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On the Correlation Effect in Peierls–Hubbard Chains

Jiří MÁLEK*, Stefan-Ludwig DRECHSLER†, Sergej FLACH[1], Eric JECKELMANN[2] and Konstantin KLADKO[3]

Leibniz-Institut für Festkörper- und Werkstoffforschung, D-01171 Dresden, PF 270116, Germany
[1]*Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Nöthnitzer Str. 33, Germany*
[2]*Philipps-Universität Marburg, Fachbereich Physik, AG Vielteilchentheorie, D-35032 Marburg, Germany*
[3]*Ingrian Networks, 475 Broadway Street, Redwood City, CA 94063, USA*

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We reexamine the dimerization, the charge and the spin gaps of a half-filled Peierls–Hubbard chain by means of the incremental expansion technique combined with density matrix renormalization group (DMRG) method. We compare our numerical findings with results recently obtained by a bosonization and a renormalization group method and found out that this approach seems to be accurate in the weakly correlated case, only. In the strongly correlated limit we found that the charge gap of the dimerized chain tends to the sum of the charge gap of the equidistant chain and the spin gap of the dimerized chain.

KEYWORDS: Peierls–Hubbard model, dimerization, charge gap, spin gap, incremental expansion and bosonization techniques, polyacetylene
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1. Introduction

The interplay of electron–electron (el–el) and electron–lattice (el–ph) interactions in the context of various phase transitions (instabilities) is one of the most challenging many-body problems in solid state physics. In particular, in the context of the longstanding debate how to describe theoretically conducting polymers like *trans*-polyacetylene and its remarkable solitonic properties,[1,2] the Peierls–Hubbard model (PHM) at half filling, considered as a minimal realistic model, became very popular.[2–14] Within this frame in the adiabatic approximation for the lattice the behavior of the dimerization amplitude as a function of the two remaining model parameters, the onsite repulsion U and the strength of the el–ph interaction is one of the central problems. To the best of our knowledge it was first addressed in 1981 by Horsch[3] who predicted on qualitative grounds a maximal dimerization at some intermediate U. This was confirmed later on and made more clear by approximate solutions obtained by Baeriswyl and Maki[5] and Kuprievich[11] within the Gutzwiller approximation and the geminal techniques, respectively. According to them the maximal dimerization occurs for weak el–ph interaction at $U \sim 4t_0$, where t_0 denotes the nearest neighbor transfer integral. Unfortunately, the region of interest is already at the border line of validity of those approaches.

The general nonmonotonous behavior of the dimerization amplitude (at weak el–ph coupling) as a function of U was confirmed by Hayden and Soos[6] and Waas *et al.*[7] who extrapolate results of exact diagonalization studies (EDS) obtained for finite even-membered rings with various boundary conditions. In the strongly correlated limit $U \gg t_0$ the PHM can be reduced to the spin–Peierls model (SPM) for which a large body of literature exists (see for instance ref. 15 and references therein). The general case of arbitrary U and intermediate as well as strong el–ph interactions has been covered by the present authors within the solitonic[12] as well as the incremental expansion method (IEM)[14] both based on self-consistent EDS.

In the context of the polyacetylene problem the charge gap has been addressed among others by Rościszewski and Oleś[10] in the framework of the extended PHM. There is now a general consensus that the Peierls mechanism, i.e. the off-diagonal el–ph interaction, enhances the charge gap compared with that of the 1D-Hubbard–Mott insulator.[7–9] The latter problem has been solved exactly by Lieb and Wu.[16]

Recently, the weak and intermediate region $U \leq 4t_0$ has been readdressed by Sugiura and Suzumura[17] who employ the bosonization technique and the renormalization group method (BRG). Applying the incremental technique supplemented by density matrix renormalization group (DMRG) calculations[13] to the original discrete PHM, we show that the BRG approach seems to be accurate in the weakly corrrelated limit, only. Finally, we consider briefly also the strongly correlated limit.

