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VARIATIONAL STUDY ON MISSING BOND-CHARGE REPULSION ON THE EXTENDED HUBBARD MODEL: EFFECTS ON POLYACETYLENE

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The variational approach is applied to the study on the effect of Coulomb interaction between electrons on the dimerization in a one-dimensional commensurability-two Peierls system, such as trans-polyacetylene. For the case of omitting direct repulsion between electrons in the bonds between sites W, it is confirmed that the weak interactions tend to enhance the dimerization; but when W is included, this enhancement will be attenuated. If $|W|$ is sufficiently large, the net effect of electron–electron interactions will reduce the magnitude of the electron–phonon-induced dimerization.

Keywords: Fermi systems, Hubbard model
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I. INTRODUCTION

The role of electron–electron (e–e) interactions in solid-state systems is a subject of intense investigation and debate. Results of mean-field theory calculations[1] show that the dimerization amplitude in the ground state decreases when an on-site Coulomb interaction U is introduced. However, longer range interactions are needed to describe many effects observed in real materials. The conventional extended Hubbard model (EHM), which, in addition to U, includes a nearest-neighbour interaction of strength V, is the simplest extension that takes into account some of the long-range interaction effects. Several authors, using various many-body techniques,[2] have found that the ground-state dimerization amplitude is enhanced when a weak Coulomb interaction V is included in the Hubbard–Peierls Hamiltonian.

Kivelson, Su, Schrieffer and Heeger (KSSH)[3] reexamined e–e interactions in the framework of tight-binding models of quasi-one-dimensional systems. They remarked that the standard extended Hubbard model, including only on-site (U) and nearest-neighbour (V) terms, has missed off-diagonal terms (W) corresponding to 'bond-charge' interaction. KSSN argued that these new terms have important physical consequences for the extended Peierls–Hubbard model of polyacetylene. In first-order perturbation theory, KSSN found, for extreme screening, that including W reverses the sign of the effects of Coulomb interactions, so that the dimerization decreases with increasing e–e interactions, and at fixed dimerization e–e interactions decrease the gap. This is consistent with the work of Wu *et al*,[4] who started from the full Coulomb interaction with any strength and range. They found that when the interaction range is of the order of the lattice constant (short range), the bond alternation monotonically decreases with increasing interaction strength. In Ref.[5] the mixed bond-site (X) and bond–bond (W) are studied; these off-diagonal terms are believed to enhance dimerization. Ref.[6] has also shown that the weak Coulomb interaction tends to increase dimerization. So the influence of bond–bond (W) on dimerization is still controversial. We focus on the effects of W on dimerization by using bosonization[7] and the self-consistent Gauss model[8] and we calculate the ground state by the variational method. We will prove that W is an important term which tends to weaken this enhancement; eventually sufficient large $|W|$ will reduce the magnitude of the electron–phonon-induced dimerization.

This paper is organized as follows. In Sec.II we give the Hamiltonian in terms of Fermi fields operators. In Sec.III we bosonize the Hamiltonian of the model. In Sec.IV we give the results of numerical calculations by the variational method, and in Sec.V the results are discussed and analysed.

II. MODEL[3]

We consider a continuum Hamiltonian which con-

sists of a one-electron term (TLM[9] model):

$$H_{\rm TLM} = \int {\rm d}x\, \psi_s^\dagger(x)\left\{ -{\rm i}\hbar v_{\rm F}\frac{\partial}{\partial x}\sigma_z + \Delta(x)\sigma_x \right\}\psi_s(x) + \int {\rm d}x \left[\frac{\hbar v_{\rm F}}{2g^2}\right]\left[\frac{\Delta(x)}{\hbar v_{\rm F}}\right]^2, \quad (1)$$

and an electron–electron interaction term:

