Solitonic approach to the dimerization problem in correlated one-dimensional systems

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Using exact diagonalizations, we consider self-consistently the lattice distortions in odd Peierls-Hubbard and spin-Peierls periodic rings in the adiabatic harmonic approximation. From the tails of the inherent spin soliton the dimerization d_∞ of regular even rings is found by extrapolations to infinite ring lengths. Considering a wide region of electron-electron on-site interaction values $U>0$ compared with the band width $4t_0$ at intermediately strong electron-phonon interaction g, known relationships obtained by other methods are reproduced and/or refined within one unified approach: an example is the maximum of d_∞ at $U \simeq 3t_0$ for $g \simeq 0.5$ and its shift to zero for $g \rightarrow g_c \approx 0.7$. The hyperbolic tangent shape of the spin soliton is retained for any U and $g \lesssim 0.6$. In the spin-Peierls limit the d_∞ are found to be in agreement with results of density-matrix-renormalization-group computations. [S0163-1829(97)50142-1]

There is a longstanding debate on the interplay of the electron-electron (el-el) interaction and the electron-phonon (el-ph) interaction in conducting polymers like *trans*-$(CH)_x$. Among a large amount of papers we refer here only to Refs. 1–6 devoted to the discussion of the origin of the observed dimerization d in the framework of the (extended) Peierls-Hubbard model (PHM). The PHM is regarded as the minimal microscopic model for conducting polymers. Special features of the interplay of on-site correlation U and off-diagonal el-ph interaction have been pointed out first in Ref. 1. Employing the Gutzwiller approximation (GA), it was shown that for weak and intermediate el-ph interaction strength, the dimerization d passes through a maximum near $U \approx 4t_0$ when U is increased after which it is suddenly suppressed. The geminal approach[6] (GEA) shows a smooth decrease of d with increasing U in the opposite strongly correlated limit. According to extrapolations based on exact diagonalizations (ED)[2,3,5] the enhancement of d due to U predicted by the GA near the maximum is overestimated. In Refs. 2 and 3 the infinite chain limit d_∞ calculated using the PHM was extrapolated from above (below) by $2n$-membered open chains ($4n+2$- membered rings). In the highly correlated limit of the 1/2-filled band case the PHM can be mapped onto the antiferromagnetic spin-1/2 Heisenberg model (AFHM) and at low temperatures a spin-Peierls phase is expected. Such dimerized phases have been observed for $CuGeO_3$ (having CuO_2 chains) and α'-NaV_2O_5. The CuO_3 chains in $Sr(Ca)_2CuO_3$ are at the threshold to the AFHM-limit.[7] In many cases of practical interest the actual d is very small and no self-consistent $d \neq 0$ is found in feasible short *even* rings.

In the present paper we show that studies of *odd* rings of comparable lengths yield reliable estimates of lattice distortions in infinite rings at arbitrary strength of el-el correlations and reasonable strength of the el-ph interaction. We exploit

the generic property of neutral odd periodic rings that their ground state is given by a spin soliton. The lattice distortions for such a ring are shown schematically in Fig. 1. The bond in front of the soliton center, i.e., between sites N and 1, is a long bond for which a_{N1}-$a_0=2u_0 \equiv d>0$ holds [a_{N1} (a_0) is the bond-length in the distorted (equidistant) state]. For large N the region far from the soliton center tends to the regularly dimerized state. Hence, varying the model parameters, insight into the behavior of d_∞ may be gained already at finite N from the study of d. For short rings ($N=3,5,\dots$), $d(N)$ exceeds significantly d_∞. This is the consequence of a strong
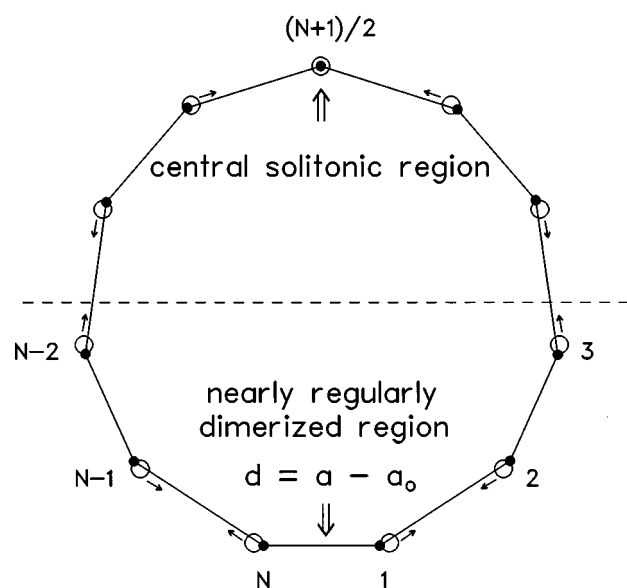