2. Models and Methods

Let us consider even-membered chains with periodic boundary conditions modeled by the Peierls–Hubbard Hamiltonian supplemented with a static harmonic lattice term

$$H = \sum_{i,s} -t_{i,i+1}\left[c^{\dagger}_{i,s}c_{i+1,s} + \text{h.c.}\right] + \frac{1}{2}Un_{i,s}n_{i,-s} + \frac{K}{2}\sum_i v_i^2, \tag{1}$$

where the bond alternation v_i has been introduced

$$v_i = u_{i+1} - u_i, \tag{2}$$

here $u_i = \pm u_0$ is the displacement of the ith lattice site in the dimerized state under consideration and K is the spring constant. We linearize the bond-length dependent transfer integral $t_{i,i+1}$

$$t_{i,i+1} = t_0 - \gamma v_i. \tag{3}$$

The strength of the off-diagonal el–ph interaction can be expressed by the dimensionless coupling constant g

$$g = \gamma/\sqrt{Kt_0} < 1. \tag{4}$$

*On leave from: Institute of Physics, ASCR, Na Slovance 2, CZ-18221 Praha 8, Czech Republic.
†E-mail: drechsler@ifw-dresden.de

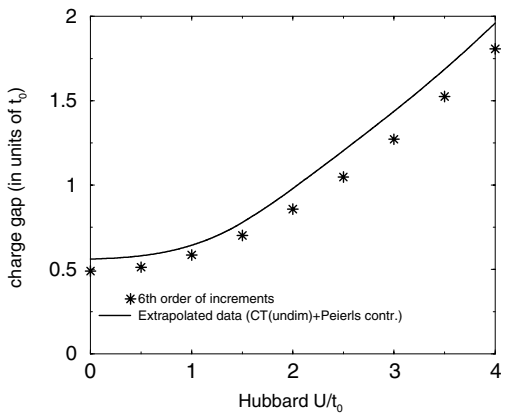

Fig. 1. Comparison of extrapolated and 6th order incremental calculations of the charge gap for the electron–phonon coupling constant $g = 0.574341$.

It is convenient to measure the dimerization amplitude $v_0 = 2u_0$ also in dimensionless units[11)]

$$d = v_0\sqrt{K/t_0} < 1. \tag{5}$$

Values of $g \sim 0.4$ to 0.5 are typical for conducting polymers. For the convenience of the reader we note that our quantities g and d are simply related to the notations used by Sugiura and Suzumura[17)]

$$\lambda = 4g^2/\pi, \quad t_{\mathrm{d}} = dgt_0. \tag{6}$$

Thus their two values of $\lambda = 0.25$, 0.42 correspond to our $g = 0.443113$ and 0.574341 (used in the calculation shown in Figs. 1, 2, 4, 5), respectively.

Let us start with the calculation of the dimerization amplitude d. Naturally in the present homogeneous dimerized case it can be obtained from the direct minimization of the total energy per site with respect to the single variable d at fixed U and g, in other words there is no need to solve the general self-consistency equations presented in ref. 12. According to the incremental expansion technique the ground state energy per site in the nth order reads[14)]

$$\epsilon^n(U,g,d) = \frac{1}{2}\left[E_{2n+2,2n+2}(U,g,d) - E_{2n,2n}(U,g,d)\right], \tag{7}$$

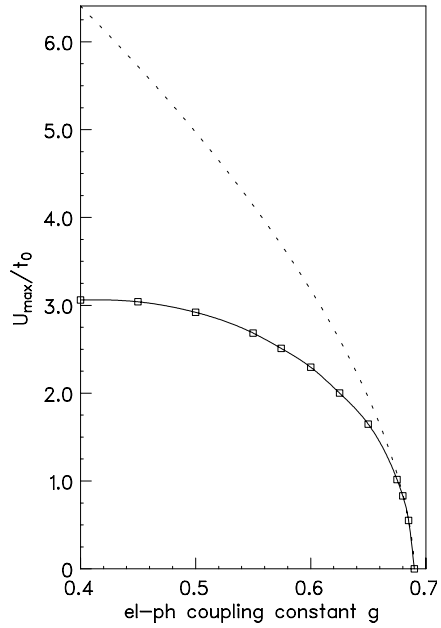

Fig. 3. The Hubbard onsite interaction $U_{\max}$ at which the maximum dimerization $d(U)$ is realized vs. electron–phonon coupling constant g (symbols, the full line as a spline interpolation for the guide to the eye). The behavior near the critical g value $g_{\mathrm{c}} \approx 0.69$ can be described by $U_{\max} \propto (g_{\mathrm{c}} - g)^{\nu}$ with $\nu \approx 0.6$ (dashed line).

where $E_{2n,2n}(U,g,d)$ is the total energy of a chain segment (finite open chain) with $2n$ electrons and $2n$ sites. The dimerization amplitude in the infinite chain limit ($N \to \infty$, where $N = 2n+2$ is the maximal number of interacting sites in the nth incremental expansion order) has been extrapolated using the empirical law (see also ref. 12)

$$d(U,g,N) = d_\infty(U,g) + \left(\sum_{i=0} a_i(U,g)/N^i\right) \times \exp(-N/2\xi(U,g)). \tag{8}$$

Notice that ξ is close to the coherence length (half-width of a soliton as obtained for instance by the solitonic method[12)] explicitly).