$$\begin{aligned} H_{\rm int} = & \sum_{ss'}\int {\rm d}x\, \hbar v_{\rm F}\{g_1\psi_{s2}^\dagger\psi_{s'1}^\dagger\psi_{s'1}\psi_{s2} \\ & + g_2\psi_{s1}^\dagger\psi_{s'2}^\dagger\psi_{s'2}\psi_{s1} \\ & + \frac{1}{2}g_3[\psi_{s1}^\dagger\psi_{s'1}^\dagger\psi_{s'2}\psi_{s2} + {\rm H.c.}] \\ & + \frac{1}{2}g_4[\psi_{s1}^\dagger\psi_{s'1}^\dagger\psi_{s'1}\psi_{s1} + \psi_{s2}^\dagger\psi_{s'2}^\dagger\psi_{s'2}\psi_{s2}]\}, \end{aligned} \quad (2)$$

where $\psi_{s1}(x)$ creates a right-moving electron of spin s, $\psi_{s2}(x)$ creates a left-moving electron of spin s, and σ_z and σ_x are Pauli matrices. When the continuum limit of the discrete model is taken, the parameters defining Eqs.(1) and (2) become the following:

$$\hbar v_f = 2t_0 a, \quad g^2 = 2\alpha^2/Kt_0,$$

the choice of nearest-neighbour hopping is $t_0 = 2.5\,{\rm eV}$, the value of the stiffness constant K is $2100\,{\rm eV/nm^2}$ and the lattice constant a is $0.122\,{\rm nm}$; these are all generally agreed.[10] α is the electron–phonon coupling constant; α=41.6 eV/nm can be used to explain some phenomenon,[2] but some authors found that α=45–60 eV/nm.[1] We take α=40–60 eV/nm in this paper. In terms of the e–e interactions model:[11]

$$\begin{aligned} g_1 &= (U - 2V + 4W)/2t_0\,, \\ g_2 &= (U + 2V)/2t_0\,, \\ g_3 &= -(U - 2V - 4W)/2t_0\,, \\ g_4 &= (U + 2V)/2t_0\,. \end{aligned}$$

The parameters U, V and W are the Coulomb interactions between electrons located on the same site, on neighbouring sites and on bonds between sites respectively. The e–e interaction can be written in its most general form as

$$\begin{aligned} H_{\rm int} &= \int\int {\rm d}r{\rm d}r'\rho(r)\,V(r-r')\,\rho(r') \\ &= \sum_{n,m,l,p,s,s'} V(n,m,l,p)\,C_{n\,s}^\dagger C_{m\,s'}^\dagger C_{l\,s'} C_{p\,s}, \end{aligned}$$

where $V(n,m,l,p)$ is the appropriate matrix element of the electron–electron interaction potential, $V(r)$,

$$V(n,m,l,p) = \int {\rm d}r{\rm d}r'\rho_{n\,p}(r)\rho_{m\,l}(r')V(r-r'),$$

in which $\rho_{n\,p}(r)$ denotes the matrix element of the electron-density operator $\hat\rho(r)$ in the local Wannier function representation, $\rho_{n\,p}(r) = \Phi_n^*(r)\,\Phi_p(r) = \langle n|\hat\rho(r)|p\rangle$. $U = 2V(0,0,0,0)$, $V = 2V(0,1,1,0)$, $W = 2V(0,1,0,1)$, where U is the most important term and V is the next important term. But, as pointed out in Ref.[3], W is as important as V or even more important. W is neglected in general reports.

III. BOSONIZATION

We will introduce Boson fields

$$\Phi_{\pm,\uparrow(\downarrow)}(x) = \frac{1}{2}\left[\phi_{\uparrow(\downarrow)}(x) \mp \int_{-\infty}^{x} \prod{}_{\uparrow(\downarrow)}(x')\,{\rm d}x'\right], \quad (3)$$

where $\phi_{\uparrow(\downarrow)}(x)$ and $\prod_{\uparrow(\downarrow)}(x)$ satisfy the commutation relations for Bose operators. Then the Fermi operators can be expressed as[7]

$$\psi_{\pm\uparrow(\downarrow)}(x) = \frac{1}{\sqrt{2\pi\epsilon}}\exp[\pm{\rm i}\sqrt{4\pi}\,\Phi_{\pm,\uparrow(\downarrow)}(x)]. \quad (4)$$

The parameter ϵ in Eq.(4) is a small distance, i.e. the lattice spacing.

