Higher order corrections to effective low-energy theories for strongly correlated electron systems

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Three well-known perturbative approaches to deriving low-energy effective theories, the degenerate Brillouin-Wigner perturbation theory (projection method), the canonical transformation, and the resolvent methods, are compared. We use the Hubbard model as an example to show how, to fourth order in hopping t, all methods lead to the same effective theory, namely the t-J model with ring exchange and various correlated hoppings. We emphasize subtle technical difficulties that make such a derivation less trivial to carry out for orders higher than second. We also show that in higher orders, different approaches can lead to seemingly different forms for the low-energy Hamiltonian. All of these forms are equivalent since they are connected by an additional unitary transformation whose generator is given explicitly. The importance of transforming the operators is emphasized and the equivalence of their transformed structure within the different approaches is also demonstrated.

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I. INTRODUCTION

There is a significant recent interest in higher-order corrections to effective low-energy theories for a broad range of strongly-correlated electronic problems.[1–4] For example, the effective low-energy Hamiltonians of the Hubbard-like models contain the so-called ring-exchange terms.[5,6] These terms can alter the basic properties of excitations,[3] or shift the balance towards a new ground state.[4] In addition, an accurate description of the experimentally observed[7] spectral weight transfer over the Mott scale also necessitates high order corrections in the hopping energy.[8,9] Although several methods exist to derive higher-order low-energy theories, the unicity of the low-energy effective theory may not be obvious. In fact, technical subtleties appear, even in a straightforward application of Brillouin-Wigner perturbation theory, that may lead to ambiguous results[10] beyond second order in the hopping. Further, unlike traditional applications of degenerate perturbation theory in which the eigenstates of the projected Hamiltonian also diagonalize the perturbation, such is not the case here.[11] The unique difficulty that arises with Hubbard-like models is that part of the kinetic energy perturbation leaves the number of doubly occupied sites unchanged and hence must still be iteratively diagonalized in the low-energy subspace.

Low-energy effective theories play a crucial role in essentially all fields of physics. When there are large energy scales that are well separated from the low-energy sector, low-energy effective theories offer the enormous advantage of being formulated in an exponentially smaller Hilbert space. The price for this simplification is that both the Hamiltonian *and* the operators take a form that is more complicated than that of the original theory. In general, this form involves n-body interactions and operators that have a finite extent in space, even if the original theory was local. For example, making use of the large energy of virtual electron-positron

pairs, Foldy and Wouthuysen derived non-relativistic quantum mechanics from the Dirac equation.[12] The local gauge coupling to the electromagnetic potential in Dirac theory yielded three interactions, Zeeman, spin-orbit, and Darwin terms, that are all nonlocal since they involve derivatives of the electromagnetic potentials. This was done with the help of a canonical transformation[12] but the Brillouin-Wigner type methods lead to the same result.[13] In the case of the Hubbard model, when the interaction U is large compared with hopping t, the second-order effective Hamiltonian in the singly-occupied subspace is the t-J model (including correlated hopping) where the spin-spin interaction is nonlocal in contrast to the original local Hubbard interaction. In higher order, n-body interactions, such as ring-exchange terms, also appear.[6] The appearance of n-body interactions and of nonlocal terms in effective low-energy theories is familiar in the Wilsonian renormalization group context.[14]

There are several ways to obtain an effective low-energy Hamiltonian,[15] two of which are widely used in condensed matter physics. The first one is the canonical transformation (CT) method, mentioned above,[12] which is based on original ideas of Van Vleck.[16] The derivation of the t-J model with ring exchange[5,6] from the Hubbard model and the derivation of the Kondo model using the Schrieffer-Wolff transformation[17] from the Anderson model, are well-known examples where the CT method was applied. A modification of that method, the continuous CT[18,19] and its predecessor,[20] has also found recent applications in the derivation of flow equations. Another equally popular method is the projection method, or degenerate Brillouin-Wigner (BW) perturbation theory. The projection method, based on ideas of Kato,[21] offers an alternative route to the derivation of, for example, the t-J model with correlated hopping.[22,23] It has been also used recently in the derivation of an effective Hamiltonian for the pyrochlores.[1] The resolvent method, based on a pro-

cedure known as Lowdin downfolding,[24] is yet another method that is available.