As the next step the gaps have been calculated for the

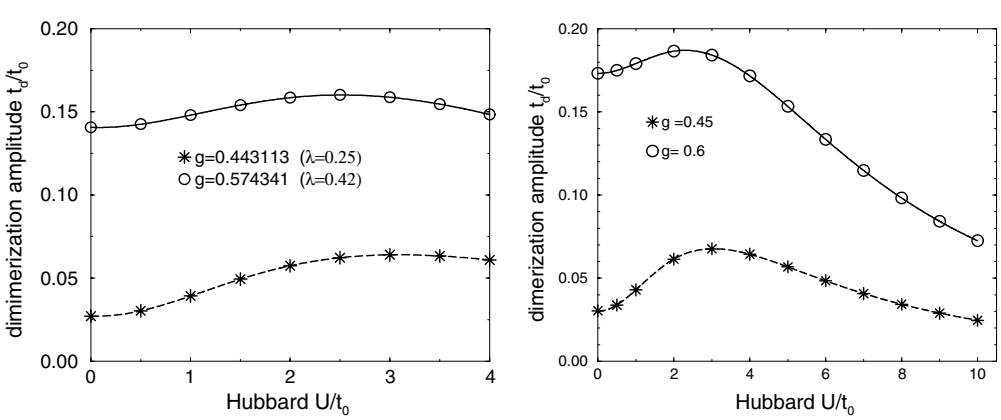

Fig. 2. The extrapolated alternating part $t_{\mathrm{d}} = gdt_0$ (dimerization) of the transfer integral t vs. on-site (Hubbard) repulsion U for the two el–ph coupling strengths considered in ref. 17 (left panel). The same as in the left panel for a larger scale of U and slightly changed el–ph coupling constants g (right panel). Full and dotted lines are spline fitted guide curves for the eye.

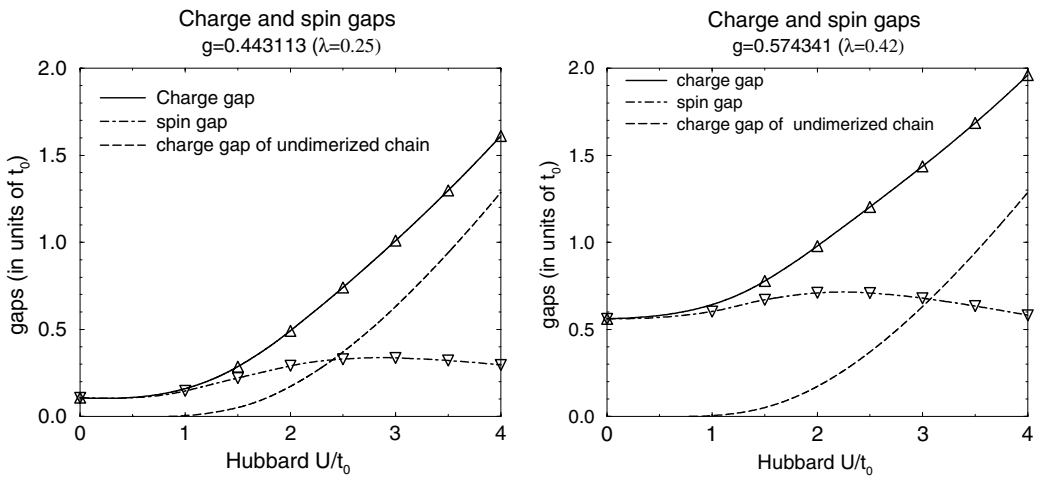

Fig. 4. The extrapolated charge and spin gaps [see eqs. (9) and (10), repectively] vs. on-site repulsion U. For comparison the charge gap of the equidistant infinite chain, i.e. the Mott–Hubbard gap (full line, no symbols) is shown, too.