We consider in this paper only the half-filled band in which there is one electron per site, thus we can bosonize the Hamiltonian of the model and we have

$$\begin{aligned} H = & \int {\rm d}x\, :G_1\left[\widetilde{\prod}_c^{\,2} + \left(\frac{\partial\widetilde\phi_c}{\partial x}\right)^2\right] \\ & + G_2\left[\widetilde{\prod}_s^{\,2} + \left(\frac{\partial\widetilde\phi_s}{\partial x}\right)^2\right] + \frac{\hbar v_{\rm F} g_3}{2\pi^2\epsilon^2}\cos 2M_c\widetilde\phi_c \\ & + \frac{2}{\pi\epsilon}\,\Delta(x)\cos M_c\widetilde\phi_c\cos M_s\widetilde\phi_s \\ & + \frac{K}{8a\alpha^2}\Delta(x)^2\,:, \end{aligned} \quad (5)$$

where the charge density wave (CDW) fields and spin density wave (SDW) fields are $\widetilde\phi_{c(s)} = \frac{1}{\sqrt{2}}(\phi_\uparrow \pm \phi_\downarrow)$.

We make a shift of $M_s\widetilde\phi_s$ to $M_s\widetilde\phi_s + \pi$ so that the potential energy in Eq.(5) will reach minimum at $\widetilde\phi_s$=0 and $\widetilde\phi_c$=0 $\left(\text{when } g_3 < \frac{\pi\Delta(x)}{\hbar v_{\rm F}}\right)$. Thus the Hamiltonian of the model becomes

$$\begin{aligned} H = & \int {\rm d}x\, :G_1\left[\widetilde{\prod}_c^{\,2} + \left(\frac{\partial\widetilde\phi_c}{\partial x}\right)^2\right] \\ & + G_2\left[\widetilde{\prod}_s^{\,2} + \left(\frac{\partial\widetilde\phi_s}{\partial x}\right)^2\right] + \frac{\hbar v_{\rm F} g_3}{2\pi^2\epsilon^2}\cos 2M_c\widetilde\phi_c \\ & - \frac{2}{\pi\epsilon}\,\Delta(x)\cos M_c\widetilde\phi_c\cos M_s\widetilde\phi_s \\ & + \frac{K}{8a\alpha^2}\Delta(x)^2\,:. \end{aligned} \quad (6)$$

The parameters M_s, M_c, G_1 and G_2 in Eqs.(5) and (6) are defined as:

$$M_s = \sqrt{2\pi}\,,$$

$$M_c = \sqrt{2\pi} \times \sqrt[4]{\frac{2\pi - 2(g_1+g_2)+g_4}{2\pi + 2(g_1+g_2)+g_4}}\,,$$

$$G_1 = \frac{\hbar v_{\rm F}}{4\pi}\sqrt{[2\pi - 2(g_1+g_2)+g_4][2\pi + 2(g_1+g_2)+g_4]}\,,$$

$$G_2 = \frac{\hbar v_{\rm F}}{4\pi}(2\pi - g_4)\,.$$

IV. VARIATIONAL PROCEDURES

We will introduce a new solvable Hamiltonian H_M to imitate H:

$$\begin{aligned} H_M = \int {\rm d}x \; :& G_1\left[\widetilde{\prod}_c^2 + \left(\frac{\partial\widetilde{\phi}_c}{\partial x}\right)^2\right] \\ &+ G_2\left[\widetilde{\prod}_s^2 + \left(\frac{\partial\widetilde{\phi}_s}{\partial x}\right)^2\right] \\ &+ (A\widetilde{\phi}_c^2 + 2B\widetilde{\phi}_c\widetilde{\phi}_s + C\widetilde{\phi}_s^2) + \frac{K}{8a\alpha^2}\Delta(x)^2 :, \end{aligned} \tag{7}$$

where A, B and C are parameters connected to the renormalized masses, and these will be determined by the variational method. The mixed term B is included to take account of the coupling between $\widetilde{\phi}_c$ and $\widetilde{\phi}_s$ in Eq.(6). By using a transformation of stretching, the free part of the Hamiltonian H_M in Eq.(7) becomes

$$\begin{aligned} H_0 = \int {\rm d}x \; :& G_1G_2\overline{\prod}_c^2 + \frac{G_1}{G_2}\left(\frac{\partial\overline{\phi}_c}{\partial x}\right)^2 \\ &+ G_1G_2\overline{\prod}_s^2 + \frac{G_2}{G_1}\left(\frac{\partial\overline{\phi}_s}{\partial x}\right)^2 :. \end{aligned} \tag{8}$$