It is well known that the BW and the CT methods give equivalent results at low (second) order, as exemplified by the t-J model with correlated hopping. Although the equivalence of these approaches in higher order might be not obvious, one intuitively expects that they are. This has been supported by Klein[15] who has given a formal proof of the equivalence between various forms of degenerate perturbation theory. Generally, in the presence of a well defined small parameter, the perturbative expansion in powers of such a parameter should not depend on the method employed. In other words, an effective low-energy theory can be presented as an nth order power series in the inverse of some large energy scale (t/U in the Hubbard model), and all methods are expected to yield equivalent forms of the theory up to that same order n.

In this paper we show in some detail how CT, resolvent and BW methods can be applied to the Hubbard model to obtain equivalent effective low-energy Hamiltonians up to fourth order, that is $O(t^4/U^3)$. By equivalence, we mean that all three methods yield Hamiltonians that are related via a unitary transformation. Although, in order to be specific, we work with the Hubbard model, it will be clear that the procedure can be trivially extended to other models, including models that involve expansion of pure spin models about the Ising limit.[3] Several new issues appear in deriving higher-order low-energy effective theories. First, one may find amusing that the low-energy Hamiltonians obtained from three different CT methods, one of Refs. 5 and 6, one of Ref. 25, and the one introduced in this work, appear to be *different* in each case. However, we show that they are all connected by an additional unitary transformation that leaves the block-diagonal form invariant.[25] That is, this unitary transformation converts these different Hamiltonians one into the other. Second, in the case of the BW method one should be careful in dealing with (i) the orthonormalization of the projected eigenstates, since the latter are not necessarily orthogonal even if the initial basis is, and (ii) the energy dependence of the expansion, since the energy should be evaluated iteratively using results from previous steps, in the spirit of Rayleigh-Schrödinger nondegenerate perturbation theory. The final low-energy theory again appears to be different from that obtained from the CT approach of Ref. 6, but a unitary transformation within the low-energy subspace shows their equivalence. Third, in the so-called resolvent method, which is similar to the BW approach but works more directly with the Hamiltonian matrix rather than with the eigenstates, one needs to perform the orthonormalization of the eigenstates in an iterative procedure. For the derivation of the t-J model with correlated hopping within this method see, e.g., Ref. 26. The fourth-order low-energy theory obtained with this method is also unitarily equivalent to the results of the BW and CT approaches.

Finally, as in Ref. 8, we emphasize that in order to compute correlation functions or spectral weight within the low-energy theory it is important to transform the operators corresponding to observables. The omission of such a transformation (see, for example, the recent work using the BW method for the pyrochlores[1,27]) has to be explicitly ad-

dressed. We also demonstrate the equivalence of the transformed structure of the operators within the different methods.

Our paper is organized as follows. Section II introduces the model and notations. Section III escribes CT methods and introduces the unitary transformation that allows us to demonstrate the equivalence of the various low-energy effective theories. Section IV is devoted to the BW method, Sec. V escribes the resolvent method and finally Sec. VI presents a generalized transformation from which all perturbative results can be derived. In Sec. VII we give a brief discussion of relevant experiments. We conclude with Sec. VIII. The Appendix contains miscellaneous results.

II. MODEL

We consider the Hubbard model, conveniently written in the form[9]

$$H = T_0 + T_1 + T_{-1} + V, \tag{1}$$

where the $O(t)$ kinetic energy operator in second quantized form has been divided into three terms by using projection operators. The first operator, T_0, includes the projection operators that ensure that the number of doubly-occupied sites does not change because of hopping. It is precisely this term that complicates the application of traditional degenerate perturbation theory to the Hubbard model. The projection operators included in the kinetic energy operators T_1 and T_{-1} make sure that these operators increase or decrease the number of doubly-occupied sites by 1, respectively. All of these terms are proportional to the hopping matrix element t. Note that generally speaking, there can be hopping matrix elements to arbitrary neighbors but we take all these terms to be of the same order in the expansion parameter t. The Hubbard on-site repulsion, written as V, is proportional to U.

