Canonical perturbation expansion of the Hubbard model

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We have incorporated the projection operators to the canonical transformation to derive an analytical infinite perturbation-expansion series. This canonical perturbation expansion (CPE) is valid if the unperturbed Hamiltonian H_0 and the perturbation H_1 can be expressed as $H_0=\sum_j P_j H P_j$ and $H_1=\sum_{j\neq k} P_j H P_k$, where P_j is the projection operator corresponding to a group of closely spaced effective one-electron orbital energies $E_{j\mu}$ with $\mu=1,2,\ldots,d_j$, and if $|E_{j\mu}-E_{j\nu}| \ll |E_{j\omega}-E_{k\delta}|$ with $j\neq k$. We have shown that the CPE is equivalent to the time-dependent perturbation theory. An extremely simple effective Hamiltonian $\tilde{H}$ is obtained when the CPE is applied to the s-band Hubbard model at the atomic limit. An explicit form of $\tilde{H}$ to the eighth order is given, and the magnetic interaction in $\tilde{H}$ is of the form of Heisenberg exchange $\vec{S}_i\cdot\vec{S}_j$, including far neighbors. We then use this form to compute the antiferromagnetic ground-state energy to the seventh order. Our result is compared with other works.

I. INTRODUCTION

The Hubbard model[1] has been extensively used in theoretical descriptions of the magnetic ordering and the Mott transition in systems which are characterized by narrow energy bands. Though the Hubbard Hamiltonian is quite simple in form, an accurate solution for the thermodynamic properties has proved difficult for the general case. Historically, the model Hamiltonian was constructed for investigating the effect of strong intra-atomic electron correlation. Near the atomic limit $U \gg W$ (U is the Hubbard parameter and W is the bare bandwidth), this model has been thoroughly studied by many authors[2–12] via various approaches. In addition, the standard perturbation method has been applied[13–18] explicitly in terms of the perturbation expansion parameter W/U. Due to the mathematical complexity in the perturbation series, most of the concrete results are restricted to the second order in W/U except for the special case of a one-dimensional chain. On the other hand, an exact numerical solution has been derived for a small ring with a maximum of six atoms for all values of U/W.[19]

It is well known that for sufficiently large U the bare energy band splits into subbands. The centers of gravity of two adjacent subbands are separated by U. To describe the motion of electrons in such a subband picture, let us first define the projection operators P_l through the equation

$$\prod_i [(1-n_{i\uparrow}n_{i\downarrow})+n_{i\uparrow}n_{i\downarrow}x]=\sum_l P_l x^l \ , \tag{1}$$

where $n_{i\sigma}$ is the number operator associated to the localized state at site i and spin σ, and the product over i runs through all the sites. P_l then projects out from a many-electron state the particular configurations each of which contains l doubly occupied sites. In terms of these projection operators we can rewrite the s-band Hubbard Hamiltonian as

$$H=\sum_{ij\sigma} t_{ij}a_{i\sigma}^{\dagger}a_{j\sigma}+U\sum_i n_{i\uparrow}n_{i\downarrow}=\sum_l P_l\left(\sum_{ij\sigma} t_{ij}a_{i\sigma}^{\dagger}a_{j\sigma}+U\sum_i n_{i\uparrow}n_{i\downarrow}\right)\sum_l P_l$$
$$=\sum_{l=0}^{\infty} P_l H P_l+\sum_{l=0}^{\infty} P_{l+1}HP_l+\sum_{l=1}^{\infty} P_{l-1}HP_l \ , \tag{2}$$

where

$$\sum_{l=0}^{\infty} P_l H P_l = P_0 \sum_{ij\sigma} t_{ij}(1-n_{i-\sigma}) a_{i\sigma}^{\dagger} a_{j\sigma}(1-n_{j-\sigma}) P_0 + \sum_{l=1}^{\infty} P_l \left\{ \sum_{ij\sigma} t_{ij}[(1-n_{i-\sigma}) a_{i\sigma}^{\dagger} a_{j\sigma}(1-n_{j-\sigma}) + n_{i-\sigma} a_{i\sigma}^{\dagger} a_{j\sigma} n_{j-\sigma}] + U \sum_i n_{i\uparrow} n_{i\downarrow} \right\} P_l \ , \tag{3a}$$

$$\sum_{l=0}^{\infty} P_{l+1} H P_l = \sum_{l=0}^{\infty} P_{l+1} \left\{ \sum_{ij\sigma} t_{ij} n_{i-\sigma} a_{i\sigma}^{\dagger} a_{j\sigma}(1-n_{j-\sigma}) \right\} P_l \ , \tag{3b}$$

$$\sum_{l=1}^{\infty} P_{l-1} H P_l = \sum_{l=1}^{\infty} P_{l-1} \left\{ \sum_{ij\sigma} t_{ij}(1-n_{i-\sigma}) a_{i\sigma}^{\dagger} a_{j\sigma} n_{j-\sigma} \right\} P_l \ . \tag{3c}$$

For convenience, we will choose a zero reference energy such that $t_{ii}=0$. Clearly, $P_l H P_l$ describes the dynamical properties of electrons within the l subband. The center of gravity of this subband locates at lU, and the subband has a finite width due to the intrasubband hoppings which do not alter the number of doubly occupied sites. $P_{l+1} H P_l$ and $P_{l-1} H P_l$, on the other hand, represent the intersubband hoppings from the l subband to the $l+1$ subband and the $l-1$ subband, respectively. Each intersubband hopping will change the energy of the system by an amount of the order U. At the strong-correlation limit $U >> t_{ij}$, the electron hopping can be treated as a perturbation. However, the hopping terms in $P_l H P_l$ contribute to the total energy linear in t_{ij}, while the leading term in the energy correction due to the hopping terms in $P_{l+1} H P_l$ and $P_{l-1} H P_l$ is proportional to t_{ij}^2/U. Consequently, a proper separation of the Hamiltonian H into an unperturbed part and a perturbation is rather crucial in the application of perturbation theory to the Hubbard model at the strong-correlation limit.

Many of the authors[13–16,18] who apply the perturbation theory to the Hubbard model start from

$$H = H(0) + H(1) \ , \tag{4}$$

where

$$H(0) = U \sum_i n_{i\uparrow} n_{i\downarrow} \ , \tag{4a}$$

$$H(1) = \sum_{ij\sigma} t_{ij} a_{i\sigma}^{\dagger} a_{j\sigma} \ . \tag{4b}$$

Since the eigenenergies of the unperturbed Hamiltonian $H(0)$ are highly degenerate, the perturbation expansions of Kato[20] and des Cloizeaux[21] have often been used. As both the intersubband and the intrasubband hoppings appear in $H(1)$, they are mixed in every higher-order term of the expansion series. Nevertheless, the energy corrections due to the intrasubband and the intersubband hoppings differ by a factor of the order W/U. Consequently, the resulting perturbation calculation becomes very tedious in practice.

The drawback of this scheme $H = H(0) + H(1)$ manifests itself when the band is not exactly half-filled. Then the lowest subband which has no doubly occupied site contains holes. It has been shown by Florencio and Chao[17] that in this case the intrasubband hopping can destroy the antiferromagnetic ordering in the strong-correlation regime. If we apply Kato's perturbation expansion to $H = H(0) + H(1)$, we have to collect all intrasubband hopping from terms of different orders and regroup them in order to fully account for the intrasubband hopping effect. Certainly this is an impossible task.

To further illustrate the different roles of intrasubband and intersubband hoppings in the strong-correlation regime, let us consider the simpler case of one electron per site. The ground state is an antiferromagnetic insulator[2–18] at the atomic limit. It is due to the virtual hopping of electrons and the coupling constant is proportional to t^2/U, where t is the nearest-neighbor hopping integral. This mechanism is just the same as $P_l H P_{l+1} H P_l$ with l referring to the lowest subband. On the other hand, let us create an electron-hole pair in the ground state, leaving one hole in the lowest subband and one electron in one of the higher subbands. Then both the electron and the hole can conduct electric current via the intrasubband hopping t. Consequently, the intrasubband hopping plays the dominating role in the Mott transition while the intersubband hopping is responsible for the magnetic ordering.

