

Electron correlation in the charge-density wave state of MX complexes

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Abstract. The effect of the electron–electron (e–e) interaction on the charge-density wave (CDW) of MX complexes is studied using the Gutzwiller variational method within the one-band model, and neglecting the quantum features of the lattice. It is found that the effect of the e–e interaction on the CDW in MX complexes is opposite to that on the BOW (bond-order wave) in the conjugated polymer, although both the CDW and BOW have the same origin, which is the dimerization of the one-dimensional lattice. The CDW is suppressed by the e–e interaction, and the BOW is initially enhanced. The physical reason for this contrast is analysed.

1. Introduction

The MX complex consists of an array of linear chains of alternating transitional metal M atoms (Pt, Pd, Ni) and halogen X atoms (Cl, Br, I), with ligands L (X, ethylamine, ethylenediamine, cyclohexanediamine, etc) attached to the metal atoms [1]. A prominent feature of this material is the great flexibility of tuning the competition between electron–phonon (e–p) and e–e interactions by chemically varying M, X and L, by pressure or by doping. Thus this kind of complex provides a unique model system to investigate both theoretically and experimentally various instabilities, broken-symmetry ground states and non-linear localized excitations governed by e–p and e–e interactions, as well as dimensionality [2–6]. On this subject, the Los Alamos group has made extensive studies with the two-band model by using quantum variational, exact diagonalization, unrestricted Hartree–Fock and perturbation methods—[7, 8].

In recent years an increasingly interesting topic in condensed matter physics is the study of electron correlation in some new materials, such as conducting polymers, high- T_c superconductors, two-dimensional electron gases, CDW systems, and so on. Such studies can give us insight into understanding many novel phenomena in these materials. This paper focuses on electron correlation in one-dimensional systems.

As is well known, one-dimensional systems possess Peierls instability caused by the e–p interaction. In systems with a half-filled band, Peierls instability produces a dimerization. Both MX complexes and conjugated polymers have a chain structure, and dimerization occurs in these two materials. But the consequences of their dimerization are different. In conjugated polymers, the dimerization of the carbon lattice changes the bond lengths, and alternating long bonds and short bonds results: this is bond alternation or BOW. In MX

chains, the dimerization of the X sublattice induces a charge disproportion in the M atoms: this is CDW. Since the Peierls instability only considers the e–p interaction, an essential issue is to ask what the effect is of the e–e interaction on the dimerization.

In the case of conjugated polymers, the above issue once caused a dispute. One school of thought declared that the dimerization should be *enhanced* by the e–e interaction [9]. The other school of thought insisted that the dimerization must be *reduced* by the e–e interaction [10]. Later this dispute was clarified by a careful consideration of the e–e interaction [11]. It was found that screening is a crucial factor. If the screening is weak, the dimerization is enhanced; if the screening is very strong, the dimerization can be reduced. In the case of weak screening, the off-diagonal part of the screened Coulomb interaction is negligible, and the on-site repulsion (Hubbard model) is dominant. Therefore, if using the Hubbard model to describe the e–e interaction, the dimerization in conjugated polymers is enhanced by it.

One naturally asks what should happen in MX chains. Will the dimerization of an MX complex be enhanced or reduced by the e–e interaction? Within the Hartree–Fock approximation, Conradson and co-workers have shown that Hubbard repulsion reduces the dimerization in the CDW of MX complexes [12]. However, electron correlation is very important in low-dimensional systems, and in this paper we go beyond the mean-field approach to study this issue. In order to make the comparison between conjugated polymers and MX complexes more transparent, the model used for the MX complex should be the same as that used for the conjugated polymer. Therefore, we take the one-band Hubbard model to describe the e–e interaction and use the Gutzwiller variational method, which was applied to study the electron correlation in conjugated polymers [13], to discover the effect of the e–e interaction on the dimerization of MX complexes. The quantum fluctuation of the lattice is neglected.

Interestingly, our results show that the effect on MX complexes is opposite to that on conjugated polymers, i.e. the dimerization in MX complexes is reduced by the e–e interaction. Section 2 presents the formulation and numerical results. In section 3, we explain the physical reason why MX chains and conjugated polymers possess such opposite behaviour when considering the effect of the e–e interaction on the dimerization.

