INCREMENTAL EXPANSIONS FOR HUBBARD-PEIERLS SYSTEMS

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The ground state energies of infinite half-filled Hubbard – Peierls chains are investigated combining 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 $3 \cdot 10^{-3}$ 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 onsite 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.

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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 a necessity to treat the Coulomb interaction in the electron subsystem. This interaction should be accounted for by including a positive Hubbard onsite interaction term in the SSH model. We refer to this extended model as to Peierls – Hubbard model (PHM). Due to strong one-dimensional quantum fluctuations a mean field theory calculation of PHM gives qualitatively wrong results, predicting a constant dimerization for small U and the abrupt disappearance of a bond order wave state upon increasing U above a certain threshold at half-filling [3]. Including many-body effects it has been shown by many authors ([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 were performed using available cluster sizes are drastically depending on the boundary conditions (see for instance [5]) and the final conclusions had to be based on extrapolations. The basic questions about the value of g_c, the behaviour of the system near the critical point, the position and the value of the dimerization maximum U_{max} as a function of the electron phonon coupling remained unanswered. The lack of accurate numerical results was making it hard to identify the values of model parameters for real systems. We show that by combining an incremental

expansion technique (IET) with numerically exact diagonalizations, one can overcome the abovementioned difficulties and perform a reliable numerical calculation of correlated one-dimensional Peierls systems in both strong and weak correlation regimes.

The quantum chemical method of increments found recently a wide region of application in condensed matter (see [6] and references therein). The IET starts with splitting a given Hamiltonian operator H into an unperturbed part H_0 and a number of perturbations $H_1 + H_2 + ...$, $H = H_0 + \sum H_i$. The hierarchy of increments is defined in the following way. The first order increment $I_k^{(1)}$ is given 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 defined 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 defined. The change of the unperturbed ground state energy of the full system is exactly given 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 where the unknown 3-body scattering matrix is expressed through 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 ([7]).

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

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

Here U is an onsite 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 reads as $H_{lat} = 1/2K \sum_i v_i^2$. Here v_i is a bond-length change (see e.g. [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 PHM amounts to finding a minimum of the full energy of the system considered as a functional of the bond length changes v_i. A remarkable proof of Lieb and Nachtergaele [8] 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 ref. [5, 4]).

Let us now formulate the incremental expansion of the PHM. A dimerised 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

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

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 PHM hamiltonian H is a sum of H_0 and a number of perturbations, formed by the (weak) bonds linking neighbouring dimers

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

. The incremental expansion is generated in the following way. The first order increment corresponds to a bond inserted between two neighbouring dimers. Due to general principles outlined above it reads as: $I^{(1)} = E_4 - 2E_2$; where E_{2n}, $n = 1, 2, ...$ denotes the ground state energy of a $2n$ sites segment cut out of the infinite chain. The second order increment is defined for a triple of neighbouring 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, hence the expression reads as: $I^{(2)} = E_6 - 2I^{(1)} - 3E_2 = E_6 - 2E_4 + E_2$. 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 (2)) the increments do not depend on site indices. One proves by induction that the expression for the n-th order increment, $n > 2$ reads as

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

In order to find the ground state energy of the infinite system one needs to count the order of increments of each order per dimer. In the infinite $1 - d$ lattice which we consider, there exists exactly one increment of each order per dimer (one makes 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, the value of the ground state energy of the infinite lattice per site is written as $\mathcal{E} = 1/2(E_2 + \sum_{n=1}^{N} I^{(n)})$. Here N is the number of increments taken into account.