These notations implicitly use the classification of the Hilbert space in subspaces with different numbers of doubly-occupied sites. Namely, every eigenfunction of the Hubbard Hamiltonian (1) can be split in the series of orthogonal pieces

$$|\psi\rangle = \sum_{m=0}^{\infty} |\psi_m\rangle = |\psi_0\rangle + |\psi_1\rangle + |\psi_2\rangle + \cdots, \tag{2}$$

where the subscript enumerates the states with $m = 0, 1, 2, \ldots$ doubly-occupied sites. Evidently, the operator V is diagonal in this basis and has the eigenvalue mU in a state containing m doubly-occupied sites. For the rest of the paper we set $U = 1$, and consider t itself as a small parameter. When a clarification is needed we will restore the actual t/U dependence of the expression.

At $t = 0$, the solution of the eigenstate equation is simply a set of highly degenerate states separated by energy U. It is assumed that U is much larger than the bandwidth (of order t) so that, with t finite, states cluster around the values mU and are separated from each other by a Mott gap where no states occur. In other words, we assume that switching on t does not lead to a crossing of levels between the lowest energy manifold, mU with $m = 0$, and all other manifolds with $m > 0$.

Evidently, many Hamiltonians can be cast in the form of Eq. (1). It suffices to have a large term in the Hamiltonian that can be easily diagonalized and leads to states that are separated by some large energy scale U. Other terms in the Hamiltonian that couple these original states and are proportional to some small parameter can be denoted by $T_{\Delta m}$ where Δm indicates that the operator couples states separated by $\Delta m U$. Although we consider only $\Delta m = -1, 0, +1$, it will be obvious how to generalize our proof to more general values of Δm.

III. CANONICAL TRANSFORMATIONS

The CT method is probably the most commonly used method to find low-energy effective theories. We briefly recall the known results for the problem at hand and then move to another version of the CT approach that gives a result that is unitarily related to the first one.

A. Method 1

To derive the higher-order effective Hamiltonian for the Hubbard model, the CT method was applied in Refs. 5 and 6. There the t^5- and t^6-order Hamiltonians were obtained for the half-filled case and t^4-order Hamiltonian was found for an arbitrary doping. We will simply repeat the basic idea and the results obtained in Ref. 6. The effective Hamiltonian was obtained from the Campbell-Baker-Hausdorff expression

$$\mathcal{H}_{eff}^{CT_1} = e^{-S} H e^{S} = H + [H,S] + \frac{1}{2!}[[H,S],S] + \cdots, \quad (3)$$

where the generator of the transformation S is truncated as

$$S = S_1 + S_2 + S_3 + \cdots,$$

where $S_n \propto t^n$. The role of each S_n in this series is to eliminate the corresponding t^n-order off-diagonal terms in the Hamiltonian in Eq. (3), which change the number of doubly-occupied sites. By assumption however, S does not contain terms that preserve the number of doubly-occupied sites. The remaining freedom to perform a unitary transformation within the singly-occupied subspace will be discussed later in this section.

Given the explicit form of the Hubbard Hamiltonian, Eq. (1), one readily finds that

$$S_1 = T_{-1} - T_1. \quad (4)$$

Using $S = S_1$ and keeping terms up to $O(t^2)$ in Eq. (3) the t-J model with correlated hopping is obtained. To derive the higher-order Hamiltonians we have to truncate S at higher order and determine the operator expression of S_n's required to eliminate the off-diagonal terms of the t^n order. These off-diagonal terms are generated by the commutators of H with $S_{n'}$'s in the previous orders. Generally, one needs n-1 terms in S to obtain the theory valid to the order t^n. We list here the generator S_2 for completeness

$$S_2 = T_0 T_{-1} - T_1 T_0 - T_{-1} T_0 + T_0 T_1, \quad (5)$$

and simply reproduce the result of the procedure described above carried out in Ref. 6 to the t^4-order,