FIG. 1. Schematic view of the lattice distortions in 1/2-filled odd rings. (Un)distorted sites are denoted by ○ (●).

first-order Jahn-Teller effect.[8] In Refs. 8 and 9 the total energy E_{tot} of odd AFHM rings has been studied for *fixed* geometries adopting rigid sharp soliton shapes. In our method *all* bonds are optimized to yield the minimum of the total energy E_{tot}. The inherent soliton exhibits a *smooth* shape. We illustrate our method considering the PHM and the AFHM, where comparison with other reliable approaches is possible. In particular, the density matrix renormalization group is used to check the extrapolated d_∞.

For the electronic part H_{el} of the total Hamiltonian $H = H_{el} + H_{lat}$ we adopt the one-band extended PHM

$$H_{el} = \sum_{i,s} t_{i,i+1}(c^\dagger_{i,s} c_{i+1,s} + \text{H.c.})$$

$$+ \sum_i (U n_{i,\uparrow} n_{i,\downarrow} + V_{i,i+1} n_i n_{i+1}), \tag{1}$$

at half filling, where $c^\dagger_{i,s}$ creates an electron with spin $s = \pm 1/2$ at site i, $n_{i,s} = c^\dagger_{is} c_{is}$ is the number operator, and $n_i = \Sigma_s n_{is}$. We linearize the bond-length dependent transfer integral t and the intersite el-el interaction V

$$t_{i,i+1} = -(t_0 - \gamma v_i), \quad V_{i,i+1} = V - \eta v_i, \tag{2}$$

where $v_i = u_{i+1} - u_i$, u_i is the displacement of the ith site relative to the undistorted state. In the adiabatic and harmonic approximation the lattice part H_{lat} reads as

$$H_{lat} = (K/2) \sum_i v_i^2, \tag{3}$$

where K is the spring constant. Via the Hellmann-Feynman theorem we obtain N self-consistent equations

$$K v_i = \Lambda/N - 2\gamma P_{i,i+1} + \eta D_{i,i+1}, \tag{4}$$

where $\Lambda = \Sigma_i (2\gamma P_{i,i+1} - \eta D_{i,i+1})$ expresses the fixed length constraint $\Sigma_i v_i = 0$, $P_{i,i+1}$ being the bond order, and $D_{i,i+1}$ denotes the density-density correlators in the ground state $|G\rangle$

$$P_{i,i+1} = \frac{1}{2} \sum_s \langle G | c^\dagger_{i,s} c_{i+1,s} + \text{H.c.} | G \rangle, \tag{5}$$

$$D_{i,i+1} = \langle G | n_i n_{i+1} | G \rangle. \tag{6}$$

The strength of the el-ph interaction can be measured by the parameter g introduced as[5]

$$g = \gamma / \sqrt{K t_0} < 1. \tag{7}$$

Note that sometimes[1] the related quantities defined as

$$\lambda_{el-ph} = 2g^2/\pi, \quad \text{or} \quad \lambda_{SSH} = 2\lambda_{el-ph}. \tag{8}$$