Thus the Hamiltonian H_M can be written as:

$$\begin{aligned} H_M = \int {\rm d}x \; :& G_1G_2\overline{\prod}_c^2 + \frac{G_1}{G_2}\left(\frac{\partial\overline{\phi}_c}{\partial x}\right)^2 \\ &+ G_1G_2\overline{\prod}_s^2 + \frac{G_2}{G_1}\left(\frac{\partial\overline{\phi}_s}{\partial x}\right)^2 \\ &+ \frac{A}{G_2}\overline{\phi}_c^2 + \frac{2B}{\sqrt{G_1G_2}}\overline{\phi}_c\,\overline{\phi}_s \\ &+ \frac{C}{G_1}\overline{\phi}_s^2 + \frac{K}{8a\alpha^2}\Delta(x)^2 :. \end{aligned} \tag{9}$$

Then we can diagonalize H_M in the momentum space with a unitary transformation,

$$\begin{aligned} H_M =& \sum_k \sqrt{\frac{G_1G_2E_1}{k^2}}\left(\widehat{\prod}_{c,k}\widehat{\prod}_{c,-k} + k^2\widehat{\phi}_{c,k}\widehat{\phi}_{c,-k}\right) \\ &+ \sqrt{\frac{G_1G_2E_2}{k^2}}\left(\widehat{\prod}_{s,k}\widehat{\prod}_{s,-k} + k^2\widehat{\phi}_{s,k}\widehat{\phi}_{s,-k}\right) \\ &+ \frac{K}{8a\alpha^2}\Delta(x)^2. \end{aligned} \tag{10}$$

The new operators in Eq.(10) are

$$\begin{aligned} \widehat{\prod}_{c,\pm k} =& \sqrt[4]{\frac{G_1G_2k^2}{E_1}} \times \left[\frac{(E_1 - M_2)}{K_1}\overline{\prod}_{c,\pm k} \right. \\ &\left. + \frac{B}{K_2\sqrt{G_1G_2}}\overline{\prod}_{s,\pm k}\right], \\ \widehat{\phi}_{c,\pm k} =& \sqrt[4]{\frac{E_1}{G_1G_2k^2}} \times \left[\frac{(E_1 - M_2)}{K_1}\overline{\phi}_{c,\pm k} \right. \\ &\left. + \frac{B}{K_2\sqrt{G_1G_2}}\overline{\phi}_{s,\pm k}\right], \\ \widehat{\prod}_{s,\pm k} =& \sqrt[4]{\frac{G_1G_2k^2}{E_2}} \times \left[\frac{(E_2 - M_1)}{K_2}\overline{\prod}_{s,\pm k} \right. \\ &\left. + \frac{B}{K_1\sqrt{G_1G_2}}\overline{\prod}_{c,\pm k}\right], \\ \widehat{\phi}_{s,\pm k} =& \sqrt[4]{\frac{E_2}{G_1G_2k^2}} \times \left[\frac{(E_2 - M_1)}{K_2}\overline{\phi}_{s,\pm k} \right. \\ &\left. + \frac{B}{K_1\sqrt{G_1G_2}}\overline{\phi}_{c,\pm k}\right]. \end{aligned}$$

The parameters in Eq.(10) are defined as

$$M_1 = \frac{G_1}{G_2}k^2 + \frac{A}{G_2}\,,$$

$$M_2 = \frac{G_2}{G_1}k^2 + \frac{C}{G_1}\,,$$

$$K_{1(2)} = \sqrt{(E_{1(2)} - M_{2(1)})^2 + \frac{B^2}{G_1G_2}}\,,$$

the spectra are

$$\sqrt{E_{1(2)}} = \sqrt{\frac{1}{2}\left[(M_1+M_2) \pm \sqrt{(M_1-M_2)^2 + \frac{4B^2}{G_1G_2}}\right]}\,.$$