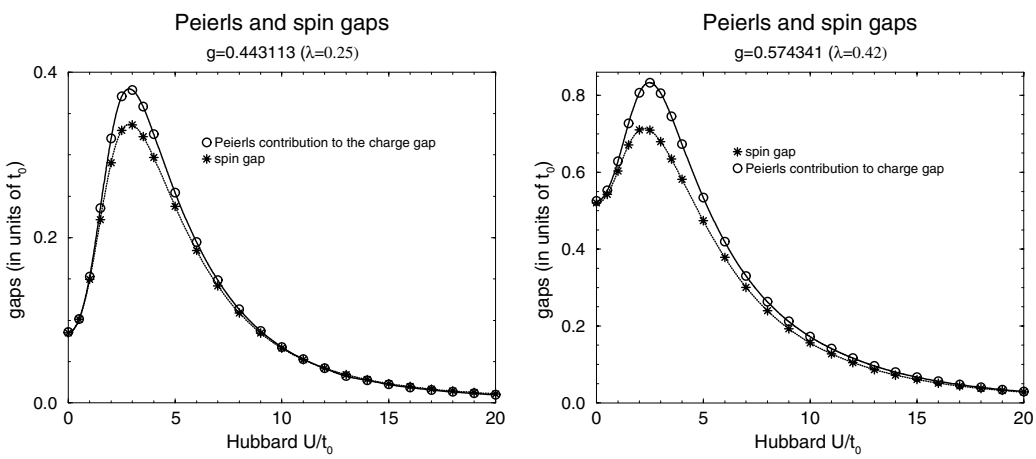

Fig. 5. The extrapolated Peierls contribution to the charge gap and the spin gap vs. on-site repulsion U for two el–ph coupling constants g.

extrapolated dimerization d_∞. In the nth order of the incremental expansion the charge gap (for definition see ref. 16) reads

$$\begin{aligned}\Delta\mathcal{E}_\rho^{(n)} \equiv \mu^+ - \mu^- &= (n+1)\big[E_{2n+3,2n+2} - E_{2n+2,2n+2}\big] \\ &\quad - n\big[E_{2n+1,2n} - E_{2n,2n}\big] \\ &\quad - (n+1)\big[E_{2n+2,2n+2} - E_{2n+1,2n+2}\big] \\ &\quad - n\big[E_{2n,2n} - E_{2n-1,2n}\big] \\ &= (n+1)\big[E_{2n+3,2n+2} - 2E_{2n+2,2n+2} + E_{2n+1,2n+2}\big] \\ &\quad - n\big[E_{2n+1,2n} - 2E_{2n,2n} + E_{2n-1,2n}\big], \end{aligned} \tag{9}$$

where $\mu^\pm$ denotes the chemical potential for adding an electron or a hole, respectively.

The spin gap $\Delta\mathcal{E}_\sigma$ can be calculated using an analogous expressions as for μ^+ [i.e. the first line of eq. (9)]

$$\begin{aligned}\Delta\mathcal{E}_s^{(n)} = (n+1)\big(E^T_{2n+2,2n+2} - E^S_{2n+2,2n+2}\big) \\ - n\big(E^T_{2n,2n} - E^S_{2n,2n}\big),\end{aligned} \tag{10}$$

where $E_{T(S)}$ is the total energy of the lowest state in the $S_z = 1(S_z = 0)$ subspace. These states correspond usually to the triplet and singlet states, respectively. For a more detailed derivation of eqs. (9), (10) and technical details of the incremental technique the reader is referred to refs. 14 and 18.

Notice that in the expression for the charge gap [eq. (9)] the corresponding multiplet notation (doublet or singlet) has been omitted for the sake of shortness. Let's note also that in ref. 17 the charge and spin gaps have been denoted by Δ_ρ and Δ_σ, respectively.

The Peierls contribution to the total charge gap as a function of U has been determined using the relation

$$\delta\mathcal{E}_\rho^{(n)}(U,g) = \Delta\mathcal{E}_\rho^{(n)}(U,g) - \Delta\mathcal{E}_\rho^{(n)}(U,0), \tag{11}$$

where $\Delta\mathcal{E}_\rho^{(n)}(U,0)$ denotes the charge gap of the undimerized chain calculated in the nth incremental order. The quantity $\delta\mathcal{E}_\rho^{(n)}(U,g)$ has then extrapolated by a polynomial fit with the leading term $\propto N^{-2}$ to the infinite chain limit $\delta\mathcal{E}_\rho(U,g)$. Finally, $\delta\mathcal{E}_\rho(U,g)$ has been added to the charge gap of the equidistant undimerized chain (sometimes called also Mott–Hubbard gap) given by the well-known Lieb–Wu solution[16]

$$\Delta\mathcal{E}_\rho(U,0) = U - 4 - 8\sum_{n=1}^{\infty}(-1)^n \times \left[\sqrt{\left(1+(nU/2)^2\right)} - nU/2\right]. \tag{12}$$

This way we circumvent some difficulties with the size dependence of the total charge gap which stem mainly from the slow size dependence of the Mott–Hubbard gap at small U.[19] In order to illustrate our extrapolation procedure described above, we show in Fig. 1 for a data set to be considered below (see Figs. 2, 4, 5), how the charge gap extrapolated to infinite chain lengths is related to the results of the 6th order of incremental expansion.