Recognizing the essential difference between these two types of electron hoppings, the starting point of the perturbation expansion in this paper is

$$H = H_0 + H_1 \ , \tag{5}$$

where

$$H_0 = \sum_{l=0}^{\infty} P_l H P_l \ , \tag{5a}$$

$$H_1 = \sum_{l=0}^{\infty} P_{l+1} H P_l + \sum_{l=1}^{\infty} P_{l-1} H P_l \ , \tag{5b}$$

and H_1 is treated as a perturbation. The unperturbed Hamiltonian H_0 at the atomic limit has been solved exactly by Klein.[22] Considering only two subbands, this scheme $H=H_0+H_1$ has been previously used by Florencio and Chao[17] and by Chao *et al.*[23]

In Sec. II we will use a canonical transformation to derive a new form of perturbation expansion. The close relation between this canonical perturbation expansion and the time-dependent perturbation theory will be demonstrated. The fact that linked-cluster theory should be employed in the future perturbation calculation then becomes obvious. For the Hubbard model at the strong-correlation regime, the infinite-expansion series can be expressed in analytical form. We then obtain an effective Hamiltonian, the explicit form of which to the eighth order will be given in Sec. III and in Appendix A. In Sec. IV we calculate the ground-state energy to the seventh order, of a half-filled band for the cases of a linear chain, a square lattice, and a simple cubic lattice. Our canonical perturbation expansion also gives the exact solution for a two-site Hubbard model, as shown in Appendix B. In Sec. V we compare our result with other works following by a concluding remark.

II. CANONICAL TRANSFORMATION

We assume that the eigenenergies $E_{i\mu}$, with $i=0,1,2,\ldots,$ and $\mu=1,2,\ldots,d_i$ of an unperturbed Hamiltonian H_0 satisfy the condition $|E_{i\mu}-E_{i\nu}| \ll |E_{i\omega}-E_{j\delta}|$, where $i\neq j$. That is, the eigenenergies of H_0 consists of disjointed regions in each of which the spectrum can be either continuous or semicontinuous.[24] The widths of such regions are much smaller than the separations between them. Let $|i\mu\rangle$ be the eigenstate corresponding to the eigenenergy $E_{i\mu}$. P_i and Q_i are, respectively, the projection operator and the eigenspace belonging to the eigenvalues $E_{i\mu}$ for all μ. We further assume that the perturbation H_1 has zero matrix elements between the eigenstates in same Q_i, i.e., $\langle i\mu|H_1|i\nu\rangle=0$. Then we can express the Hamiltonian $H=H_0+H_1$ in the general form

$$H_0=\sum_i P_i H P_i \ , \tag{6a}$$

$$H_1=\sum_{i,j}{}' P_i H P_j \ , \tag{6b}$$

where the primed sum excludes the terms with $i=j$.

Consider the canonical transformed effective Hamiltonian

$$\tilde{H}(\epsilon)=e^{-i\epsilon S}(H_0+\epsilon H_1)e^{i\epsilon S} \ , \tag{7}$$

where ϵ is formally treated as small except at the end of calculation we set $\epsilon=1$. If we expand the exponential function in power series and use the notation

$$[[A,B]]_n=[A,[A,[\cdots,[A,B]]\cdots]] \ ,$$

with n commutators at the right-hand side, then we can rewrite the effective Hamiltonian as

$$\tilde{H}(\epsilon)=H_0+\epsilon(H_1-i[S,H_0]) + \sum_{n=2}^{\infty}\frac{(-i\epsilon)^n}{n!}([[S,H_0]]_n+in[[S,H_1]]_{n-1}) \ . \tag{8}$$

We will search an operator S such that

$$H_1-i[S,H_0]=0 \ . \tag{9}$$

Substituting $[S,H_0]=-iH_1$ into (8), we obtain

$$\tilde{H}(\epsilon)=H_0+\sum_{n=2}^{\infty}\frac{(n-1)(-i)^{n-1}\epsilon^n}{n!}[[S,H_1]]_{n-1} \ . \tag{10}$$

To derive an expression for S, we can substitute (6a) and (6b) into (9) and then apply the projection operators P_j and P_k to (9) from both sides to get

$$P_jHP_k(1-\delta_{jk})+iP_jHP_j(P_jSP_k)-i(P_jSP_k)P_kHP_k=0 \ . \tag{11}$$

For $j\neq k$, the above equation reduces to

$$P_jHP_j(P_jSP_k)-(P_jSP_k)P_kHP_k=iP_jHP_k \ . \tag{12}$$

The operators $P_jHP_j=P_jH_0P_j$ and $P_kHP_k=P_kH_0P_k$ at the left-hand side will be approximated by their proper expectation values of the energy. From (6b) we see that the right-hand side of (12), $P_jHP_k=P_jH_1P_k$ represents the coupling between one state in the k eigenspace and one in the j eigenspace. P_jHP_j and P_kHP_k then correspond, respectively, to the energies of the final and the initial states which are coupled by P_jHP_k. Since $|E_{j\mu}-E_{j\nu}| \ll |E_{j\omega}-E_{k\delta}|$, P_jHP_j can be well approximated by E_j, where E_j is the mean energy of $E_{j\mu}$ over all μ. Hence we have

$$P_jSP_k=iP_jHP_k/(E_j-E_k) \quad \text{for } j\neq k \ . \tag{13}$$

If $j=k$, we can use (6a) to rewrite (12) as

$$[P_jH_0P_j,P_jSP_j]=0 \ . \tag{14}$$

The general solution is[25]

$$P_jSP_j=\sum_i P_izP_i \ , \tag{15}$$

where z is an arbitrary operator. To illustrate the effect of P_jSP_j, let us consider the basis $\{|\psi_j\rangle\}$ of H. Using the transformation (7) with $\epsilon=1$, $\{|\psi_j\rangle\}$ is transformed into a basis $\{|\tilde{\psi}_j\rangle=e^{-iS}|\psi_j\rangle\}$ of $\tilde{H}$. As P_jSP_j does not depend on H_1, we can now assume $H_1=0$ and so $P_jSP_k=0$ for $j\neq k$. Furthermore, we have

$$S=\sum_{jk}P_jSP_k=\sum_j P_jSP_j=\sum_j P_jZP_j \ ,$$

where Z is also an arbitrary operator. Since $[P_jZP_j,P_jH_0P_j]=0$, we have

$$\tilde{H}=\exp\left(-i\sum_j P_jZP_j\right)H_0\exp\left(i\sum_j P_jZP_j\right)=H_0 \ .$$

Therefore, $\{|\psi_j\rangle\}=\{|j\mu\rangle\}$ and

$$\{|\tilde{\psi}_j\rangle\}=\left\{\exp\left(-i\sum_k P_kZP_k\right)|j\mu\rangle\right\}$$

$$=\{\exp(-i\zeta_{j\mu})|j\mu\rangle\} \ ,$$

where $\zeta_{j\mu}$ is the eigenvalue of P_jZP_j with respect to the state $|j\mu\rangle$ because P_jZP_j and $P_jH_0P_j$ commute. The effect of the P_jSP_j terms in the canonical transformation is thus simply to add a phase factor to each eigenstate of the basis. Since the basis can be uniquely defined only within a phase factor, we can choose a constant phase factor for the entire basis. Hence we have

$$P_jSP_j=\gamma P_j \ , \tag{16}$$

where γ is an arbitrary real constant.

