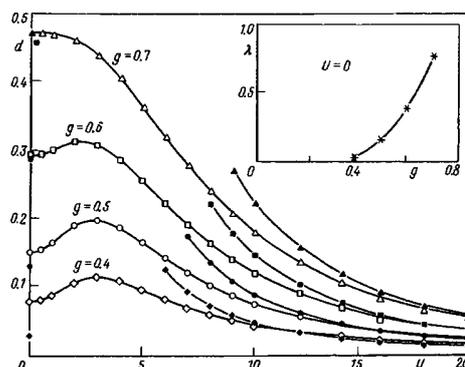


FIG. 2. Dimerization versus U for different values of g . Open symbols — IET results for $N=5$, filled symbols for $U=0$ — exact results, filled symbols for $U>5$ — results for Heisenberg chains with IET and $N=8$. The solid lines are guides to the eye. Inset: g dependence of the exponent λ of the obtained functional dependence of the relative error on $(2N+2)$ for $U=0$ (see text).

dependence of $\lambda(g)$ is shown in the inset of Fig. 2. A crossover is detected around $g=0.4$, with λ being suppressed to rather small values for $g \leq 0.4$. That implies that for small values of U the IET method using exact diagonalizations is confined to values of the coupling constant $g > 0.4$ if high precision is required. In Fig. 2 we present the dependence of $d(U)$ for $g=0.5, 0.6$, and 0.7 (open symbols). For $g=0.5, 0.6$ the dimerization d first increases with U , and then decreases after reaching a maximum. For $g=0.7$ is a monotonically decreasing function of U . Therefore the system has a qualitatively different behavior for weak and strong couplings g , as predicted by the GA theory. On the other hand, our results agree well with the extrapolated values of d obtained within the solitonic approach.⁴

We performed more calculations of $d(U)$ to obtain the dependence of the position of the maximum U_{\max} on the coupling g (see Fig. 3). In particular, we find $U_{\max}(g)$ to be a monotonically decreasing function with $U_{\max}=0$ at a critical coupling g_c . Since our method yields very small errors for $g \geq 0.6$ we can estimate the critical coupling g where

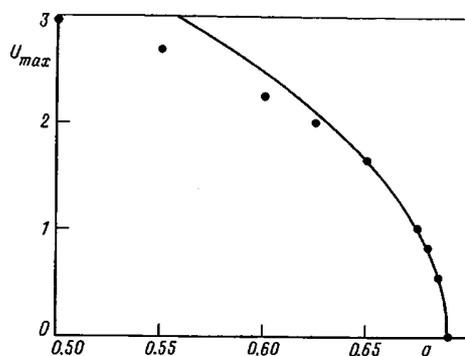


FIG. 3. Dependence of U_{\max} on the coupling g for the Hubbard-Peierls chains with IET and $N=5$. Circles — numerical results; line — best fit (see text).

$U_{\max}=0$ with high accuracy $R_d < 10^{-3}$. It is found $g_c=0.69$. The GA prediction $g_c > 0.74$ overestimates this result slightly. The GA gives the position of the dimerization maximum as $U_{\max}=4t$ for g far below g_c . Our numerical calculation gives $U_{\max} \approx 3t$. The small- U behavior of d is found to be $d \sim U^2$, which is consistent with the GA approach. Furthermore the GA approach predicts that d is an analytic function of U^2 . Then it follows that $U_{\max}(g)$ close to g_c varies as $\kappa(g_c - g)^{1/2}$, which is what we find in Fig. 3 ($\kappa \approx 8.25$).

For large values of U the system is equivalent to the Heisenberg spin-exchange model, with J_i given by $J_i = 4t_i^2/U$. We have calculated the spin-Peierls transition in this system separately, using the formula (4) and $N=8$. The results for the dimerization are plotted in Fig. 2 (filled symbols). Note that the dimerization $d(U)$ for the Hubbard and Heisenberg chains converge for large U , which supports the correctness of our calculations. For the spin-Peierls transition Inagaki and Fukuyama¹² found an asymptotic formula

$$\frac{32g^2}{\pi\sqrt{1+D}} \left(\frac{t}{U} \right)^{3/2}, \quad (5)$$

where D is a constant which was assumed to be of the order of 1/2. Our results confirm this choice.

The above results show that the IET can be a key method for numerical study of the static properties of one-dimensional Peierls systems. Our recent calculations show that it can be equally well applied to spin-Peierls systems with frustration.¹³ We believe also that this method could be applied to higher dimensional systems, namely to the Peierls transition in the two-dimensional Hubbard model. Since cancellation of the lower-order energies does not take place in the two-dimensional Hubbard model, the analog of formula (4) contains the energies of clusters of all sizes.

To further underline the applicability of the IET, we consider the *dynamical* properties of finite Hubbard—Peierls systems. The dynamics of classical degrees of freedom (phonons) Q_i interacting on a lattice generically allows for time-periodic and spatially localized solutions, namely, discrete breathers, if the equations of motion include non-linear terms (see Ref. 14 and citations therein). These discrete breather solutions can be localized on as few as three neighboring sites. If the electron–phonon coupling is taken into account and the Born–Oppenheimer approximation is used, the electronic subsystem generates an additional potential for the classical phonon degrees of freedom. To find once again the discrete breather solutions numerically, one needs the electronic energy $\mathcal{E}(\{Q_i\})$ as a function of the phonon degrees of freedom. For a lattice with L sites this amounts to calculating the ground-state energy of the electronic system L times on each time step in order to find the gradient of H_{el} . Precalculating the function H_{el} on a grid is also impossible since it is a function of prohibitively many variables. In the static dimerization case, where it is known that the target state is a bond conjugate state, this problem is avoided, since there is only one variable d .

Again the IET helps to overcome this problem. Consider a finite chain with periodic boundary conditions. The first-order increment $I^{(1)}(x)$, which does not depend on the site index, is obtained by fixing all the $Q_i=0$ except one with $Q_i=x$, and calculating the change of the electronic energy as a function of x , $I^{(1)}(x) = \mathcal{E}(x) - \mathcal{E}(0)$. The second

order increment is obtained by fixing all phonon variables $Q_i=0$ except $Q_l=x$ and $Q_m=y$. Then the energy of the electronic system will depend on $k=l-m$, x and y . The second order increment is $I_k^{(2)}(x,y)=\mathcal{E}(x,y)-I^{(1)}(x)-I^{(1)}(y)-\mathcal{E}(0)$. The higher-order increments are found in the same manner. Our calculations (see Ref. 15 for a detailed discussion) show that taking into account increments of first and second order is enough to calculate the ground-state energy of a 14-site Hubbard chain with periodic boundary conditions for an arbitrary configuration of $\{Q_i\}$. The relative error is less than 10^{-3} . The increments are calculated on a two-dimensional grid to generate smooth functions. With the help of these functions the lattice dynamics can be calculated using ordinary molecular dynamics techniques.

In this paper we combined the IET with an exact-diagonalization method. It is known that the DMRG is especially accurate when applied to large but finite open chains, where one can achieve higher and higher accuracy by iteratively repeating the DMRG procedure.¹⁶ Taking this into account, we think that the combination of the IET with the DMRG technique can significantly improve calculations.

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