$$\mathcal{H}_{eff}^{(4),CT_1} = V + T_0 - T_{-1}T_1 + T_{-1}T_0T_1 - \frac{1}{2}(T_{-1}T_1T_0 + T_0T_{-1}T_1)$$

$$+ (T_{-1}T_1)^2 - \frac{1}{2}T_{-1}^2T_1^2 - T_{-1}T_0^2T_1 + T_{-1}T_0T_1T_0$$

$$+ T_0T_{-1}T_0T_1 - \frac{1}{2}(T_{-1}T_1T_0^2 + T_0^2T_{-1}T_1). \quad (6)$$

The value of V is taken to be zero since we are in the singly-occupied subspace. In deriving this expression the identity $T_{-1}|\psi_0\rangle = 0$, where $|\psi_0\rangle$ is any of the singly-occupied states, is used.

We would like to add an interesting technical detail to the discussion of this method. The t^3-term in the generator, S_3, although necessary to eliminate the t^3-order off-diagonal terms in Eq. (3), does not contribute to $\mathcal{H}_{eff}^{(4),CT_1}$ explicitly. That is, the 4th-order effective Hamiltonian of Eq. (6) can be obtained using $S = S_1 + S_2$ only, simply neglecting the remaining off-diagonal terms. Similarly, the diagonal terms in the 3rd-order Hamiltonian $\mathcal{H}_{eff}^{(3)}$ are all generated by S_1 alone. This is because the original Hubbard Hamiltonian does not contain any "bare" off-diagonal terms of order higher than t. All such higher-order off-diagonal terms are the result of commutations of T-terms. This shows some additional internal structure of the model. Since we will need the generator S_3 for the discussion of the transformed operators but it was not written out explicitly in Ref. 6, we present it in the Appendix, Eq. (A1).

The expression for the $\mathcal{H}_{eff}^{(4),CT_1}$ in Eq. (6) seems to have all possible combinations of T_0, T_{-1}, and T_1, except for one "missing term:" $T_0T_{-1}T_1T_0$. Although there is no general principle which would require presence of such a term in the effective Hamiltonian, its absence makes one curious about its whereabouts. The fate of this term will be clarified in Sec. III C.

B. Method 2

In the same spirit, a different way to formulate an effective theory using the CT approach is to apply consecutive unitary transformations

$$\mathcal{H}_{eff}^{CT_2} = \dots e^{-\widetilde{S}_3} e^{-\widetilde{S}_2} e^{-\widetilde{S}_1} H e^{\widetilde{S}_1} e^{\widetilde{S}_2} e^{\widetilde{S}_3} \dots.$$

We call this the "consecutive CTs" approach. The idea for each $\widetilde{S}_n$ is to eliminate the off-diagonal terms of the nth order remaining from the previous, $n-1$ order CT. In each of the transformations the expansion formula Eq. (3) is applied and all terms up to a desired order in t are kept. Thus, after $\widetilde{U}_1 = e^{\widetilde{S}_1}$ is applied to the original Hamiltonian the off-diagonal terms of order $O(t)$ are eliminated and show up only in $O(t^2)$. The next transformation moves the off-diagonal terms to $O(t^3)$, and so on. Generally, the generators $\widetilde{S}_n$ in this approach are different from the ones in the previous approach, that is $\widetilde{S}_n \neq S_n$. However, one can check that for the Hubbard model generators $\widetilde{S}_1 = S_1$ and $\widetilde{S}_2 = S_2$, Eqs. (4) and (5). Note that $\widetilde{S}_3$ is indeed different from S_3.

We would like to remark that the derivation of the higher-order effective Hamiltonian within this "consecutive CTs" approach is more straightforward than the approach of Ref. 6. Also, the absence of the $\widetilde{S}_3$ contribution to $\mathcal{H}_{eff}^{(4)}$ is much less enigmatic here. Namely, since $\widetilde{S}_3$ is the off-diagonal order t^3 operator, its only commutator which can give $O(t^4)$ contribution to the Hamiltonian is with the off-diagonal operator of the order t. However, after $e^{\widetilde{S}_1}$ is applied the only operator of order t remaining in the transformed Hamiltonian is the *diagonal* operator T_0. This removes the need to know the explicit form of $\widetilde{S}_3$, although it is formally still necessary to eliminate the off-diagonal t^3-order terms in $\mathcal{H}_{eff}^{(4)}$.