The justification of (16) manifests itself in the close relation between the canonical perturbation expansion and the time-dependent perturbation theory. Let us formally define the "interaction representation" for the operator S in (7) as

$$S(\tau)=\exp(iH_0\tau)S\exp(-iH_0\tau) \ . \tag{17}$$

Applying the projection operators from both sides, we obtain

$$P_jS(\tau)P_k=P_j\left(\prod_\mu\exp(iP_\mu HP_\mu\tau)\right)$$

$$\times S\left(\prod_\nu\exp(-iP_\nu HP_\nu\tau)\right)P_k$$

$$=\exp(iP_jHP_j\tau)P_jSP_k\exp(-iP_kHP_k\tau)$$

$$=\exp(iH_0\tau)P_jSP_k\exp(-iH_0\tau) \ . \tag{18}$$

It satisfies the "equation of motion"

$$i\frac{d}{d\tau}P_jS(\tau)P_k=[P_jS(\tau)P_k,H_0](1-\delta_{jk}) \ . \tag{19}$$

We can also define the perturbation in the interaction representation as

$$H_1(\tau)=\exp(iH_0\tau)H_1\exp(-iH_0\tau) \ . \tag{20}$$

Then, by applying the projection operators to (9) from both sides and using (20), we get

$$P_jH_1(\tau)P_k(1-\delta_{jk})-i[P_jS(\tau)P_k,H_0]=0 \ .$$

Therefore, (19) becomes

$$\frac{d}{d\tau}P_jS(\tau)P_k=-P_jH_1(\tau)P_k(1-\delta_{jk}) \ , \tag{21}$$

which has the solution

$$P_jS(\tau)P_k=-\int_{-\infty}^{\tau}P_jH_1(\tau)P_k\,d\tau \quad \text{for } j\neq k \tag{22a}$$

and

$$P_jS(\tau)P_j=P_jS(\tau=0)P_j=P_jSP_j=\sum_i P_izP_i \ . \tag{22b}$$

If we denote $\bar{S}=\sum_{j,k}{}' P_jSP_k$ and $\bar{S}(\tau)=\exp(iH_0\tau)\bar{S}\exp(-iH_0\tau)$, (22a) yields the relation

$$\bar{S}=\bar{S}(0)=-\int_{-\infty}^{0}H_1(\tau)\,d\tau \ . \tag{23}$$

It is well known in the time-dependent perturbation theory that the time-development operator is defined as

$$U(0,-\infty)=T\exp\left(-i\int_{-\infty}^{0}H_1(\tau)\,d\tau\right) \ .$$

Therefore, we have $U(0,-\infty)=Te^{i\bar{S}}$, where T is the time-ordering operator. Note that $U(0,-\infty)$ is a function of $\bar{S}$ instead of S. Since $\bar{S}$ does not contain P_jSP_j, P_jSP_j thus plays no role in the perturbation expansion.

Using (6b), (13), and (16), and $\sum_j P_j=1$, the commutators in (10) can be expressed as

$$[[S,H_1]]_n=\left[\left[\sum_j P_jSP_j,H_1\right]\right]_n+\left[\left[\sum_{jk}{}' P_jSP_k,H_1\right]\right]_n=[[\gamma,H_1]]_n+\left[\left[\sum_{jk}{}' P_jSP_k,H_1\right]\right]_n$$

$$=\left[\left[\sum_{jk}{}' P_jSP_k,-i\sum_{\mu\nu}{}'(E_\mu-E_\nu)P_\mu SP_\nu\right]\right]_n \ .$$

By mathematical induction, we arrive at the general formula

$$[[S,H_1]]_n = i(-1)^{n-1} \sum_{\text{all } k_m}{}'' \left[\sum_{j=0}^{n+1} \frac{(-1)^j(n+1)!}{j!(n+1-j)!} E_{k_{j+1}}\right] P_{k_1} S P_{k_2} S \cdots S P_{k_{n+2}} \ , \tag{24}$$

where the double-primed summation is restricted to $k_m \neq k_{m+1}$ for all m. Substituting (24) into (10), we have the effective Hamiltonian as

$$\tilde{H}(\epsilon) = H_0 - \sum_{n=2}^{\infty} \frac{(n-1)(i\epsilon)^n}{n!} \sum_{\text{all } k_m}{}'' \left[\sum_{j=0}^{n} \frac{(-1)^j n!}{j!(n-j)!} E_{k_{j+1}}\right] P_{k_1} S P_{k_2} S \cdots S P_{k_{n+1}} \ . \tag{25}$$

III. EFFECTIVE HAMILTONIAN FOR THE s-BAND HUBBARD MODEL

In this section we will apply (25) to the s-band Hubbard model. From Eqs. (3a)–(3c) and (5a)–(5b), we see that H_0 consists of separated subbands and H_1 couples only the adjacent subbands. Therefore, in (25) we have $k_{m+1} = k_m \pm 1$. Let us define $u_{m-1} = k_m - k_1$ for $m \geq 2$ and $u_0 = 0$. Since the centers of gravity of two adjacent subbands are separated by the intraatomic correlation energy U, hence $E_{k_{m+1}} - E_{k_m} = (u_m - u_{m-1})U = \pm U$. Using (13) and the relation

$$\begin{aligned} \sum_{j=0}^{n} \frac{(-1)^j n!}{j!(n-j)!} E_{k_{j+1}} &= \sum_{j=1}^{n} \frac{(-1)^j (n-1)!}{(j-1)!(n-j)!} (E_{k_{j+1}} - E_{k_j}) \\ &= \sum_{j=1}^{n} \frac{(-1)^j (n-1)!}{(j-1)!(n-j)!} (u_j - u_{j-1}) U \end{aligned} \tag{26}$$

the effective Hamiltonian $\tilde{H} = \tilde{H}(\epsilon = 1)$ of (25) can be rewritten

$$\begin{aligned} \tilde{H} = H_0 + \sum_{n=2}^{\infty} \frac{n-1}{n! U^{n-1}} \sum_{k,\{u_j\}} &\left[\sum_{j=1}^{n} \frac{(-1)^j (n-1)!}{(j-1)!(n-j)!} (u_{j-1} - u_j)\right] \left[\prod_{j=1}^{n} (u_j - u_{j-1})\right] \\ &\times P_k H P_{k+u_1} H P_{k+u_2} H \cdots H P_{k+u_n} \ . \end{aligned} \tag{27}$$

Note that in the above equation we have $u_j - u_{j-1} = \pm 1$. We will use the notations

$$C(u_1, u_2, \ldots, u_n) = \frac{-n+1}{n!} \sum_{j=1}^{n} \frac{(-1)^j (n-1)!}{(j-1)!(n-j)!} (u_j - u_{j-1}) \left[\prod_{j=1}^{n} (u_j - u_{j-1})\right] \tag{28}$$

and

$$\langle k, u_1, u_2, \ldots, u_n \rangle = P_k H P_{k+u_1} H P_{k+u_2} H \cdots H P_{k+u_n} \ . \tag{29}$$

Then the effective Hamiltonian has the final simple form

$$\tilde{H} = H_0 + \sum_{n=2}^{\infty} u^{-n+1} \sum_{k,\{u_j\}} C(u_1, u_2, \ldots, u_n) \langle k, u_1, u_2, \ldots, u_n \rangle \ . \tag{30}$$

Since $u_j - u_{j-1} = \pm 1$, all allowed channels $\langle k, u_1, u_2, \ldots, u_n \rangle$ for given k and the coefficients $C(u_1, u_2, \ldots, u_n)$ of (28) can be generated on computer to as large number n as desired. Using the symmetry properties

$$C(-u_1, -u_2, \ldots, -u_n) = (-1)^{n+1} C(u_1, u_2, \ldots, u_n) \ , \tag{31}$$

the computation effort can be reduced by a factor $\frac{1}{2}$. The explicit expressions for $\tilde{H}^{(n)}$ with $n \leq 8$ are given by (A3)–(A9) in Appendix A.