3. Results and Discussion

Let us start with the discussion of our numerical results obtained up to 6th order in the incremental expansion using the method of exact diagonalization for the Peierls–Hubbard Hamiltonian of the chain segments. All results have been extrapolated as mentioned in the previous section. Dimerization amplitudes t_d are shown in Fig. 2. From the comparison with Fig. 4 of ref. 17 one realizes reasonable agreement in the weak coupling region $U/t_0 < 1.5$. But at $U/t_0 = 4$ we found a nearly twice as large value for the dimerization amplitude in comparison with the results shown in ref. 17. This is mainly caused by the shift of the maximum position $U_\mathrm{max}[g]$ to higher U-values and to a more pronounced asymmetric shape of the whole curve (see Fig. 2, right panel). Notice that in Fig. 4 of ref. 17 there is essentially no shift of the maximum dimerization towards smaller U-values with increasing el–ph interaction λ as it should be.[5,7,12] In the weak coupling limit it should tend to $U_\mathrm{max}(0) \approx 3t_0$ whereas U_max tends to zero for $g \to g_\mathrm{c} \approx 0.69$ as shown in Fig. 3 (for more details the interested reader is referred to our previous work in ref. 14). This is in contrast with the statement of $U_\mathrm{max} = 2.2 \pm 0.1$ for $0.2 \le \lambda \le 0.5$ made in ref. 17. Furthermore, the difference $\delta d = d(U_\mathrm{max}) - d(0)$ *decreases* with increasing g contrarily with the results shown in Fig. 4 of ref. 17, where it increases by a factor of two. The same problem is also evident from the inspection of Fig. 3 of ref. 17. For λ approaching the critical value $\lambda_\mathrm{c} \approx 0.606189$ mentioned above, the $t_\mathrm{d}(U=0)$ curve should intersect all t_d-curves at finite U, because for all el–ph constants $\lambda > \lambda_\mathrm{c}$ the maximal dimerization is already reached in the uncorrelated limit $U = 0$. (Strictly speaking, their figure Fig. 3 shows only $\lambda \le 0.6$, i.e. slightly below λ_c. Anyhow, no visible change in the slope of the $t_\mathrm{d}(\lambda)$-curves with finite U approaching the closely lying critical point λ_c can be detected.)

The charge and the spin gaps are shown in Figs. 4 and 5. One readily realizes (i) that $\delta\mathcal{E}_\rho(U,g)$ is always positive, i.e. the Peierls mechanism *enhances* the total charge gap and (ii) it follows closely the spin gap. Roughly speaking, there are three regions: the weakly coupled one $U/t_0 \le 1.5$, the intermediately coupled and the strongly coupled ones. In the first one correlation effects can be neglected and the charge gap being almost coinciding with the spin gap is dominated by the el–ph interaction. In the second intermediate region the Peierls mechanism yields a substantial contribution to the total charge gap. This is of interest for conducting polymers, where $U \sim U_\mathrm{max} \sim 3t_0$. In the strongly coupled spin–Peierls region it becomes small tending to the spin gap (see Fig. 5). Both quantitities vanish in the same fashion with increasing U. In other words a remarkably simple relation

$$\Delta\mathcal{E}_\rho(U,g) \approx \Delta\mathcal{E}_\rho(U,0) + \Delta\mathcal{E}_s, \tag{13}$$

holds in that limit. To the best of our knowledge this nontrivial relation has not been reported in the literature. In principle, it might be useful to detect the opening of a spin gap (in addition to direct measurements of the magnetic susceptibility) by high-precision optical measurements of the change of the charge gap below a spin Peierls-transtion. Quite interestingly, the dimerization, the Peierls-contribution to the charge gap as well as the spin gap exhibit a very similar dependence on U. From this observation one might suggest that all those three quantities are mainly described by the spin degrees of freedom (see also ref. 12, where an effective spin–Peierls model has been proposed to describe the dimerization $d(U,g)$ even analytically).