Surprisingly, the final 4th order result of the "consecutive CTs" approach is *different* from $\mathcal{H}_{eff}^{(4),CT_1}$ Eq. (6):

$$H_{eff}^{(4),CT_2} = H_{eff}^{(4),CT_1} + \frac{1}{2}(T_0^2 T_{-1}T_1 + T_{-1}T_1 T_0^2) - T_0 T_{-1}T_1 T_0.$$

(7)

The difference concerns the above-mentioned "missing term" $T_0 T_{-1}T_1 T_0$ and the terms $T_0^2 T_{-1}T_1$ and $T_{-1}T_1 T_0^2$. In fact, in this version of the effective theory the original "missing term" is found, but the two analogous terms are missing. This "mystery" is unveiled below.

C. Additional unitary transformation

Let us first make the following observation. One can consider the following unitary transformation:

$$\mathcal{H}_{eff}' = e^{-S_0}\mathcal{H}_{eff}^{CT_1}e^{S_0},$$

(8)

with the generator

$$S_0 = \gamma(T_0 T_{-1}T_1 - T_{-1}T_1 T_0),$$

(9)

where γ is a real number and plays the role of an "angle of rotation." Note that such a generator: (i) is explicitly anti-Hermitian, (ii) is diagonal (does not change the number of doubly-occupied sites), (iii) is $O(t^3)$, and (iv) is real. The operator S_0 is the lowest order operator satisfying (i)–(iv) which one can construct using T_0 and $T_{\pm 1}$. It is also the only operator of such kind in the $O(t^3)$ order. Therefore, the only contribution from such a transformation to $\mathcal{H}_{eff}'$ will be from the $[T_0, S_0]$ commutator and it will generate additional terms of t^4-order of the form

$$\delta\mathcal{H}_{eff} = \gamma(T_0^2 T_{-1}T_1 + T_{-1}T_1 T_0^2 - 2T_0 T_{-1}T_1 T_0).$$ (10)

As we will see, the multiplicity of Hamiltonians that arise once the high energy scale is eliminated all differ by the terms appearing in $\delta\mathcal{H}_{eff}$. Choosing the "angle of rotation" $\gamma = 1/2$ and applying the transformation S_0 to the $\mathcal{H}_{eff}^{(4),CT_1}$, Eq. (6), one readily obtains $\mathcal{H}_{eff}^{(4),CT_2}$, Eq. (7). As a result $T_{-1}T_1 T_0^2 + $H.c. are replaced by the "missing term" $T_0 T_{-1}T_1 T_0$. Clearly, different choices of the "angle of rotation" will give different fractions of those terms in the result. In fact, a recent study, Ref. 25, used a continuous CT approach to the Hubbard model and obtained an effective Hamiltonian which would be equivalent to the choice $\gamma = 1/4$ in Eq. (9).

Thus the 4th-order effective Hamiltonian for the Hubbard model can take an infinite number of unitary equivalent *forms*, all connected by the transformation in Eqs. (8) and (9). All these models possess the same energy spectrum and correlation functions and thus are equivalent. From this point of view, the reader should not be surprised when, in the next section, we find that the BW method gives a result that is different from Eq. (6).

Although the unitary equivalence of the models is a rather natural property, it is certainly unfamiliar in lower-order effective theories. Furthermore, such a unitary equivalence should be common to all higher-order theories. As the order of the perturbation theory is increased the number of block-diagonal, anti-Hermitian operators one can construct will also grow, providing one with a broader variety of unitarily equivalent forms of the effective Hamiltonian and corresponding operators.