Let us consider the case that the bare energy band is no more than half filled. Then for the ground state all subbands except the lowest one (the P_0 subband) are empty. If we are interested in the ground-state energy correction, we need only those channels $\langle k, u_1, u_2, \ldots, u_n \rangle$ with $k = u_n = 0$. Starting from the lowest subband, an odd number of intersubband hoppings $P_k H P_{k+u_1} H \cdots H P_{k+u_n}$ can never generate a final state with only the lowest subband occupied. Therefore, the terms in (30) with n equal to odd integers do not contribute to the ground-state energy correction. To the seventh order, the effective Hamiltonian can then be expressed by selecting the proper terms from (A3), (A5), and (A7) as

$$P_0\tilde{H}P_0 = P_0H_0P_0 - U^{-1}\langle 0,1,0\rangle + \tfrac{1}{2}U^{-3}(2\langle 0,1,0,1,0\rangle - \langle 0,1,2,1,0\rangle) - \tfrac{1}{72}U^{-5}(16\langle ,1,0,1,0,1,0\rangle$$
$$+ \langle 0,1,0,1,2,1,0\rangle + \langle 0,1,2,1,0,1,0\rangle - 14\langle 0,1,2,1,2,1,0\rangle + 6\langle 0,1,2,3,2,1,0\rangle) \quad . \tag{32}$$

We should point out that the above equation contains errors from two sources. First, the approximated solution (13) generally introduces errors of order $(t/U)^m$, $m \geq 3$, in $\tilde{H}$. Further, projection to $P_j\tilde{H}P_j$ introduces errors of order $(t/U)^m$, $m \geq 4$.

IV. GROUND-STATE ENERGY

From the relation $U(0,-\infty) = T\exp(i\bar{S})$ derived in Sec. II, one would expect that the linked-cluster theory should be incorporated to (32) in our energy calculation. The validity of the linked-cluster expansion in the canonical perturbation theory has been proved by Klein.[26] The proof is for the very general case, and applies to our problem with $P_jSP_j = \gamma P_j$.

Using the linked diagrammatic expansion, the operators $\langle 0,u_1,u_2,\ldots,0\rangle$ in (32) can be evaluated without difficulty. For one electron per site, their explicit expression are given by (A16)–(A23) in Appendix A. These operators can be built up from two fundamental elements $t_{ij}^2 \nu_{i-\sigma}\nu_{j\sigma}$ and $t_{ij}^2 S_i^{\sigma}S_j^{-\sigma}$, where $\nu_{i\sigma} = (1-n_{i-\sigma})n_{i\sigma}$ and $S_i^{\sigma} = a_{i\sigma}^{\dagger}a_{i-\sigma}$. These two fundamental elements correspond to the longitudinal (electron-virtual-hopping) and the transverse (double-spin-flip) components of the Heisenberg exchange interaction $\vec{S}_i \cdot \vec{S}_j$. If we restrict ourselves to the nearest-neighbor hopping, it is not difficult to find out that $\langle 0,1,0\rangle$ contains the nearest neighbor $\vec{S}_i \cdot \vec{S}_j$, $\langle 0,1,0,1,0\rangle$ and $\langle 0,1,2,1,0\rangle$ contain the nearest and the next-nearest neighbor $\vec{S}_i \cdot \vec{S}_j$, while $\langle 0,1,0,1,0,1,0\rangle$, $\langle 0,1,0,1,2,1,0\rangle$, $\langle 0,1,2,1,0,1,0\rangle$, $\langle 0,1,2,1,2,1,0\rangle$, and $\langle 0,1,2,3,2,1,0\rangle$ contain the nearest, and next-nearest, and the third-nearest neighbor $\vec{S}_i \cdot \vec{S}_j$.

The effective Hamiltonian (32) to the second order has been investigated in detail,[23] indicating that the ground state of a strongly correlated half-filled narrow band is antiferromagnetic. Strictly speaking, the ground state is certainly not the pure Néel state. To find the exact ground state is outside the scope of the present paper. Nevertheless, Oguchi[27] has shown that the correction due to spin-wave interactions in a Heisenberg antiferromagnet is negligibly small for practical purpose. Consequently, we will substitute (A16)–(A23) into (32) to calculate the energy per electron $E = \langle P_0\tilde{H}P_0\rangle/N$ of the antiferromagnetic (Néel) ground state to the seventh order.

In the regime of very strong correlation, we can retain only the nearest-neighbor hopping integral t. Then all the t_{ij}'s in (A16)–(A23) are constant t, and the calculation of E reduces to simple countings of linked diagrams. We will restrict our calculations to a linear chain, a square lattice and a simple cubic lattice. For these cases, the counting of linked diagrams corresponding to (A16)–(A23) can be readily done without difficulty. Let Z be the coordination number and $W = 2Zt$ be the bare bandwidth. If $N\eta(0,u_1,u_2,\ldots,0)$ represents the number of linked diagrams associated to the $\langle 0,u_1,u_2,\ldots,0\rangle$ term in (32), then we have

$$\eta(0,1,0) = Z \quad ,$$
$$\eta(0,1,0,1,0) = 4[Z + Z(Z-1)] \quad ,$$
$$\eta(0,1,2,1,0) = 2Z(Z-2) \quad ,$$
$$\eta(0,1,0,1,0,1,0) = 8[2Z + 6Z(Z-1) + 3Z(Z-1)^2 + Z(Z-1)(Z-2)] \quad ,$$
$$\eta(0,1,0,1,2,1,0) = 8[Z(Z-1)^2 + 6Z(Z-2) + 2Z(Z-2)^2] = \eta(0,1,2,1,0,1,0) \quad ,$$
$$\eta(0,1,2,1,2,1,0) = 8[2Z(Z-1)^2 + 4Z(Z-2) + Z(Z-1)(Z-2)] \quad ,$$

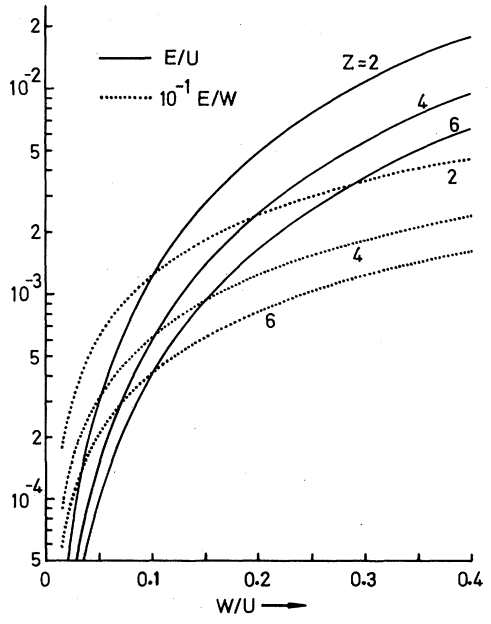

FIG. 1. Ground-state energy per electron E/U and E/W as functions of W/U, for a linear chain ($Z=2$), a sqaure lattice ($Z=4$), and a simple cubic lattice ($Z=6$).

and

$$\eta(0,1,2,3,2,1,0) = 24Z(Z-1)(Z-2) \ .$$

The ground-state energy per electron is then obtained from (32) as

$$E = -\frac{U}{4Z}\left(\frac{W}{U}\right)^2 + \frac{U(3Z+2)}{16Z^3}\left(\frac{W}{U}\right)^4 - \frac{U(23Z^2-34Z+51)}{288Z^5}\left(\frac{W}{U}\right)^6 + O\left(\left(\frac{W}{U}\right)^8\right) \ . \tag{33}$$

In Fig. 1, we present the results of E/U and E/W as functions of W/U.

For the special case of a half-filled two-site Hubbard model, the infinite perturbation series in (27) can be summed up exactly. The basis consists of only six two-electron states, and we find that the effective Hamiltonian $\tilde{H}$ of (27) can be diagonalized analytically. The result, as shown in Appendix B, agrees with the exact solution. We should remind the reader that (27) is derived from (25) which is obtained with a proper choice of $\sum_i P_i z P_i$ in (15), namely, the choice of (16). Therefore, the fact that (18) yields the exact solution is another indirect proof that (16) is a reasonable choice.