2. Formulation and results

As mentioned in the introduction, in order to make the comparison between MX complexes and conjugated polymers more transparent, the MX chain is described by a one-band Hubbard model, although a more precise description needs the two-band model [7, 8]. The one-band Hamiltonian is

$$\hat{H} = -T \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + \text{HC}) + \omega \sum_i q_i^2 / 2 + \sqrt{S\omega} \sum_{i\sigma} (q_i - q_{i+1}) n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

where $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ denote the creation and annihilation operators of an electron at site i with spin σ , $n_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma}$; T is the transfer energy of an electron between neighbouring M atoms, ω the elastic constant of the X sublattice, q_i the displacement of X atoms, S the electron–lattice coupling and U the Hubbard parameter of the e–e interaction. In this paper we only consider the effect of the e–e interaction on the CDW; the quantum effects of the

lattice vibration will be studied in another paper. The movement of the X atoms is therefore treated classically and their kinetic energy is dropped.

By introducing

$$Q_i = \sqrt{\omega/S} q_i \quad \hat{h} = \hat{H}/T \quad s = S/T \quad u = U/T$$

the Hamiltonian (1) is converted into a dimensionless form:

$$\hat{h} = - \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + \text{HC}) + s \sum_i Q_i^2/2 + s \sum_{i\sigma} (Q_i - Q_{i+1}) n_{i\sigma} + u \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (2)$$

When the band is half-filled, the Peierls instability produces a dimerization, and

$$Q_i = (-1)^i \bar{v}$$

where \bar{v} is the amplitude of the dimerization. The electronic Hamiltonian is then

$$\hat{h}_e = - \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + \text{HC}) + 2s\bar{v} \sum_i (-1)^i n_{i\sigma} + u \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (3)$$

In order to apply the Gutzwiller variational method [13], it is necessary to get an effective single-particle (mean-field) Hamiltonian, which can be easily obtained from \hat{h}_e by the Hartree-Fock approximation

$$\hat{h}_0 = \sum'_{k\sigma} \Psi_{k\sigma}^\dagger \mathcal{H} \Psi_{k\sigma} \quad (4)$$

where

$$\mathcal{H} = \begin{pmatrix} \epsilon_k & \Delta \\ \Delta & -\epsilon_k \end{pmatrix} \quad \Psi_{k\sigma} = \begin{pmatrix} c_{k\sigma} \\ c_{k-Q\sigma} \end{pmatrix}$$

with the prime denoting summation in the region from $-\pi/2$ to $\pi/2$, $Q = \pi$, and

$$c_{k\sigma} = \frac{1}{\sqrt{N}} \sum_l e^{-ikl} c_{l\sigma} \quad \epsilon_k = -2 \cos k$$

with 2Δ the mean field gap.

Unlike the conjugated polymer, Hubbard repulsion affects the ground state of MX complexes even in the Hartree-Fock approximation [12]. To clarify the effect of electron correlation, we determined the gap parameter Δ by minimizing the mean-field energy of the system, giving

$$\frac{1}{8s - u} = \frac{1}{\pi \sqrt{4 + \Delta^2}} K \left(\frac{2}{\sqrt{4 + \Delta^2}} \right) \quad (5)$$

where $K(x)$ is a complete elliptic integral of the first kind.

The Gutzwiller variational function of the ground state is then [6]

$$|\psi\rangle = e^S|0\rangle \quad (6)$$

where $|0\rangle$ is the ground state of the mean-field Hamiltonian (4), and S describes the correlation effect which is unfavourable to double occupation. In conjugated polymers, since the carbon atoms are equivalent, only one correlation parameter η is needed and the Gutzwiller *ansatz* is [13]

$$S = -\frac{1}{2}\eta \sum_i n_{i\uparrow}n_{i\downarrow}. \quad (7)$$

However, in MX chains with a CDW ground state, the charge density is different in odd and even sites, and one global parameter is no longer appropriate. In the following discussion, we introduce two parameters, η_+ and η_- , to describe the correlations at even and odd sites:

$$S = -\frac{1}{2}\left(\eta_+ \sum_{i=\text{even}} n_{i\uparrow}n_{i\downarrow} + \eta_- \sum_{i=\text{odd}} n_{i\uparrow}n_{i\downarrow}\right) \equiv -\frac{1}{2}(\eta_+ V_+ + \eta_- V_-). \quad (8)$$

The total energy per site of the ground state is

$$\varepsilon(\eta_+, \eta_-, \bar{v}) = \frac{1}{2}s\bar{v}^2 + N^{-1} \frac{\langle \psi | \hat{h}_e | \psi \rangle}{\langle \psi | \psi \rangle}. \quad (9)$$