We average H with respect to the ground state of H_M and obtain

$$E_h = E_A + E_B + E_C + E_D + E_E + \frac{K}{8a\alpha^2}\Delta(x)^2, \tag{11}$$

$$E_A = \sum_k \frac{\sqrt{G_1G_2}}{2}[\sqrt{E_1} + \sqrt{E_2}], \tag{12}$$

$$\begin{aligned} E_B = \sum_k \frac{G_1k^2}{2G_2}\Bigg[& \frac{(E_1 - M_2)^2}{K_1^2}\sqrt{\frac{G_1G_2}{E_1}} \\ &+ \frac{B^2}{K_1^2G_1G_2}\sqrt{\frac{G_1G_2}{E_2}}\Bigg], \end{aligned} \tag{13}$$

$$\begin{aligned} E_C = \sum_k \frac{G_2k^2}{2G_1}\Bigg[& \frac{(E_2 - M_1)^2}{K_2^2}\sqrt{\frac{G_1G_2}{E_2}} \\ &+ \frac{B^2}{K_2^2G_1G_2}\sqrt{\frac{G_1G_2}{E_1}}\Bigg], \end{aligned} \tag{14}$$

$$E_D = \frac{\hbar v_F g_3 L}{2\pi^2\epsilon^2}\exp\Big\{\sum_k \frac{-M_c^2}{G_2 L}\Big[\frac{(E_1-M_2)^2}{K_1^2}\sqrt{\frac{G_1G_2}{E_1}} + \frac{B^2}{K_1^2 G_1 G_2}\sqrt{\frac{G_1G_2}{E_2}}\Big]\Big\}, \quad (15)$$

$$E_E = \frac{-2\Delta L}{\pi\epsilon}\cosh\Big\{\sum_k \frac{M_c M_s B}{2LK_1K_2\sqrt{G_1G_2}} \cdot \Big[\frac{E_1-M_2}{\sqrt{E_1}} + \frac{E_2-M_1}{\sqrt{E_2}}\Big]\Big\} \cdot \exp\Big\{\sum_k \frac{-M_c^2}{4G_2L}\Big[\frac{(E_1-M_2)^2}{K_1^2}\sqrt{\frac{G_1G_2}{E_1}} + \frac{B^2}{K_1^2G_1G_2}\sqrt{\frac{G_1G_2}{E_2}}\Big] + \frac{-M_s^2}{4G_1L}\Big[\frac{(E_2-M_1)^2}{K_2^2}\sqrt{\frac{G_1G_2}{E_2}} + \frac{B^2}{K_2^2G_1G_2}\sqrt{\frac{G_1G_2}{E_1}}\Big]\Big\}, \quad (16)$$

where L is the length of the space.

E_H should be minimized with respect to the parameters A, B and C. We believe that the parameter B is a small quantity, so we first calculate A and C without B, and then consider the correction of B.

(i) Without hybridization (B=0)

The parameter ϵ is regarded as a scale; we take $\epsilon = 1$. We transfer the summation into an integration, from $\frac{\delta E_H}{\delta A} = 0$, $\frac{\delta E_H}{\delta C} = 0$ and large cut-off momentum approximation. We obtain two equations:

$$\frac{1}{4} + \Big[\frac{1}{2\sqrt{AG_1}} - \frac{1}{A\sqrt{\frac{A}{G_1}}}\Big] \cdot \Big[2\Delta\beta\Big(\frac{1}{2}\sqrt{\frac{C}{G_2}}\Big)^{\frac{1}{2}}\Big(\frac{1}{2}\sqrt{\frac{A}{G_1}}\Big)^{(\beta+1)} - \frac{2\beta\hbar v_F g_3}{\pi}\Big(\frac{1}{2}\sqrt{\frac{A}{G_1}}\Big)^{(4\beta+1)}\Big] = 0, \quad (17)$$

$$\frac{1}{4} + \Big[\frac{1}{2\sqrt{CG_2}} - \frac{1}{C\sqrt{\frac{C}{G_2}}}\Big] \cdot \Big[\Delta\Big(\frac{1}{2}\sqrt{\frac{A}{G_1}}\Big)^{\beta}\Big(\frac{1}{2}\sqrt{\frac{C}{G_2}}\Big)^{\frac{3}{2}}\Big] = 0, \quad (18)$$