are used. Values of $g \sim 0.4$ to 0.5 typical for conducting polymers are regarded as weak to intermediate coupling constants. Following Refs. 5 and 6 we shall use hereafter the dimensionless dimerization defined as

$$d = 2u_0 \sqrt{K/t_0} < 1. \tag{9}$$

The parameter δ frequently used to describe the modulation of the transfer integral $t_{i,i+1} = t_0(1 + (-1)^{i+1}\delta)$ in the dimerized state[1-3] is related to d by $\delta = gd$. In the limit $U/t_0 \gg 1$ the low-energy physics of the 1/2-filled PHM ring [Eq. (1)] can be described by the AFHM

$$H_{sp} = \sum_i J_{i,i+1} \vec{S}_i \vec{S}_{i+1}, \quad \text{with} \quad J_{i,i+1} \approx \frac{4t_{i,i+1}^2}{U - V_{i,i+1}}, \tag{10}$$

where the exchange integral is given to 2nd order perturbation theory in t_0/U. Using Eq. (2) we find

$$J_{i,i+1} = J_0 - \gamma_{sp} v_i = J_0 [1 + (-1)^{i+1}\delta_{sp}], \tag{11}$$

where $\gamma_{sp} = 2\gamma J_0/t_0$ and $\delta_{sp} = 2gd$ characterizes the regular spin-Peierls state for $\eta = 0$. We shall use the AFHM also out of the limit $U \gg t_0$ for the case $V = 0$ adopting an effective exchange integral $J = J(U/t_0)$ given by the relation $J_{ij} = (2/\pi) v_{sp} t_{ij}$ and the spin velocity v_{sp} taken from the Bethe-Ansatz solution for the equidistant infinite Hubbard ring[10] (hereafter $a_0 = 1$, $\hbar = 1$)

$$J_{i,i+1} = \frac{4}{\pi} \frac{t_{i,i+1} I_1(z_{i,i+1})}{I_0(z_{i,i+1})}, \quad z_{i,i+1} = \frac{2}{\pi U} t_{i,i+1}, \tag{12}$$

where I_n, $(n = 0,1)$ are modified Bessel functions.

Using the Lánczos-method, the Hamiltonians [Eqs. (1) and (10)] have been diagonalized exactly for finite rings with periodic boundary conditions starting with a given set $\{v_{n,(0)}\}$. The AFHM has been treated using the spinless fermion technique[11] resulting in analogous self-consistent equations as for the PHM. Then the corresponding ''ground-state'' eigenvector $|G\rangle$ has been used to calculate the next set of lattice order parameters $\{v_{n,(1)}\}$ using Eq. (4). The iteration was continued until the maximal deviations of E_{tot} and all $v_{n,(j)}$ between two iteration steps j and $j+1$ became smaller than the required accuracy of 10^{-7} to 10^{-8} (see Refs. 3 and 12). Here rings composed of up to $N = 13$ sites (PHM) and $N = 23$ (AFHM) have been studied. The ED computer limitations to rings where finite-size effects are still important can be circumvented at least for *even* membered regularly dimerized AFHM rings and reasonable el-ph (sp-ph) interaction strength applying the density matrix renormalization group technique[13] (DMRG) with typical discarded errors of the order 10^{-6}.

At first we consider the one-particle Su-Schrieffer-Heeger model (SSH) (PHM: $U,V = 0$) where very long odd rings can be treated numerically. The infinite even ring problem is reduced to a transcendental equation for d_∞:

$$\frac{1}{\lambda_{SSH}} = \frac{K(k) - E(k)}{k^2}, \quad \text{with} \quad k = \sqrt{1 - (gd_\infty)^2}, \tag{13}$$