Expanding e^S to second order in η_+ and η_- , the total energy per site is

$$\begin{aligned} \varepsilon(\eta_+, \eta_-, \bar{v}) = & \frac{1}{2}s\bar{v}^2 + \frac{1}{N} \{ \langle 0 | \hat{h}_e | 0 \rangle_c - \frac{1}{2} [\eta_+ \langle 0 | \{ V_+, \hat{h}_e \} | 0 \rangle_c + \eta_- \langle 0 | \{ V_-, \hat{h}_e \} | 0 \rangle_c] \\ & + \frac{1}{8} [\eta_+^2 \langle 0 | \{ V_+, \{ V_+, \hat{h}_e \} \} | 0 \rangle_c + \eta_+ \eta_- \langle 0 | \{ V_+, \{ V_-, \hat{h}_e \} \} | 0 \rangle_c \\ & + \eta_+ \eta_- \langle 0 | \{ V_-, \{ V_+, \hat{h}_e \} \} | 0 \rangle_c + \eta_-^2 \langle 0 | \{ V_-, \{ V_-, \hat{h}_e \} \} | 0 \rangle_c] \} \end{aligned} \quad (10)$$

where $\{A, B\} = AB + BA$, and the subscript c means only the connected diagrams are taken into account. We introduce the correlation functions as [13]

$$P_{ij} \equiv \langle 0 | c_{i\sigma}^\dagger c_{j\sigma} | 0 \rangle \quad Q_{ij} \equiv \langle 0 | c_{i\sigma} c_{j\sigma}^\dagger | 0 \rangle = \delta_{ij} - P_{ij}. \quad (11)$$

It is easy to verify that

$$P_{ij} = P_{ji} \quad Q_{ij} = Q_{ji}. \quad (12)$$

Details of the calculation of P_{ij} are given in appendix A.

The ground state is obtained by minimizing the total energy. Minimizing the energy with respect to these two correlation parameters we obtain

$$\eta_+ = -\frac{2(A_+B_- - A_-C)}{C^2 - B_+B_-} \quad \eta_- = -\frac{2(A_-B_+ - A_+C)}{C^2 - B_+B_-} \quad (13)$$

where

$$\begin{aligned} A_{\pm} &= \langle 0 | \{V_{\pm}, \hat{h}_e\} | 0 \rangle_c \\ B_+ &= \langle 0 | \{V_+, \{V_+, \hat{h}_e\}\} | 0 \rangle_c \quad B_- = \langle 0 | \{V_-, \{V_-, \hat{h}_e\}\} | 0 \rangle_c \\ C &= \frac{1}{2} [\langle 0 | \{V_+, \{V_-, \hat{h}_e\}\} | 0 \rangle_c + \langle 0 | \{V_-, \{V_+, \hat{h}_e\}\} | 0 \rangle_c]. \end{aligned}$$

So the total energy is written as

$$\varepsilon(\bar{v}) = \frac{1}{2}s\bar{v}^2 + \frac{1}{N} [\langle 0 | \hat{h}_e | 0 \rangle_c - \frac{1}{4}\eta_+ \langle 0 | \{V_+, \hat{h}_e\} | 0 \rangle_c - \frac{1}{4}\eta_- \langle 0 | \{V_-, \hat{h}_e\} | 0 \rangle_c]. \quad (14)$$

The explicit expressions for A_{\pm} , B_{\pm} , C and $\langle 0 | \hat{h}_e | 0 \rangle_c$ in terms of the correlation functions defined in (11) can be found in appendix B. Minimizing the total energy with respect to \bar{v} , the amplitude of dimerization \bar{v} and the correlation parameters η_+ , η_- can be determined through numerical calculation. Since the function $P_{n,n+m}$ decreases as $\exp(-|m|\Delta)$ for large m [13], we truncate the series by assuming $P_{ij} = 0$ if $|i - j| \geq 5$. The results are shown in figures 1 and 2. Here, we choose an intermediate electron-lattice coupling strength of CDW, $s = 0.5$ [4].