where parameter β is

$$\beta = \frac{1}{2}\sqrt{\frac{2\pi - 2(g_1+g_2)+g_4}{2\pi+2(g_1+g_2)+g_4}}.$$

The parameters A and C in the two equations should satisfy the condition that E_h takes the minimum value. By using numerical simulation technique, we find the relationship between dimerization and the electron–phonon coupling constant when we take $U = 4$, $V = -2$, $W = 0, -1, -1.5$ respectively. From this we have found three very straight curves: $\delta_{1(1)}$, $\delta_{1(2)}$, $\delta_{1(3)}$ (see Fig.1).

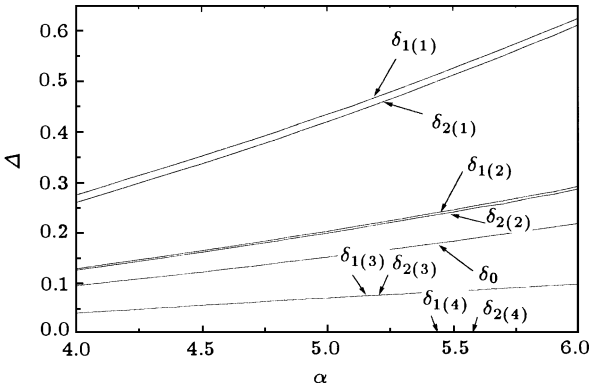


Fig.1. The dimerization (scaled in $1/\epsilon$) versus electron–phonon coupling constant when $U = 4$, $V = -2$, $W = 0, -1, -1.5, -2$ respectively.

(ii) With hybridization ($B \neq 0$)

We will take A and C which we have obtained from calculation in (i), and we will also determine whether M_1 and M_2 have a point of intersection. After calculation, we conclude that under the conditions that $U = 4$, $V = -2$, $0 \geq W \geq -2$, M_1 and M_2 have no point of intersection. We suppose the parameter B is a small quantity. It can be proved lately that our assumption is self-consistent. If M_1 and M_2 have no point of intersection, then $|M_1 - M_2| \gg 2B/\sqrt{G_1G_2}$. We expand the expression of E_1 and E_2 in which $2B/\sqrt{G_1G_2}$ is regarded as a small quantity, and we also transfer the summation into integration. From numerical calculation we conclude that in Eq.(16) the influence of the hyperbolic cosine term is much smaller than that of the exponential term, so we can approximately take it as unity. By using a numerical simulation technique, we can determine the parameter B corresponding to the minimal E_h which is less than 0.0001. We also find the relationship between dimerization and the electron–phonon (e–ph) coupling constant, from which we obtain three very straight curves: $\delta_{2(1)}$, $\delta_{2(2)}$, $\delta_{2(3)}$ (see Fig.1).

V. DISCUSSION AND SUMMARY

1. If we neglect $H_{\rm int}$ and only keep $H_{\rm TLM}$ in our model, in the same way, after bosonization and variation, we can obtain the relationship between the dimerization Δ and the e–ph coupling constant α from one-dimensional free-field theory. The line δ_0 (see

Fig.1) is a reference line in our discussion, when we include the influence of $H_{\rm int}$. If the line δ is located above the line δ_0, this indicates that the influence of net Coulomb strength will increase the dimerization; otherwise, it will decrease the dimerization.