V. DISCUSSION

The s-band Hubbard model at the atomic limit has been extensively investigated because when $U >> W$, the perturbation theory is valid. Kato's perturbation expansion[20] has been applied to (4), (4a), and (4b) in most of these works. Let us first summarize Kato's theory. Assume that $H(0)$ has a discrete m-fold degenerate level $E_\mu(0)$. We designate the associated projection operators as $P_\mu(0)$. As the perturbation $H(1)$ is turned on, $E_\mu(0)$ and $P_\mu(0)$ evolve, respectively, into E_μ and P_μ. Kato has derived the perturbation series

$$HP_\mu = E_\mu(0)P_\mu + \sum_{n=1}^{\infty}(-1)^{n-1}\sum_{(k_1+k_2+\cdots+k_{n+1}=n-1)} D^{k_1}H(1)D^{k_2}H(1)\cdots H(1)D^{k_{n+1}} \ , \tag{34}$$

where $D^0 = -P_\mu(0)$ and

$$D^k = \{[1-P_\mu(0)]/[E_\mu(0)-H(0)]\}^k$$

for $k \geq 1$.

We note that $H(1)$ consists of both the intrasubband and the intersubband hoppings. Since $1-P_\mu(0)$ includes all the subbands except the μth, a term in (34) containing a factor $D^{k_1}H(1)D^{k_2}$ with $k_1, k_2 \neq 0$ has both the intrasubband hopping $P_\nu(0)H(1)P_\nu(0)$ and the intersubband hopping $P_\omega(0)H(1)P_\nu(0)$, where $\nu \neq \mu$, $\omega \neq \mu$, and $\omega \neq \nu$. On the other hand, $D^0H(1)D^0$ represents only the intrasubband hopping. Two complications are then introduced in the computation. The intrasubband hopping opens lots of channels and thus largely increases the number of diagrams to be evaluated. One finds such additional terms in Eq. (2.17) of Klein and Seitz.[14] As far as the intersubband hopping, $P_\omega(0)H(1)P_\nu(0)$ with $\omega \neq \nu$, is concerned, the corresponding energy denominator appeared in (34) is $1/[E_\mu(0)-E_\omega(0)]$ or $1/[E_\mu(0)-E_\nu(0)]$ instead of $1/[E_\omega(0)-E_\nu(0)] = \pm 1/U$. Consequently, a simple form as (28)–(30) cannot be derived from (34). Klein and Seitz[28] have tried to avoid this complication by using (5), (5a), and (5b). However, they only apply the conventional second-order perturbation theory to a linear chain. For higher-order corrections or for higher-dimensional systems the conventional perturbation series is too complicated to be solved.

In our canonical perturbation expansion we discover that $P_j S P_j$ cannot be determined uniquely, because it corresponds to adding a phase factor to each unperturbed eigenstate of a complete basis of H_0. Nevertheless, we have shown that the choice of these phase factors has no effect on the final result. For convenience, we have chosen a constant phase factor corresponding to the solution (16).

Most of the perturbation calculations on the Hubbard model are performed for the special case of one electron per site, in order to eliminate the complication caused by the intrasubband hopping as a perturbation. Since we have separated the intrasubband and the intersubband hoppings, and the intrasubband hopping is part of the unperturbed Hamiltonian, we can apply our result to any value of electron density. Some work along this line including higher-order perturbation correction will be reported in the future.

Recently, Takahashi[18] has applied Kato's theory to the Hubbard model and obtains the ground-state energy per electron

$$E = -\frac{1.313U}{4Z}\left(\frac{W}{U}\right)^2 + \frac{0.665(3Z+2)U}{16Z^3}\left(\frac{W}{U}\right)^4 \tag{35}$$

for the linear chain,

$$E=-\frac{1.16U}{4Z}\left(\frac{W}{U}\right)^2+\frac{0.62(3Z+2)}{16Z^3}\left(\frac{W}{U}\right)^4 \tag{36}$$

for the square lattice, and

$$E=-\frac{1.10U}{4Z}\left(\frac{W}{U}\right)^2+\frac{0.55(3Z+2)}{16Z^3}\left(\frac{W}{U}\right)^4 \tag{37}$$

for the simple cubic lattice. Takahashi's results are exact through 4th order. Hence, our expansion (33) works better for high-dimensional systems than the lower-dimensional ones.

Finally, we should point out that the usefulness of (25) is not restricted to the Hubbard model. Any system with effective one-electron orbital energies satisfying the conditions[24] specified at the beginning of Sec. II can be tackled with this approach. For example, (25) can be used in the studies of magnetic resonances which have equally spaced energy levels.

APPENDIX A

Let us rewrite the effective Hamiltonian (27) as

$$\tilde{H}=H_0+\sum_{n=2}^{\infty}\tilde{H}^{(n)} , \tag{A1}$$

where

$$\tilde{H}^{(n)}=U^{-n+1}\sum_{k,\{u_j\}}C(u_1,u_2,\ldots,u_n)\langle k,u_1,u_2,\ldots,u_n\rangle . \tag{A2}$$

Since $u_j-u_{j-1}=\pm1$, we can easily generate by computer the following results (the dots represent image terms):

$$\tilde{H}^{(2)}=-U^{-1}\sum_k(\langle k,1,0\rangle+\cdots) , \tag{A3}$$

$$\tilde{H}^{(3)}=\tfrac{2}{3}U^{-2}\sum_k(\langle k,1,2,1\rangle-2\langle k,1,0,1\rangle+\langle k,1,0,-1\rangle+\cdots) , \tag{A4}$$

$$\begin{aligned}\tilde{H}^{(4)}=-\tfrac{1}{4}U^{-3}\sum_k(&\langle k,1,2,3,2\rangle-3\langle k,1,2,1,2\rangle+2\langle k,1,2,1,0\rangle+3\langle k,1,0,1,2\rangle\\&-4\langle k,1,0,1,0\rangle+\langle k,1,0,-1,-2\rangle+\cdots) ,\end{aligned} \tag{A5}$$

$$\begin{aligned}\tilde{H}^{(5)}=\tfrac{1}{15}U^{-4}\sum_k(&\langle k,1,2,3,4,3\rangle-4\langle k,1,2,3,2,3\rangle+3\langle k,1,2,3,2,1\rangle+6\langle k,1,2,1,2,3\rangle\\&-7\langle k,1,2,1,2,1\rangle-2\langle k,1,2,1,0,1\rangle+3\langle k,1,2,1,0,-1\rangle-4\langle k,1,0,1,2,3\rangle\\&+3\langle k,1,0,1,2,1\rangle+8\langle k,1,0,1,0,1\rangle-7\langle k,1,0,1,0,-1\rangle-2\langle k,1,0,-1,0,1\rangle+3\langle k,1,0,-1,0,-1\rangle\\&-2\langle k,1,0,-1,-2,-1\rangle+\langle k,1,0,-1,-2,-3\rangle+\cdots) ,\end{aligned} \tag{A6}$$

$$\begin{aligned}\tilde{H}^{(6)}=-\tfrac{1}{72}U^{-5}\sum_k(&\langle k,1,2,3,4,5,4\rangle-5\langle k,1,2,3,4,3,4\rangle+4\langle k,1,2,3,4,3,2\rangle+10\langle k,1,2,3,2,3,4\rangle\\&-11\langle k,1,2,3,2,3,2\rangle-5\langle k,1,2,3,2,1,2\rangle+6\langle k,1,2,3,2,1,0\rangle-10\langle k,1,2,1,2,3,4\rangle\\&+9\langle k,1,2,1,2,3,2\rangle+15\langle k,1,2,1,2,1,2\rangle-14\langle k,1,2,1,2,1,0\rangle+\langle k,1,2,1,0,1,0\rangle\\&-5\langle k,1,2,1,0,-1,0\rangle+4\langle k,1,2,1,0,-1,-2\rangle+5\langle k,1,0,1,2,3,4\rangle-6\langle k,1,0,1,2,3,2\rangle\\&+\langle k,1,0,1,2,1,0\rangle-15\langle k,1,0,1,0,1,2\rangle+16\langle k,1,0,1,0,1,0\rangle\\&+10\langle k,1,0,1,0,-1,0\rangle-11\langle k,1,0,1,0,-1,-2\rangle+5\langle k,1,0,-1,0,1,2\rangle-4\langle k,1,0,-1,0,1,0\rangle\\&-10\langle k,1,0,-1,0,-1,0\rangle+9\langle k,1,0,-1,-1,-2\rangle+5\langle k,1,0,-1,-2,-1,0\rangle\\&-6\langle k,1,0,-1,-2,-1,-2\rangle+\langle k,1,0,-1,-2,-3,-4\rangle+\cdots) ,\end{aligned} \tag{A7}$$