where K and E denote complete elliptical integrals. The results for up to $N = 601$ sites are shown in Fig. 2. Starting from small N, d passes at first by a minimum at $N \approx 2\xi$, the width of a soliton in an infinite ring. For weak el-ph coupling $\xi \gg 1$, $d_{min}/d_\infty \approx 0.86$ at $2\xi/N \approx 0.92$. Below that minimum all curves, for which $N > 2\xi$ holds, approach a nearly universal curve, pass a very small maximum near 6ξ, and tend finally to d_∞ from above.[14] Since for correlated problems
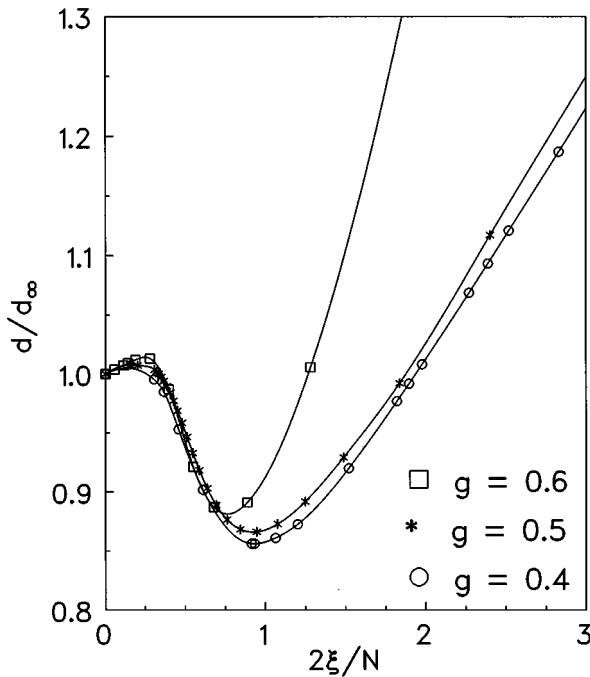
FIG. 2. Reduced dimerization in odd SSH rings vs reciprocal ring length $1/N$ for various el-ph interactions g. The ring length N is given in units of the soliton width $2\xi = 2/(g d_\infty)$.

FIG. 3. Dimerization in the Peierls-Hubbard model vs on-site energy U for the el-ph coupling $g = 0.5$. In deriving the improved lower bound, Eqs. (13)–(15) have been used.

only relatively short rings can be treated exactly, a strong nonmonotonous behavior could cause problems in extrapolating to d_∞. Fortunately, our calculations indicate that at least in the AFHM limit the depth of the first minimum at finite N is strongly suppressed.

Let us now consider how the on-site interaction U affects d. As shown in Fig. 3 starting from $U = 0$, d increases with U and has a maximum at $U_{max} \sim 3t_0$, after which d starts to decrease smoothly. Both behaviors are similar to the GA and GEA predictions, respectively. Quantitatively, however, we obtain $U_{max}(g) \approx 3.12t_0$ for $g \sim 0.5$. For $0.5 < g < 0.6$, U_{max} starts to decrease. Finally, when $g \rightarrow g_c \approx 0.7$, $U_{max} \rightarrow 0$. For comparison we note that the GA's results are $U_{max} \approx 4t_0$ for $g < g_c = 0.76$. The ED results of Ref. 5 yield $g_c = 0.75 \pm 0.04$ slightly above our result. Above g_c, there is no enhancement of d due to U. Turning to larger rings, we first adopt a $1/N$ extrapolation (dashed curve) and arrive at a rough lower bound being crudest for small U. An improved bound is achieved connecting the exact $U = 0$ point with the $1/N$ extrapolation upshifted to the AFHM limit (see below). To avoid an artificial minimum, we omit the $U = t_0$ point. Thus for $g = 0.5$ we obtain $0.174 < d_{\infty,max} \lesssim d_{N=13} \approx 0.2$. Instead the GA[6] gives $d_{max} \approx 0.31$. For $U \gg t_0$, $g \lesssim 0.5$ the $d_{PHM} \rightarrow d_{AFHM}$ from above. To compare our d with the continuum model result of Inagaki et al.,[16] we rewrite their dimerization as