D. Operators

It is important to note that in a low-energy effective theory all operators should be transformed along with the Hamiltonian. Then the expectation values of the observables can be calculated in the singly-occupied manifold. The transformation is different depending on which canonical transformation method is used. Using the first CT above, the standard expression for the transformation is

$$\widetilde{O} = e^{-S}Oe^{S} = O + [O,S] + \frac{1}{2!}[[H,O],O] + \cdots.$$

Again, we consider as an example the operator O_1, which increases the number of doubly-occupied sites by one. Using $S = S_1 + S_2$ from Eqs. (4) and (5) and utilizing the property $T_{-1}|\psi_0\rangle = 0$ we obtain, to the order t^2

$$\widetilde{O}_1 = -T_{-1}O_1 + (T_{-1}T_0 - T_0 T_{-1})O_1,$$

which coincides with the expression we will obtain with the BW method, Eq. (34). To obtain the next-order expression for the transformed operator one needs to know an explicit expression for the generator S_3 [see Appendix, Eq. (A1)]. Using it, some algebra reveals that, to order t^3

$$\widetilde{O}_1 = -T_{-1}O_1 + (T_{-1}T_0 - T_0 T_{-1})O_1 + \frac{3}{2}T_{-1}T_1 T_{-1}O_1$$

$$- \frac{1}{2}T_{-1}^2 T_1 O_1 - T_0^2 T_{-1}O_1 - T_{-1}T_0^2 O_1 + 2T_0 T_{-1}T_0 O_1$$

$$+ \frac{1}{2}T_{-1}O_1 T_{-1}T_1 - \frac{1}{2}T_{-1}^2 O_1 T_1,$$

(11)

which should be compared with the result of the BW method given in the Appendix, Eq. (A2).

IV. BRILLOUIN-WIGNER METHOD

We proceed to show, up to order $O(t^4)$ $[=O(t^4/U^3)]$ for the Hamiltonian, that degenerate BW perturbation theory can be organized in the spirit of the Rayleigh-Schrödinger (RS)

perturbation theory to lead to the same low-energy effective theory for Hamiltonian and operators as the consecutive CT method. We will take a detailed approach that shows all the subtleties.

Let us consider one eigenstate $|\psi\rangle$ of the full Hamiltonian (1) with the eigenvalue E. It obeys the Schrödinger equation

$$(E - T_0 - V - T_1 - T_{-1})|\psi\rangle = 0. \tag{12}$$

Although we have not explicitly written quantum numbers for E and $|\psi\rangle$, we have to remember that we have a matrix equation with many eigenvalues and corresponding eigenstates. We look for the effective theory that describes the states that evolve from the lowest energy sector, $m=0$, taking into account virtual excitations into $m>0$ states perturbatively. One can also write effective theories that are valid for any of the subspaces[28] with $m>0$.

A. BW expression for $|\psi\rangle$

We would like to rewrite the eigenstate $|\psi\rangle$ in a way that will allow us to take into account higher-energy sectors with $m \geq 1$ through an iterative procedure. Let Q be a projection operator that removes all components of $|\psi\rangle$ that are in the $m=0$ (singly-occupied) subspace. We have $[Q, E-T_0-V] = 0$ since T_0+V does not change double-occupancy. One can find then an iterative expression for $Q|\psi\rangle$ directly from the Schrödinger equation Eq. (12)

$$Q|\psi\rangle = \frac{1}{E - T_0 - V} Q(T_1 + T_{-1})|\psi\rangle. \tag{13}$$

Inversion of the operator $E-T_0-V$ does not cause any problem when there is a Mott gap since the denominator has only nonvanishing eigenvalues. Indeed, $E-T_0$ is at most of order of the bandwidth (proportional to t) while the operator Q ensures that the smallest value that V takes is U. The complete eigenvector $|\psi\rangle$ has components in the $m=0$ subspace $|\psi_0\rangle \equiv (1-Q)|\psi\rangle$ that we need to determine. We assume that $|\psi_0\rangle$ is a member of an orthonormal subspace $\langle\psi_0'|\psi_0\rangle = \delta_{\psi_0',\psi_0}$. The subscript 0 to a ket means that it has components only in the $m=0$ subspace. This procedure leads to the standard BW expression for $|\psi\rangle$[29]

$$|\psi\rangle = |\psi_0\rangle + \frac{1}{E - T_0 - V} Q(T_1 + T_{-1})|\psi\rangle, \tag{14}$$