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 per site number of increments of a given order grows rapidly with the order of the increment. This special property of one dimension leads to the following result:

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

Formula (4) is quite remarkable, since the calculation of ground state properties amounts to the exact diagonalization of two open chains whose length differs by two. Note that expressions of the type (4) were intuitively used before in quantum chemical calculations (see for instance [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 the 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 the Fig. 1, where the exact $\mathcal{E}(U)$ dependence for $t = 1$ (solid line) is plotted against the results of (4) (open circles). The relative error R_E decays algebraically with growing order of 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 – for $N = 6$ typically below 0.1%. 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 used to achieve comparable precision.
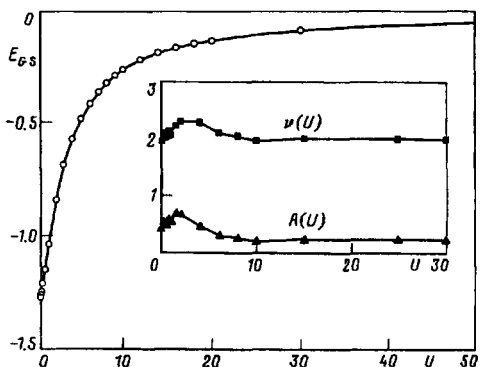

Fig.1. Ground state energy of the equidistant Hubbard model at half filling. Solid line - exact result [10], open circles - IET result for $N = 5$ (see text). Inset: U-dependence of prefactor A and exponent ν of the found functional dependence of the relative error on $(2N + 2)$ (see text)
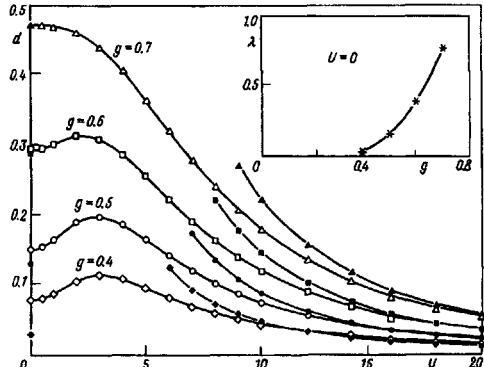
Fig.2. Dimerization versus U for different values of g. Open symbols - IET results for $N = 5$, filled symbols for $U = 0$ - exact results, filled symbols for $U > 5$ - results for Heisenberg chains with IET and $N = 8$. Solid lines are guides to the eye. Inset: g-dependence of the exponent λ of the found functional dependence of the relative error on $(2N + 2)$ for $U = 0$ (see text)

Next we show the results of calculations of the dimensionless dimerization in the PHM as a function of U and g (Fig.2). For $U = 0$ the value of $d(g)$ is known exactly [1] (see filled symbols at $U = 0$ 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 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 sufficient precision is requested. 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 monotonously decreasing function of U. Therefore the system has a qualitatively different behaviour for weak and strong couplings g, as predicted by the GA theory. On the other hand, our results well agree with the extrapolated values of d obtained within the solitonic approach [4].
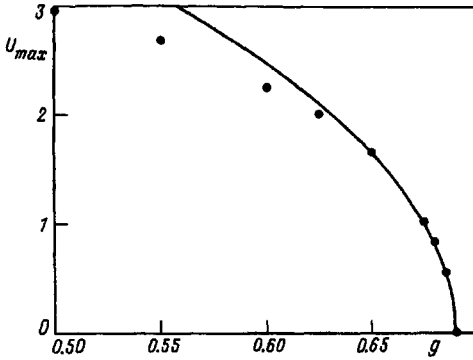
Fig.3. Dependence of U_{max} on the coupling g for the Hubbard–Peierls chains with IET and $N = 5$. Circles - numerical results; line - fit (see text)

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). Especially we find $U_{max}(g)$ to be a monotonously 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 $U_{max} = 0$ 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 $U_{max} \simeq 3t$. The small U behaviour 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 Fukuyama [12] found an asymptotic formula

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

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 studying the static properties of one-dimensional Peierls systems. Our recent calculations show that it can be equally good 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. The cancellation of the lower order energies does not take place in the two-dimensional Hubbard model so the analogue of the formula (4) contains energies of the clusters of all sizes.

To further underline the applicability of the IET, we consider *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 incorporate nonlinear terms (see [14] and citations therein). These discrete breathers solutions can be localized on as

few as three neighbouring 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 numerically find again discrete breathers solutions, 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 $Q_l = x$, 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 reads as $I_k^{(2)}(x, y) = \mathcal{E}(x, y) - I^{(1)}(x) - I^{(1)}(y) - \mathcal{E}(0)$. In the same manner higher order increments are found. Our calculations (see [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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