$$d = \frac{g^2}{\pi \sqrt{1+\kappa}} \left(\frac{\partial J_0}{\partial t_0} \right)^2 \left(\frac{t_0}{J_0} \right)^{1/2} \rightarrow c g^2 \left(\frac{4t_0}{U-V} \right)^{3/2}, \quad (14)$$

where $c = (4/\pi)\sqrt{2/3} \approx 1.04$ for $\kappa = 0.5$ [see Eq. (10) and Refs. 15–18]. Applying Eq. (14) to intermediately correlated cases, we adopt the effective exchange integral J defined by Eq. (12) and arrive at an *analytic* expression (the dashed-
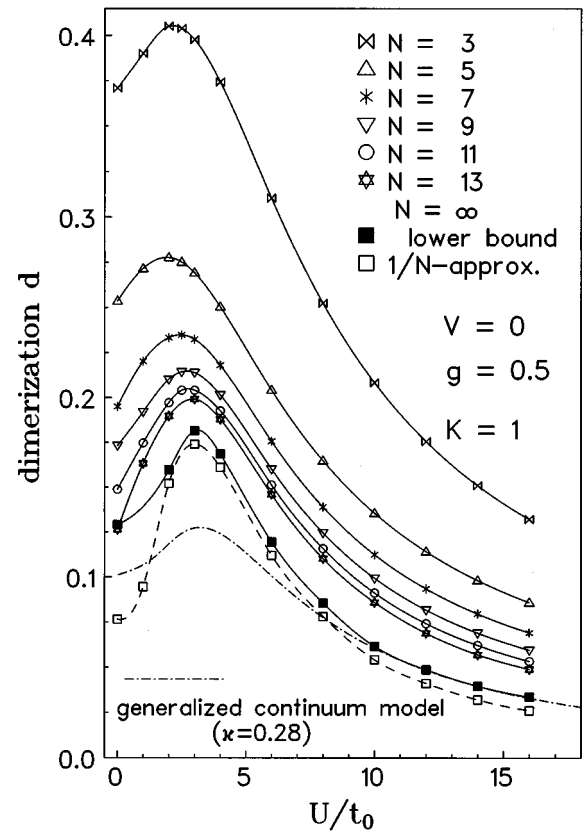
dotted curve in Fig. 3).[18] Surprisingly it exhibits similar shape and magnitude as the weak coupling ($g \lesssim 0.5$) ED curves. In particular its $U_{max}/t_0 = 3.21$ is close to 3.12 mentioned above. This suggests that even in the case of conducting polymers, being clearly outside the usual AFHM regime, the dimerization is mainly governed by the (always present) spin degrees of freedom and to less extent by the charge degrees of freedom. In the usual case $U > 2V$, the V and its derivative η [see Eq. (2)] enhance d. For $U \gg t_0$, V and $\eta = 0$ one can replace $U \rightarrow U - V$.

For long rings $N > 2\xi$, d_N values close to d_∞ can be expected. Then $d = d(N)$ might be approximated by

$$d(N) = d_\infty + \sum_{l=1}^{l_{max}} \frac{A_l}{N^l} \exp\left(\frac{-N}{2\xi} \right) + \dots . \quad (15)$$