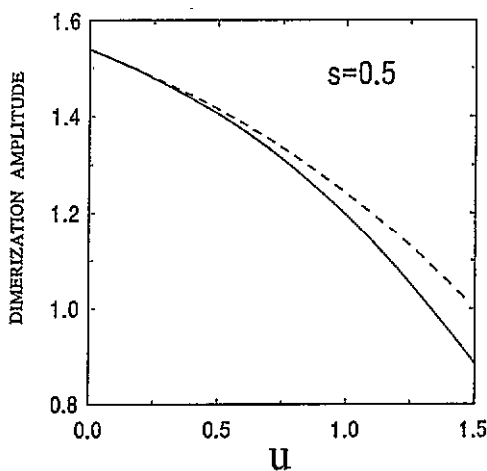


Figure 1. The dependence of dimerization on the electron interaction parameter u for $s = 0.5$. The broken curve is the mean-field result.

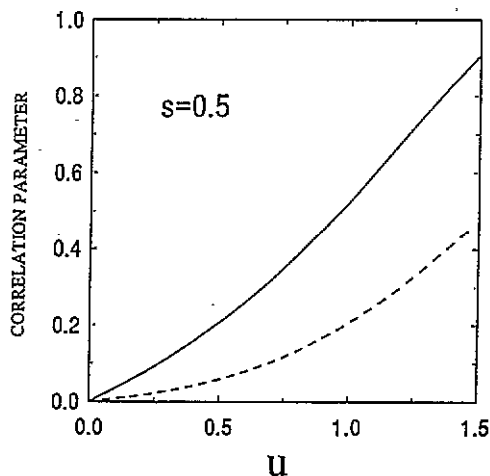


Figure 2. The dependencies of correlation parameters on u for $s = 0.5$. Full and broken curves correspond to η_+ and η_- respectively.

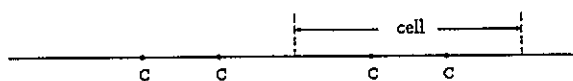
Figure 1 shows the dependence of the dimerization on the e - e interaction for electron-lattice coupling $s = 0.5$. It demonstrates that the dimerization of MX complexes is reduced by the e - e interaction. This behaviour is contrary to that of conjugated polymers. In the next section we analyse why these two systems show such opposite behaviour.

In figure 1, the broken curve is the mean-field result; the full curve is the result after taking account of electron correlation. The mean-field approximation only counts the electrostatic and exchange effects of the e - e interaction, but no correlation. So figure 1 also indicates that the electron correlation further reduces the dimerization.

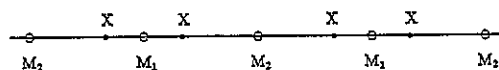
Figure 2 demonstrates the dependences of correlation parameters on the Hubbard parameter u . The full and broken curves describe the even-site correlation parameter η_+ and odd-site correlation parameter η_- respectively. The curves show that, for the realistic e - e interaction $U \sim T$, the correlation parameters are smaller than unity; this ensures the expansion in (10) is reasonable.

3. Discussion

It has been seen that the e - e interaction has opposite effects on the dimerizations of MX complexes and conjugated polymers. In order to understand the physical origin behind such a contrast, it is necessary to look at the chain structures and the consequences of dimerization in these two systems.



(a) Polyacetylene



(b) MX Complex

Figure 3. The dimerizations in polyacetylene and MX complexes.

The prototype conjugated polymer is polyacetylene, in which the chain consists of carbon atoms. Before dimerization, all the carbon atoms are equally separated, a unit cell contains only one atom and each carbon atom possess one π electron. After dimerization, two neighbouring C atoms constitute a unit cell, which is shown in figure 3(a), and each unit cell has two π electrons. It should be noted that these two C atoms in the cell are equivalent to each other; they should equally share two π electrons existing in this cell. This means that each C atom still possesses one π electron. Thus in polyacetylene, no

matter how large the dimerization may be, there is always one electron in each site, and no double occupation. Thus the Hubbard repulsion will not obstruct the dimerization. On the other hand, as was pointed out in [14], the Hubbard repulsion prevents the mixture of long and short bonds; this effect favours bond alternation. Therefore dimerization in conjugated polymers is enhanced by the e–e interaction.

The MX complex has other characteristics. In the MX chain, M is fixed; only the X sublattice undergoes dimerization. Before dimerization, X sits in the middle point between two neighbouring M atoms; all the M atoms are equivalent and have the same amount of charge. After dimerization (see figure 3(b)) two neighbouring atoms M_1 and M_2 are no longer equivalent: M_2 has higher electron affinity than M_1 , and some electrons are transferred from M_1 to M_2 . Consequently, double occupation appears. The Hubbard repulsion is unfavourable to the double occupation, so the dimerization in MX chains is suppressed by the e–e interaction.