$$\tilde{H}^{(7)}=\frac{1}{420}U^{-6}\sum_k(\langle k,1,2,3,4,5,6,5\rangle-6\langle k,1,2,3,4,5,4,5\rangle+5\langle k,1,2,3,4,5,4,3\rangle+15\langle k,1,2,3,4,3,4,5\rangle$$
$$-16\langle k,1,2,3,4,3,4,3\rangle-9\langle k,1,2,3,4,3,2,3\rangle+10\langle k,1,2,3,4,3,2,1\rangle-20\langle k,1,2,3,2,3,4,5\rangle$$
$$+19\langle k,1,2,3,2,3,4,3\rangle+26\langle k,1,2,3,2,3,2,3\rangle-25\langle k,1,2,3,2,3,2,1\rangle+5\langle k,1,2,3,2,1,2,3\rangle$$
$$-4\langle k,1,2,3,2,1,2,1\rangle-11\langle k,1,2,3,2,1,0,1\rangle+10\langle k,1,2,3,2,1,0,-1\rangle+15\langle k,1,2,1,2,3,4,5\rangle$$
$$-16\langle k,1,2,1,2,3,4,3\rangle-9\langle k,1,2,1,2,3,2,3\rangle+10\langle k,1,2,1,2,3,2,1\rangle-30\langle k,1,2,1,2,1,2,3\rangle$$
$$+31\langle k,1,2,1,2,1,2,1\rangle+24\langle k,1,2,1,2,1,0,1\rangle-25\langle k,1,2,1,2,1,0,-1\rangle+5\langle k,1,2,1,0,1,2,3\rangle$$
$$-4\langle k,1,2,1,0,1,2,1\rangle-11\langle k,1,2,1,0,1,0,1\rangle+10\langle k,1,2,1,0,1,0,-1\rangle+10\langle k,1,2,1,0,-1,0,1\rangle$$
$$-11\langle k,1,2,1,0,-1,0,-1\rangle-4\langle k,1,2,1,0,-1,-2,-1\rangle+5\langle k,1,2,1,0,-1,-2,-3\rangle-6\langle k,1,0,1,2,3,4,5\rangle$$
$$+5\langle k,1,0,1,2,3,4,3\rangle+12\langle k,1,0,1,2,3,2,3\rangle-11\langle k,1,0,1,2,3,2,1\rangle-9\langle k,1,0,1,2,1,2,3\rangle$$
$$+10\langle k,1,0,1,2,1,2,1\rangle+3\langle k,1,0,1,2,1,0,1\rangle-4\langle k,1,0,1,2,1,0,-1\rangle+26\langle k,1,0,1,0,1,2,3\rangle$$
$$-25\langle k,1,0,1,0,1,2,1\rangle-32\langle k,1,0,1,0,1,0,1\rangle+31\langle k,1,0,1,0,1,0,-1\rangle-11\langle k,1,0,1,0,-1,0,1\rangle$$
$$+10\langle k,1,0,1,0,-1,0,-1\rangle+17\langle k,1,0,1,0,-1,-2,-1\rangle$$
$$-16\langle k,1,0,1,0,-1,-2,-3\rangle-9\langle k,1,0,-1,0,1,2,3\rangle$$
$$+10\langle k,1,0,-1,0,1,2,1\rangle+3\langle k,1,0,-1,0,1,0,1\rangle-4\langle k,1,0,-1,0,1,0,-1\rangle$$
$$+24\langle k,1,0,-1,0,-1,0,1\rangle-25\langle k,1,0,-1,0,-1,0,-1\rangle-16\langle k,1,0,-1,0,-1,-2,-1\rangle$$
$$+19\langle k,1,0,-1,0,-1,-2,-3\rangle-11\langle k,1,0,-1,-2,-1,0,1\rangle+10\langle k,1,0,-1,-2,-1,0,-1\rangle$$
$$+17\langle k,1,0,-1,-2,-1,-2,-1\rangle-16\langle k,1,0,-1,-2,-1,-2,-3\rangle$$
$$-4\langle k,1,0,-1,-2,-3,-2,-1\rangle+5\langle k,1,0,-1,-2,-3,-2,-3\rangle$$
$$-2\langle k,1,0,-1,-2,-3,-4,-3\rangle+\langle k,1,0,-1,-2,-3,-4,-5\rangle+\cdots),\tag{A8}$$

$$\tilde{H}^{(8)}=-\frac{1}{2880}U^{-7}\sum_k(\langle k,1,2,3,4,5,6,7,6\rangle-7\langle k,1,2,3,4,5,6,5,6\rangle+6\langle k,1,2,3,4,5,6,5,4\rangle+21\langle k,1,2,3,4,5,4,5,6\rangle$$
$$-22\langle k,1,2,3,4,5,4,5,4\rangle-14\langle k,1,2,3,4,5,4,3,4\rangle+15\langle k,1,2,3,4,5,4,3,2\rangle-35\langle k,1,2,3,4,3,4,5,6\rangle$$
$$+34\langle k,1,2,3,4,3,4,5,4\rangle+42\langle k,1,2,3,4,3,4,3,4\rangle-41\langle k,1,2,3,4,3,4,3,2\rangle+14\langle k,1,2,3,4,3,2,3,4\rangle$$
$$-13\langle k,1,2,3,4,3,2,3,2\rangle-21\langle k,1,2,3,4,3,2,1,2\rangle+20\langle k,1,2,3,4,3,2,1,0\rangle+35\langle k,1,2,3,2,3,4,5,6\rangle$$
$$-36\langle k,1,2,3,2,3,4,5,4\rangle-28\langle k,1,2,3,2,3,4,3,4\rangle+29\langle k,1,2,3,2,3,4,3,2\rangle-56\langle k,1,2,3,2,3,2,3,4\rangle$$
$$+57\langle k,1,2,3,2,3,2,3,2\rangle+49\langle k,1,2,3,2,3,2,1,2\rangle-50\langle k,1,2,3,2,3,2,1,0\rangle+\langle k,1,2,3,2,1,2,3,2\rangle$$
$$-7\langle k,1,2,3,2,1,2,1,2\rangle+6\langle k,1,2,3,2,1,2,1,0\rangle+21\langle k,1,2,3,2,1,0,1,2\rangle-22\langle k,1,2,3,2,1,0,1,0\rangle$$
$$-14\langle k,1,2,3,2,1,0,-1,0\rangle+15\langle k,1,2,3,2,1,0,-1,-2\rangle-21\langle k,1,2,1,2,3,4,5,6\rangle+20\langle k,1,2,1,2,3,4,5,4\rangle$$
$$+28\langle k,1,2,1,2,3,4,3,4\rangle-27\langle k,1,2,1,2,3,4,3,2\rangle+\langle k,1,2,1,2,3,2,3,2\rangle-7\langle k,1,2,1,2,3,2,1,2\rangle$$
$$+6\langle k,1,2,1,2,3,2,1,0\rangle+56\langle k,1,2,1,2,1,2,3,4\rangle-55\langle k,1,2,1,2,1,2,3,2\rangle-63\langle k,1,2,1,2,1,2,1,2\rangle$$
$$+62\langle k,1,2,1,2,1,2,1,0\rangle-35\langle k,1,2,1,2,1,0,1,2\rangle+34\langle k,1,2,1,2,1,0,1,0\rangle+42\langle k,1,2,1,2,1,0,-1,0\rangle$$
$$-41\langle k,1,2,1,2,1,0,-1,-2\rangle-14\langle k,1,0,1,0,1,2,3,4\rangle+15\langle k,1,2,1,0,1,2,3,2\rangle$$
$$+7\langle k,1,2,1,0,1,2,1,2\rangle-8\langle k,1,2,1,0,1,2,1,0\rangle$$
$$+35\langle k,1,2,1,0,1,0,1,2\rangle-36\langle k,1,2,1,0,1,0,1,0\rangle-28\langle k,1,2,1,0,1,0,-1,0\rangle$$