Note that in contrast with the general PHM case, $d(N)$ for $4n$ and $4n+2$ AFHM rings can be described by *one* smooth curve.[8] The $d_{even} \rightarrow d_\infty$ from below, just opposite to odd rings. To be specific, we consider one typical example. We estimate for the upper curve shown in Fig. 4, $d_{odd,\infty} = 0.0765$, $l_{max} = 1$, $A_{1,odd} \approx 0.5$ and $\xi_{odd} = 5.26$. The even ring curve tends from below to a slightly larger value $d_{even,\infty} = 0.078$ and $A_{1,even} = -11.8$. The exponent $\xi_{even} = 1.85$ differs significantly from ξ_{odd}. From the soliton shape $(-1)^n v_n \approx d_N \tanh(n/\xi_N)$, we deduced at $N = 23$, $\xi_N \approx 5$, $d_N \approx 0.08$, whereas the continuum model[17] yields $\xi = 3\pi t_0/(16 J_0 g^2) = 4.91$. The fit of the even curve can be
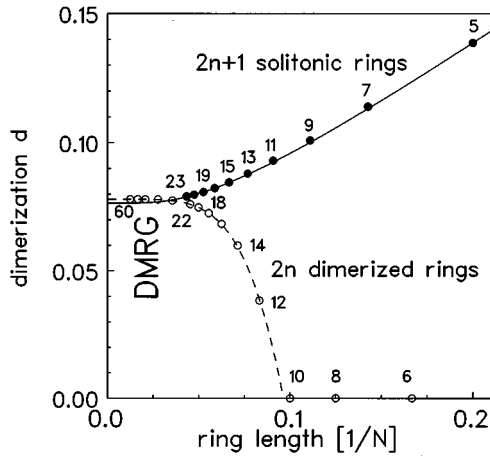
FIG. 4. Size dependence of the dimerization d for even ($\circ$) and odd ($\bullet$) periodic spin-Peierls rings. Even rings are treated by ED until $N=22$. The d for $N=28$ to 60 are obtained by the DMRG. The parameter set used $\gamma_{sp}=0.4$, $J=1/3$, $K=1$ corresponds to $U=13$, $V=t_0=1$, $\eta=0$, and $g=0.6$ for the PHM. The full and the dashed curves are the fits by Eq. (15).

somewhat improved adopting $l_{max}=4$. Then with $A_1=A_3=0$ and $A_2=-3.5$, $A_4=-2040$ one arrives at the same $\xi=5.26$ as in the odd case for $l_{max}=1$. Taking the DMRG values for $N=60$, we conclude that the accuracy of the solitonic estimate of d_∞ is ~ 2 to 3%. The continuum theory[16] [Eq. (14)] predicts, for $\kappa=0.5$, $d_\infty=0.07203$, a value slightly below our discrete results. According to our numerical finding we would recommend to use $\kappa \approx 0.279$. Fitting alternatively the curvature of d_{odd} at large N by a parabola, one

arrives at an extrapolated very shallow minimum at *finite* ring length ($N_{min} \approx 29$ sites for the present parameters). Then the slightly smaller $d_{\infty,odd}$ compared with $d_{\infty,even}$ might be viewed as a hint for a tiny minimum at *finite N* generic for d_{odd} being the deepest in the SHH case (see Fig. 2). Raising g, the soliton becomes narrower. Thus at large g any minimum should be accessible by the ED. With increasing g the $d_{odd}(1/N)$ curves become flatter. Small minima were detected for $g=0.9$, 0.85 at $N=N_{min}=17$, 21, respectively. Anyhow, the $1/N$ extrapolation of d_{odd} (d_{even}) from accessible $N \leq N_{min}$ yields a lower (upper) bound of d_∞.

To summarize, an efficient approach to the dimerization problem of correlated 1D models has been presented. It is based on exact diagonalizations of odd ring Hamiltonians combined with a self-consistent treatment of the classical lattice degrees of freedom. Known dependences of the bond alternation on the el-el and el-ph coupling strengths obtained by other approximations valid in different parameter regimes have been reproduced and refined within one unified method. The $1/N$ extrapolation to the infinite rings gives a lower bound for any correlation strength. With the aid of the Bethe-Ansatz solution for the spin velocity, even in the intermediate coupling regime a sizeable part of the dimerization can be described by an effective spin-Hamiltonian gaining thus insights in the dimerization mechanism of conducting polymers. The DMRG is found to be a valuable supplementary tool to our solitonic method.

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