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Appendix A. Calculation of the correlation functions

The mean-field Hamiltonian (4) can be diagonalized

$$\hat{h}_0 = \sum_{k\sigma} E_k (A_{k\sigma}^\dagger A_{k\sigma} - B_{k\sigma}^\dagger B_{k\sigma}) \quad (\text{A1})$$

with

$$E_k = \sqrt{\epsilon_k^2 + \Delta^2} \quad (\text{A2})$$

where $A_{k\sigma}^\dagger$ and $B_{k\sigma}^\dagger$ are creation operators of conduction and valence bands; their wavefunctions are

$$\begin{pmatrix} \langle 2n-1|k_c \rangle & \langle 2n|k_c \rangle \\ \langle 2n-1|k_v \rangle & \langle 2n|k_v \rangle \end{pmatrix} = \frac{1}{\sqrt{N}} e^{ik2n} \begin{pmatrix} e^{-ik} \alpha_k & \beta_k \\ -e^{-ik} \beta_k & \alpha_k \end{pmatrix} \quad (\text{A3})$$

where the subscripts c and v indicate conduction and valence bands, and

$$\alpha_k = \frac{1}{\sqrt{2E_k}} (\sqrt{E_k - \epsilon_k} - \sqrt{E_k + \epsilon_k}) \quad (\text{A4a})$$

$$\beta_k = -\frac{1}{\sqrt{2E_k}} (\sqrt{E_k + \epsilon_k} + \sqrt{E_k - \epsilon_k}). \quad (\text{A4b})$$

Using these wavefunctions, the correlation function P_{ij} can be obtained:

$$P_{n,n+2m} = \sum_k \langle k_v | n \rangle \langle n + 2m | k_v \rangle = \frac{1}{2\pi} \int_{-\pi/2}^{\pi/2} dk e^{i2mk} \left(1 - (-1)^n \frac{\Delta}{E_k} \right) \quad (\text{A5a})$$

$$P_{n,n+2m-1} = \sum_k \langle k_v | n \rangle \langle n + 2m - 1 | k_v \rangle = -\frac{1}{2\pi} \int_{-\pi/2}^{\pi/2} dk e^{i(2m-1)k} \frac{\epsilon_k}{E_k}. \quad (\text{A5b})$$

Obviously $P_{n,n+2m}$ depends on the parity of n , and the charge density of the CDW is different at odd and even sites. We only consider the correlation of two sites not far away from each other ($|i - j| \leq 4$):

$$P_{nn} = \frac{1}{2} - (-1)^n \frac{\Delta}{\pi \sqrt{4 + \Delta^2}} K \left(\frac{2}{\sqrt{4 + \Delta^2}} \right) \quad (\text{A6a})$$

$$P_{n,n+1} = \frac{1}{2\pi} \left[\sqrt{4 + \Delta^2} E \left(\frac{2}{\sqrt{4 + \Delta^2}} \right) - \frac{\Delta^2}{\sqrt{4 + \Delta^2}} K \left(\frac{2}{\sqrt{4 + \Delta^2}} \right) \right] \quad (\text{A6b})$$

$$P_{n,n+2} = -(-1)^n \frac{1}{2\pi} \left[\Delta \sqrt{4 + \Delta^2} E \left(\frac{2}{\sqrt{4 + \Delta^2}} \right) - \frac{\Delta^3 + 2\Delta}{\sqrt{4 + \Delta^2}} K \left(\frac{2}{\sqrt{4 + \Delta^2}} \right) \right] \quad (\text{A6c})$$

$$P_{n,n+3} = \frac{3}{2\sqrt{\Delta^2 + 4}} \left[F \left(\frac{1}{2}, \frac{1}{2}; 3; \frac{4}{4 + \Delta^2} \right) - F \left(\frac{1}{2}, \frac{1}{2}; 2; \frac{4}{4 + \Delta^2} \right) \right] \quad (\text{A6d})$$

$$P_{n,n+4} = -(-1)^n \frac{\Delta}{\pi \sqrt{\Delta^2 + 4}} \left[\frac{3\pi}{2} F \left(\frac{1}{2}, \frac{1}{2}; 3; \frac{4}{4 + \Delta^2} \right) - 2\pi F \left(\frac{1}{2}, \frac{1}{2}; 2; \frac{4}{4 + \Delta^2} \right) + K \left(\frac{2}{\sqrt{4 + \Delta^2}} \right) \right] \quad (\text{A6e})$$

where $E(x)$ is a complete elliptic integral of the second kind and $F(\alpha, \beta; \gamma; z)$ is the hypergeometric function.