which can be solved perturbatively by iteration. Using $T_{-1}|\psi_0\rangle = 0$ and the fact that we cannot come back to the $m=0$ subspace in any of the intermediate steps ($QT_{-1}T_1|\psi_0\rangle = 0$) we find, iterating Eq. (14) three times,

$$|\psi\rangle = \left[1 + \frac{1}{E - T_0 - V}T_1 + \left(\frac{1}{E - T_0 - V}T_1\right)^2 \right.$$
$$\left. + \left(\frac{1}{E - T_0 - V}T_1\right)^3 + \frac{1}{E - T_0 - V}T_{-1}\left(\frac{1}{E - T_0 - V}T_1\right)^2 \right]$$
$$\times |\psi_0\rangle + \cdots. \tag{15}$$

We took into account the projection operators Q so that the above equation contains only the terms for which Q equals

unity. The above equation Eq. (15) generates the usual Brillouin-Wigner perturbation theory. One recognizes that the second term and the last term in Eq. (15) are components of the eigenvector in the subspace with $m=1$ doubly-occupied site $|\psi_1\rangle$, while the third and the fourth terms are components with $m=2$ ($|\psi_2\rangle$) and $m=3$ ($|\psi_3\rangle$) doubly-occupied sites, respectively. This form (without $|\psi_3\rangle$) suffices for our derivation of the effective theory to order $O(t^4)$. With this effective Hamiltonian, one will be able to find the component of the eigenstate in the singly occupied subspace $|\psi_0\rangle$. Given $|\psi_0\rangle$, all the components of the eigenvector $|\psi\rangle$ in the $m=1$ and $m=2$ subspaces are already completely determined by Eq. (15).

The subsequent treatment of Eq. (15) to generate a low-energy theory is the following. The denominators $(E-T_0 -V)^{-1}$ are not singular because they correspond to the energy in the bands with $m>0$. Using $V \gg E-T_0$, one has to expand the energy denominators in Eq. (15) to the required order in t. Let us list here the results of such an expansion of Eq. (15) order by order ($U=1$). We find

$$|\psi^{(0)}\rangle = |\psi_0^{(0)}\rangle, \tag{16}$$

$$|\psi^{(1)}\rangle = (1 - T_1)|\psi_0^{(1)}\rangle, \tag{17}$$

$$|\psi^{(2)}\rangle = (1 - T_1 - (E - T_0)T_1)|\psi_0^{(2)}\rangle, \tag{18}$$

$$|\psi^{(3)}\rangle = \left(1 - T_1 + T_0T_1 - T_1E - \frac{1}{2}T_{-1}T_1^2 - T_1E^2 - T_0^2T_1 \right.$$
$$\left. + 2T_0T_1E + \frac{1}{2}T_1^2 - \frac{1}{2}T_1T_0T_1 + \frac{3}{4}T_1^2E - \frac{1}{4}T_0T_1^2 \right)|\psi_0^{(3)}\rangle, \tag{19}$$

where the superscript describes the order of approximation, that is $|\psi_0^{(3)}\rangle$ is the component of the third-order eigenstate $|\psi^{(3)}\rangle$ in the singly-occupied, $m=0$ subspace: $|\psi_0^{(3)}\rangle = (1 -Q)|\psi^{(3)}\rangle$. Note that, as usual, the order t^{n-1} in the expansion of the eigenvector $|\psi\rangle$ correspond to the order t^n in the matrix elements of the Hamiltonian and of the corresponding energy.[30] That is, one computes the first-order $E^{(1)}$ using zeroth-order eigenstates $|\psi^{(0)}\rangle$, the second-order theory $H^{(2)}$ is formulated with the first-order basis $|\psi^{(1)}\rangle$, etc. Thus, for the fourth-order effective Hamiltonian we will need $|\psi^{(3)}\rangle$. Another detail concerns the explicit dependence of $|\psi^{(2)}\rangle$ and $|\psi^{(3)}\rangle$ in Eqs. (18) and (19) on the energy E. This issue will be resolved later by evaluating E in iterative manner.