From our calculations it becomes clear that there is *no* visible hump in the charge gap curve (see Fig. 4 of ref. 17) near the region where the dimerization amplitude $t_\mathrm{d}(d)$ and the spin gap reach their maximum. Note that in ref. 17 the calculated charge gap at $U = 4t_0$ is *smaller* than the Lieb–Wu prediction [see eq. (12)]. At first glance this might imply a *negative* impact of the Peierls mechanism. Nevertheless, in Sugiura and Suzumura's approach the charge gap is *also* enhanced by the Peierls mechanism (due to the enhancement of the umklapp scattering by the coupling to the phonons) although both gaps, the total charge gap and the Mott–Hubbard gap, are clearly underestimated.[20]

Finally, below we report also on some incremental expansion results where due to the application of the DMRG-method to open chain segments rather high orders of IEM could be considered. Furthermore, charge gaps obtained from total energy differences of long open chains (denoted as standard open chain results) will be provided, where the well-known definition of the charge gap[16]

$$\Delta\mathcal{E}_\rho(U,g,N) = E(+e,U,g) - 2E(0,U,g) + E(-e,U,g,N), \tag{14}$$

has been used. Here $E(0,U,g,N)$ and $E(\pm e,U,g,N)$ denotes the total energy of the neutral and charged open chain, respectively, at fixed d. For instance, for $g = 0.4$ and $U/t_0 = 4$ in the 31st incremental order one arrives at $d = 0.10591$ (0.10590). Here and below, the numbers in brackets denote the results obtained by the extrapolation of the incremental data calculated up to the 6th order. With that dimerization we obtained in the 63rd order the charge gap $\Delta\mathcal{E}_\rho/t_0 = 1.4992$ (1.5195) whereas the standard open chain result for $N = 128$ sites is $\Delta\mathcal{E}_\rho/t_0 = 1.5077$. Since the charge gap of the undimerized chain calculated from eq. (12) equals to 1.2867 one realizes a significant enhancement of the charge gap due to the finite dimerization. At the same incremental orders and open chain lengths as mentioned above, for $g = 0.45$ (which is very close to $\lambda = 0.25$ considered in ref. 17), and for $U/t_0 = 2$ we found $d = 0.13575$ (0.13650) and $\Delta\mathcal{E}_\rho/t_0 = 0.5208$ (0.5127) whereas the standard open chain result is $\Delta\mathcal{E}_\rho/t_0 = 0.5374$ [compare with 0.1728 from eq.

(12). For $g = 0.5$ and the same $U/t_0 = 2$ as above we have now $d = 0.18578$ (0.18580) and $\Delta\mathcal{E}_\rho/t_0 = 0.6696$ (0.6764) whereas the standard open chain result is $\Delta\mathcal{E}_\rho/t_0 = 0.6828$. For the same $g = 0.5$ but $U/t_0 = 7$, one arrives at $d = 0.11977$ and $\Delta\mathcal{E}_\rho/t_0 = 3.9734$ (3.9925). The standard open chain result is $\Delta\mathcal{E}_\rho/t_0 = 3.9777$ whereas eq. (12) yields 3.7720, only.

Thus the open chain results [eq. (14)] provide an *upper* bound whereas the incremental technique [eq. (9)] results in a *lower* bound for the charge gap. The incremental technique yields excellent results for the gaps in the intermediate and strongly correlated regime whereas in the weakly correlated regime slight deviations occur, if one restricts oneself to sixth order dictated by the computational facilities available for exact diagonalization at present. Due to an exponential size dependence in the dimerization amplitude [see eq. (8)] it gives excellent results for this quantity even here. Anyhow, the incremental expansion technique combined with DMRG method provides a very powerful tool to evaluate with high accuracy the dimerization amplitude, the charge gap as well as the spin gap for all physically relevant U and g values.

To conclude, from the critical comparison of our discrete calculations with the bosonization (continuum) approach proposed by Sugiura and Suzumura[17] one has the impression that their formalism in the present form yields accurate results only in the weakly correlated region $0 \leq U/t_0 \leq 1.5$. It might be interesting to elucidate to what extent such an approach might be improved for instance in the spirit of the finite-band approach proposed by Gammel[21] to eliminate shortcomings of the continuum models[22,23] for the discrete SSH-model[1] for noniteracting particles. Alternatively, an improved and extended effective spin–Peierls model based on the description proposed in ref. 12 would be noteworthy, too, at least in the intermediately strong correlated case where the maximum of the dimerization occurs for weak el–ph interaction. Finally, the Peierls contribution to the charge gap is always positive. It tends to the spin gap approaching the latter in limiting uncorrelated and highly correlated cases.

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