Appendix B. Explicit expressions for A_{\pm} , B_{\pm} , C and $\langle 0 | \hat{h}_e | 0 \rangle_c$

Using the correlation functions defined in (11) we have

$$\langle 0 | \hat{h}_e | 0 \rangle_c = \sum_i [-4P_{i,i+1} + 4s\bar{v}(-1)^i P_{ii} + uP_{ii}^2] \quad (\text{B1})$$

$$A_{\pm} \equiv \langle 0 | \{V_{\pm}, \hat{h}_e\} | 0 \rangle_c = \sum_i [-2C_{\pm}(i, i+1) - 2C_{\pm}(i+1, i) + 4s\bar{v}(-1)^i C_{\pm}(i, i)] + 2uW_{\pm} \quad (\text{B2})$$

where

$$C_{\pm}(i, j) = \sum_{m=\pm} P_{mm}(P_{mj}Q_{mi} + P_{im}Q_{jm}) \quad (\text{B3})$$

$m = +$ or $m = -$ means that the summation is only over even or odd sites, and

$$W_{\pm} = \sum_{m=\pm} \sum_i (2P_{ii} P_{mm} P_{im} Q_{im} + P_{im}^2 Q_{im}^2) \quad (B4)$$

$$B_{\pm} \equiv \langle 0 | \{V_{\pm}, \{V_{\pm}, \hat{h}_e\}\} | 0 \rangle_c = \sum_i [-2D_{\pm}(i, i+1) - 2D_{\pm}(i+1, i) + 4s\bar{v}(-1)^i D_{\pm}(i, i)] + 4u\tilde{W}_{\pm} \quad (B5)$$

where

$$D_{\pm}(i, j) = \sum_{mn=\pm} D(m, n, i, j) \equiv \sum_{mn=\pm} \left[4P_{nm} Q_{nm} P_{nn} (P_{mj} Q_{mi} + Q_{mj} P_{mi}) + P_{nn} P_{mm} [(Q_{ni} P_{mj} + P_{ni} Q_{mj})(Q_{nm} - P_{nm}) + 2(Q_{mi} Q_{nj} P_{nm} - P_{mi} P_{nj} Q_{nm})] + P_{nm}^2 [-(Q_{ni} P_{mj} + P_{ni} Q_{mj}) Q_{nm} + 2Q_{mi} Q_{nj} Q_{nm}] + Q_{nm}^2 [(Q_{ni} P_{mj} + P_{ni} Q_{mj}) P_{nm} - 2P_{mi} P_{nj} P_{nm}] \right] \quad (B6)$$

and

$$\tilde{W}_{\pm} = \sum_{mn=\pm} \tilde{W}(m, n) \equiv \sum_{mn=\pm} \sum_i \left[2P_{ii} P_{mm} P_{nn} (P_{im} Q_{mn} Q_{ni} - Q_{im} P_{mn} P_{ni}) + 6P_{mm} P_{nn} P_{im} Q_{im} P_{in} Q_{in} + 2P_{ii} [P_{mn}^2 Q_{mn} Q_{im} (Q_{in} - 2P_{in}) - Q_{nn}^2 P_{im} P_{mn} (P_{in} - 2Q_{in})] + (Q_{im} P_{nn} P_{ni} - P_{im} Q_{mn} Q_{ni})^2 \right] \quad (B7)$$

$$C \equiv \frac{1}{2} [\langle 0 | \{V_+, \{V_-, \hat{h}_e\}\} | 0 \rangle_c + \langle 0 | \{V_-, \{V_+, \hat{h}_e\}\} | 0 \rangle_c] = \sum_i [-(D_{+-}(i, i+1) + D_{-+}(i, i+1)) - (D_{+-}(i+1, i) + D_{-+}(i+1, i))] + 2s\bar{v}(-1)^i (D_{+-}(i, i) + D_{-+}(i, i))] + 2u(\tilde{W}_{+-} + \tilde{W}_{-+}) \quad (B8)$$

where

$$D_{+-}(i, j) = \sum_{m=+,n=-} D(m, n, i, j) \quad D_{-+}(i, j) = \sum_{m=-,n=+} D(m, n, i, j)$$

$$\tilde{W}_{+-} = \sum_{m=+,n=-} \tilde{W}(m, n) \quad \tilde{W}_{-+} = \sum_{m=-,n=+} \tilde{W}(m, n).$$

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