$$
\begin{aligned}
&+29\langle k,1,2,1,0,1,0,-1,-2\rangle-21\langle k,1,2,1,0,-1,0,1,2\rangle\\
&+20\langle k,1,2,1,0,-1,0,1,0\rangle+28\langle k,1,2,1,0,-1,0,-1,0\rangle\\
&-27\langle k,1,2,1,0,-1,0,-1,-2\rangle+\langle k,1,2,1,0,-1,-2,-1,-2\rangle-7\langle k,1,2,1,0,-1,-2,-3,-2\rangle\\
&+6\langle k,1,2,1,0,-1,-2,-3,-4\rangle+7\langle k,1,0,1,2,3,4,5,6\rangle-8\langle k,1,0,1,2,3,4,5,4\rangle+\langle k,1,0,1,2,3,4,3,2\rangle\\
&-28\langle k,1,0,1,2,3,2,3,4\rangle\\
&+29\langle k,1,0,1,2,3,2,3,2\rangle+21\langle k,1,0,1,2,3,2,1,2\rangle-22\langle k,1,0,1,2,3,2,1,0\rangle+28\langle k,1,0,1,2,1,2,3,4\rangle\\
&-27\langle k,1,0,1,2,1,2,3,2\rangle-35\langle k,1,0,1,2,1,2,1,2\rangle+34\langle k,1,0,1,2,1,2,1,0\rangle-7\langle k,1,0,1,2,1,0,1,2\rangle\\
&+6\langle k,1,0,1,2,1,0,1,0\rangle+14\langle k,1,0,1,2,1,0,-1,0\rangle-13\langle k,1,0,1,2,1,0,-1,-2\rangle-42\langle k,1,0,1,0,1,2,3,4\rangle\\
&+43\langle k,1,0,1,0,1,2,3,2\rangle+35\langle k,1,0,1,0,1,2,1,2\rangle-36\langle k,1,0,1,0,1,2,1,0\rangle+63\langle k,1,0,1,0,1,0,1,2\rangle\\
&-64\langle k,1,0,1,0,1,0,1,0\rangle-56\langle k,1,0,1,0,1,0,-1,0\rangle+57\langle k,1,0,1,0,1,0,-1-2\rangle+7\langle k,1,0,1,0,-1,0,1,2\rangle\\
&-8\langle k,1,0,1,0,-1,0,1,0\rangle+\langle k,1,0,1,0,-1,0,-1,-2\rangle-28\langle k,1,0,1,0,-1,-2,-1,0\rangle\\
&+29\langle k,1,0,1,0,-1,-2,-1,-2\rangle\\
&+21\langle k,1,0,1,0,-1,-2,-3,-2\rangle-22\langle k,1,0,1,0,-1,-2,-3,-4\rangle+14\langle k,1,0,-1,0,1,2,3,4\rangle\\
&-13\langle k,1,0,-1,0,1,2,3,4\rangle-21\langle k,1,0,-1,0,1,2,1,2\rangle+20\langle k,1,0,-1,0,1,2,1,0\rangle\\
&+7\langle k,1,0,-1,0,1,0,1,2\rangle-8\langle k,1,0,-1,0,1,0,1,0\rangle\\
&+\langle k,1,0,-1,0,1,0,-1,-2\rangle-49\langle k,1,0,-1,0,-1,0,1,2\rangle+48\langle k,1,0,-1,0,-1,0,1,0\rangle\\
&+56\langle k,1,0,-1,0,-1,0,-1,0\rangle-55\langle k,1,0,-1,0,-1,0,-1,-2\rangle+28\langle k,1,0,-1,0,-1,-2,-1,0\rangle\\
&-27\langle k,1,0,-1,0,-1,-2,-1,-2\rangle-35\langle k,1,0,-1,0,-1,-2,-3,-2\rangle\\
&+34\langle k,1,0,-1,0,-1,-2,-3,-4\rangle+21\langle k,1,0,-1,-2,-1,0,1,2\rangle-22\langle k,1,0,-1,-2,-1,0,1,0\rangle\\
&-14\langle k,1,0,-1,-2,-1,0,-1,0\rangle+15\langle k,1,0,-1,-2,-1,0,-1,-2\rangle-42\langle k,1,0,-1,-2,-1,-2,-1,0\rangle\\
&+43\langle k,1,0,-1,-2,-1,-2,-1,-2\rangle+35\langle k,1,0,-1,-2,-1,-2,-3,-2\rangle\\
&-36\langle k,1,0,-1,-2,-1,-2,-3,-4\rangle+14\langle k,1,0,-1,-2,-3,-2,-1,0\rangle\\
&-13\langle k,1,0,-1,-2,-3,-2,-1,-2\rangle-21\langle k,1,0,-1,-2,-3,-2,-3,-2\rangle\\
&+20\langle k,1,0,-1,-2,-3,-2,-3,-4\rangle+7\langle k,1,0,-1,-2,-3,-4,-3,-2\rangle\\
&-8\langle k,1,0,-1,-2,-3,-4,-3,-4\rangle+\langle k,1,0,-1,-2,-3,-4,-5,-6\rangle+\cdots)\ . \qquad \text{(A9)}
\end{aligned}
$$

In the above expressions the dots represent the image terms which are generated from the existing terms by applying the symmetry properties (28).

The operators in (29) can be derived using (3a)–(3c), (5a), (5b), (26), and the linked-cluster theory. Let us define

$$\nu_{j\sigma}=(1-n_{j-\sigma})n_{j\sigma}\ , \qquad \text{(A10)}$$

$$S_j^{\sigma}=a_{j\sigma}^{\dagger}a_{j-\sigma}\ , \qquad \text{(A11)}$$

$$D(\sigma;i,j)=\nu_{i-\sigma}\nu_{j\sigma}-S_i^{\sigma}S_j^{-\sigma}\ , \qquad \text{(A12)}$$

$$D(i,j)=\sum_{\sigma}D(\sigma;i,j)\ , \qquad \text{(A13)}$$

$$R(\sigma;i,j)=\nu_{i-\sigma}S_j^{\sigma}-S_i^{\sigma}\nu_{j-\sigma}\ , \qquad \text{(A14)}$$

and

$$Q(i,j;k,l)=\sum_{\sigma}[D(\sigma;i,k)D(\sigma;j,l)+R(\sigma;j,l)R(-\sigma;i,k)]\ . \qquad \text{(A15)}$$

Including only the linked diagrams, we obtain for one electron per site,

$$\langle 0,1,0\rangle = \sum_{\{j_i\}} t_{j_2 j_1}^2 D(j_2,j_1) \ , \tag{A16}$$

$$\langle 0,1,0,1,0\rangle = 2\sum_{\{j_i\}} [t_{j_2 j_1}^4 D(j_2,j_1)^2 + 2t_{j_3 j_2}^2 t_{j_2 j_1}^2 D(j_3,j_2) D(j_2,j_1)] \ , \tag{A17}$$

$$\begin{aligned}\langle 0,1,0,1,0,1,0\rangle = 4\sum_{\{j_i\}} [&t_{j_2 j_1}^6 D(j_2,j_1)^3 + 6t_{j_3 j_2}^2 t_{j_2 j_1}^4 D(j_3,j_2) D(j_2,j_1)^2 \\ &+ 6t_{j_4 j_3}^2 t_{j_3 j_2}^2 t_{j_2 j_1}^2 D(j_4,j_3) D(j_3,j_2) D(j_2,j_1) + 2t_{j_4 j_1}^2 t_{j_3 j_1}^2 t_{j_2 j_1}^2 D(j_4,j_1) D(j_3,j_1) D(j_1,j_1)] \ ,\end{aligned} \tag{A18}$$

$$\langle 0,1,2,1,0\rangle = -2\sum_{\{j_i\}} t_{j_1 j_4} t_{j_3 j_2} t_{j_4 j_3} t_{j_2 j_1} Q(j_4 j_2; j_3 j_1) \ , \tag{A19}$$