2. We take $U = -2V = 4$.[12] When W is neglected ($U = 4, V = -2, W = 0$), $\delta_{1(1)}$ and $\delta_{2(1)}$ are located above δ_0, this means that in the extended Hubbard model, the net Coulomb strength increases the dimerization. Reference [3] indicates that $V = W$ for reasonable forms of the Wannier function and $V(r) = V_0\delta(r)$. If we approximate $V(r)$ by Gaussian screening and also approximate the Wannier functions in terms of Gaussians, from straightforward calculation we can show $W \approx V$. Since different materials may have quite different relations among X, U, V and W, and the value of W is uncertain, we will take the parameter W which varies from zero to V, thus we can find the influence of W on dimerization. It can be seen in Fig.1 that the curves Δ-α drop monotonically with W changing from zero, -1.0, -1.5, to -2.0. When $|W|$ is larger than a certain value, the contribution of the weakened e–e interaction to the magnitude of the dimerization is negative. If W changes to -2 corresponding to $g_1 = g_2 = g_4 = 0$, the potential terms in Eq.(6) are marginally irrelevant and will be renormalized to zero. In this special case, the Hamiltonian of the model in Eq.(6) can be renormalized to free model, we assert qualitatively that the dimerization is zero—that is, $\delta_{1(4)}$(without hybridization)=$\delta_{2(4)}$(with hybridization)=0!—(see Fig.1).

The Hamiltonian (6) contains an interaction term between CDW and SDW, therefore one must take account of the influence of hybridization between them. We find that $\delta_{2(1)}$(with hybridization) is located below $\delta_{1(1)}$(without hybridization), so are the $\delta_{2(2)}$ with respect to $\delta_{1(2)}$ and the $\delta_{2(3)}$ with respect to $\delta_{1(3)}$. This indicates that the influence of hybridization will diminish the magnitude of dimerization. The influence of hybridization will decrease with the increase of $|W|$, and $\delta_{2(2)}$ is much closer to $\delta_{1(2)}$ than $\delta_{2(1)}$ to $\delta_{1(1)}$. Thus $\delta_{2(3)}$ and $\delta_{1(3)}$ are almost overlapping and we can hardly distinguish one from the other.

3. Previous studies established that the diagonal Coulomb interaction terms (U, V) enhance dimerization substantially for weak (to intermediate) values. This is generally agreed. Here we are mainly interested in the effects of off-diagonal terms. Conclusions based on weak-coupling perturbation theory,[5] including all terms to second order, suggest that U, V and X enhance dimerization while W suppresses it; overall Coulomb interactions enhance dimerization. But perturbation theory about the effects of off-diagonal terms on dimerization is not valid for realistic, self-consistent values of the Coulomb interaction parameters.[5]

The exact diagonalizations and strong-coupling perturbation analysis of dimerization[5] suggest that for intermediate-strength e–e interaction, dimerization increases slightly with the addition of small W, and the extended Peierls–Hubbard models without off-diagonal terms will underestimate the enhancement of dimerization caused by Coulomb interactions. But the results are based on the assumption that W is a small quantity ($U \gg W$) and can almost be neglected. Whether W is a small quantity is still an open question.

There are several variational studies for the full-screened Coulomb interaction. The first study used a Jastrow variational ansatz[4] to examine quantitatively the effect of e–e interactions on dimerization, and the second undertook a detailed qualitative analysis of the validity of the Hubbard model using only the assumption that the overlap integrals decay more rapidly with distance than does the interelectronic potential.[13] The results of both these studies indicate that for all except short screening length and for weak (to intermediate) e–ph coupling, dimerization is enhanced by Coulomb effects. Reference [4] also indicates that for repulsion in short range, dimerization will decrease with increasing strength. But Ref.[6] has shown that the weak Coulomb interaction is in favour of the lattice dimerization, and this has been demonstrated by extensive numerical calculations.[14–18] These theories are contrary to Ref.[4] in short range (of the order of a lattice); some of the authors did not include W in their work, others did but supposed that $U > V \gg W$ or $U \gg W = V$. So, whether W is a small quantity and what is the effect of W on dimerization are still under investigation. In this paper, we take $V < 0$ and $W \approx V$. When W is adjusted from zero to V, we can find out the influences of W on dimerization. Our conclusions suggest that when $|W|$ increases from zero but less than a certain value (about $0.6V$), the enhancement of the diagonal terms on dimerization will be attenuated, but the net Coulomb interaction will still enhance dimerization. If $|W|$ increases further, the net Coulomb interaction will decrease dimerization. When $W = V$, dimerization is destroyed. The true physical value of W may

be in the range of $(0.6V, V)$. Our conclusion is consistent with the work of Wu *et al.*,[4] thus we conclude that the influence of W is important and will decrease dimerization rather than increase it. This is reasonable from a physical point of view.

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