$$\begin{aligned}\langle 0,1,0,1,2,1,0\rangle = 8\sum_{\{j_i\}} t_{j_1 j_4} t_{j_3 j_2} t_{j_4 j_3} t_{j_2 j_1} &[t_{j_2 j_1}^2 D(j_2,j_1) + t_{j_3 j_2}^2 D(j_3,j_2) \\ &+ t_{j_3 j_1}^2 D(j_3,j_1) + t_{j_5 j_1}^2 D(j_5,j_1) + t_{j_5 j_2}^2 D(j_5,j_2)] Q(j_4 j_2; j_3 j_1) \\ + 8\sum_{\{j_i\}} t_{j_4 j_3}^2 t_{j_3 j_2}^2 t_{j_2 j_1}^2 &D(j_4,j_3) D(j_3,j_2) D(j_2,j_1) \ ,\end{aligned} \tag{A20}$$

$$\begin{aligned}\langle 0,1,2,1,0,1,0\rangle = &\text{ obtained from } \langle 0,1,0,1,2,1,0\rangle \text{ by changing the order of} \\ &Q \text{ and the curly bracket in the first summation} \ ,\end{aligned} \tag{A21}$$

$$\begin{aligned}\langle 0,1,2,1,2,1,0\rangle = &8\sum_{\{j_i\}} t_{j_1 j_4} t_{j_3 j_2} t_{j_4 j_3} t_{j_2 j_1} [t_{j_3 j_2}^2 D(j_3,j_2) + 2t_{j_5 j_2}^2 D(j_5,j_2)] Q(j_4 j_2; j_3 j_1) \\ &16\sum_{\{j_i\}} t_{j_4 j_3}^2 t_{j_3 j_2}^2 t_{j_2 j_1}^2 D(j_4,j_3) D(j_2,j_1) + 16\sum_{\{j_i\},\sigma} t_{j_1 j_5} t_{j_2 j_4} t_{j_5 j_2} t_{j_3 j_2} t_{j_4 j_3} t_{j_2 j_1} \{R(-\sigma;j_1 j_5) \\ &\times [\nu_{j_3\sigma} R(\sigma;j_2 j_4) - S_{j_3}^{\sigma} D(\sigma;j_2 j_4) + D(\sigma;j_2 j_5)[S_{j_3}^{\sigma} R(-\sigma;j_2 j_4) - \nu_{j_3\sigma} D(-\sigma;j_2 j_4)]\} \\ &+ 4\sum_{\{j_i\},\sigma} t_{j_5 j_4} t_{j_1 j_6} t_{j_6 j_5} t_{j_3 j_2} t_{j_4 j_3} t_{j_2 j_1} \\ &\times \{D(\sigma;j_4 j_5)[D(\sigma;j_6 j_1) D(\sigma;j_2 j_3) + R(\sigma;j_1 j_6) R(-\sigma;j_3 j_2)] \\ &- R(\sigma;j_5 j_4)[R(-\sigma;j_1 j_6) D(\sigma;j_2 j_3) - D(\sigma;j_1 j_6) R(-\sigma;j_3 j_2)]\} \ ,\end{aligned} \tag{A22}$$

and

$$\begin{aligned}\langle 0,1,2,3,2,1,0\rangle = 12\sum_{\{j_i\},\sigma} t_{j_5 j_2} t_{j_3 j_6} t_{j_1 j_4} t_{j_6 j_5} t_{j_4 j_3} t_{j_2 j_1} &\{D(\sigma;j_2 j_5)[D(\sigma;j_6 j_3) D(\sigma;j_4 j_1) + R(\sigma;j_3 j_6) R(-\sigma;j_1 j_4)] \\ &- R(\sigma;j_5 j_2)[R(-\sigma;j_3 j_6) D(\sigma;j_4 j_1) - D(\sigma;j_3 j_6) R(-\sigma;j_1 j_4)]\} \ .\end{aligned} \tag{A23}$$

APPENDIX B

For a two-site Hubbard model, there are only two subbands: the lower subband has no doubly occupied site while the upper subband contains only one doubly occupied site. Therefore,

$$H_0 = t\sum_{ij\sigma}{}' (1-n_{i-\sigma}) a_{i\sigma}^{\dagger} a_{j\sigma} (1-n_{j-\sigma}) + \left(t\sum_{ij\sigma}{}' n_{i-\sigma} a_{i\sigma}^{\dagger} a_{j\sigma} n_{j-\sigma} + u\sum_i n_{i\uparrow} n_{i\downarrow} \right) \ , \tag{B1}$$

$$P_1HP_2 = t\sum_{ij\sigma}{}' (1-n_{i-\sigma})a_{i\sigma}^{\dagger}a_{j\sigma}n_{j-\sigma} \ , \tag{B2}$$

$$P_2HP_1 = t\sum_{ij\sigma}{}' n_{i-\sigma}a_{i\sigma}^{\dagger}a_{j\sigma}(1-n_{j-\sigma}) \ , \tag{B3}$$

Substituting (B2) and (B3) into (24), we obtain the simple form

$$\tilde{H} = H_0 + \alpha U[(P_1HP_2HP_1 - P_2HP_1HP_2)/2t^2] + \beta U[(P_1HP_2 - P_2HP_1)/t] \ , \tag{B4}$$

where

$$\alpha = \frac{1}{4}\sum_{n=0}^{\infty}(-1)^{n+1}(2n+1)[(2n+2)!]^{-1}\left(\frac{4t}{U}\right)^{2n+2} \ , \tag{B5}$$

$$\beta = \frac{1}{4}\sum_{n=0}^{\infty}(-1)^{n+1}(2n+2)[(2n+3)!]^{-1}\left(\frac{4t}{U}\right)^{2n+3} \ . \tag{B6}$$

Let the two sites be labeled as 1 and 2. Then the eigenstates of H_0 consists of $a_{1\uparrow}^{\dagger}a_{2\uparrow}^{\dagger}|0\rangle$, $a_{1\uparrow}^{\dagger}a_{2\downarrow}^{\dagger}|0\rangle$, $a_{1\uparrow}^{\dagger}a_{2\uparrow}^{\dagger}|0\rangle$, $a_{1\downarrow}^{\dagger}a_{2\downarrow}^{\dagger}|0\rangle$, $a_{1\downarrow}^{\dagger}a_{1\downarrow}^{\dagger}|0\rangle$, and $a_{2\downarrow}^{\dagger}a_{2\downarrow}^{\dagger}|0\rangle$. The Hamiltonian matrix of $\tilde{H}$ with respect to these states can be diagonalized analytically and the eigenenergies are $\epsilon_1 = 0$, $\epsilon_2 = U$, and $\epsilon_{\pm} = \frac{1}{2}U[1 \pm (1+16\alpha^2+16\beta^2-8\alpha)^{1/2}]$. Using the expressions of α and β from (B5) and (B6), we obtain

$$4(\alpha^2+\beta^2) - 2\alpha = \frac{x^2}{4} + \frac{1}{4}\sum_{n=0}^{\infty}(-1)^n x^{2n+6}K(n) \ , \tag{B7}$$

where $x = 4t/U$ and

$$K(n) = \frac{2(2n+5)}{(2n+6)!} - \frac{2n+3}{2(2n+4)!} + \sum_{m=0}^{n}\left[\frac{(2m+2)(2n-2m+2)}{(2m+3)!(2n-2m+3)!} - \frac{(2m+1)(2n-2m+3)}{(2m+2)!(2n-2m+4)!}\right] \ . \tag{B8}$$

$K(n)$ is too complicated to be evaluated analytically. However, a computer calculation gives $K(n) = 0$ for all values of n. Therefore, we have

$$\epsilon_{\pm} = \tfrac{1}{2}U[1 \pm (1+16t^2/U^2)^{1/2}] \ . \tag{B9}$$

ϵ_1 is a triplet but ϵ_2 and $\epsilon_{\pm}$ are nondegenerate. These are just the exact solutions of a two-site Hubbard model for all values of t and U.

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