One can see that in all orders the full eigenstate $|\psi\rangle$ is built from the $m=0$ states $|\psi_0\rangle$ by including the off-diagonal transitions to the upper-band. The zeroth-order approximation $|\psi^{(0)}\rangle$ Eq. (16) corresponds to taking only the first term in Eq. (15) and neglecting all the upper-band excitations. For the first-order approximation $|\psi^{(1)}\rangle$, we needed to include the second term in Eq. (15). Using that $E-T_0$ will be of the order of t we have simply neglected $E-T_0$ in the denominator which yielded the first-order state, Eq. (17). The second-order state $|\psi^{(2)}\rangle$ is obtained from the first three terms in the BW series Eq. (15). In the third term we can neglect $E-T_0$ again, but the second term needs to be expanded in $E-T_0$.

This leads to the second-order state given in Eq. (18). A term of the form $T_1^2/2$, which does not contribute to the effective Hamiltonian to that order, was dropped although it can appear in certain observables. To obtain the effective Hamiltonian valid to order t^4 one has to generate the third-order wave function $|\psi^{(3)}\rangle$ from Eq. (15). This is obtained from the contributions of all terms in Eq. (15), although the fourth term $\propto T_1^3$ can be neglected since it only contributes to the effective theory to order t^6. The expansion of the denominators provides us with the E-, and E^2-dependent terms in the resulting expression for $|\psi^{(3)}\rangle$, Eq. (19). Let us emphasize here that in the E-dependent terms of the second- and third-order eigenfunctions, one should expand E as well, and keep only the terms to the required order. Thus, for $|\psi^{(2)}\rangle$ we will only need the expression for E that is valid up to order t, while for $|\psi^{(3)}\rangle$ order t^2 is required.

We also point out that Eqs. (16)–(19) relate the "full" eigenstate $|\psi\rangle$ to the the state in the "projected," $m=0$ subspace. Since our goal is to have a low-energy theory which operates with the projected $|\psi_0\rangle$ states only, one should take into account the fact that although the eigenstates are orthonormal $\langle\psi'|\psi\rangle=\delta_{\psi',\psi}$ this is not true for the $m=0$ component alone, that is $\langle\psi_0'|\psi_0\rangle\neq\delta_{\psi_0',\psi_0}$. This is evident from Eq. (2). Therefore, if one wishes to obtain an effective theory that takes the usual Hermitian form, one needs to orthonormalize the projected basis to the required order in t. This difficulty will appear in higher order, but let us first reproduce the well-known second-order results.

B. Derivation of the *t-J* model

We begin with the zeroth-order approximation $|\psi^{(0)}\rangle$ given in Eq. (16). Since the eigenfunction involves only the $m=0$ subspace, the diagonal part of the Hamiltonian (1) solely contributes to the eigenvalue equation

$$\langle\psi'^{(0)}|H|\psi^{(0)}\rangle=\langle\psi_0'^{(0)}|T_0|\psi_0^{(0)}\rangle=E\delta_{\psi_0',\psi_0}. \quad (20)$$

Therefore, $\mathcal{H}_{eff}^{(1)}\equiv T_0$ is our effective Hamiltonian to order t. We rewrite Eq. (20), for future reference, as

$$T_0|\psi_0^{(0)}\rangle=E|\psi_0^{(0)}\rangle. \quad (21)$$

To next order, we need the first-order state $|\psi^{(1)}\rangle$ from Eq. (17). One can see that the states $|\psi_0^{(1)}\rangle$ in Eq. (17) are still orthonormal to order t, that is $\langle\psi'^{(1)}|\psi^{(1)}\rangle=\langle\psi_0'^{(1)}|\psi_0^{(1)}\rangle+O(t^2)=\delta_{\psi',\psi}$. With these states one obtains

$$\langle\psi'^{(1)}|H|\psi^{(1)}\rangle=\langle\psi_0'^{(1)}|T_0-T_{-1}T_1|\psi_0^{(1)}\rangle=E\langle\psi_0'^{(1)}|\psi_0^{(1)}\rangle+O(t^3)$$
$$=E\delta_{\psi_0',\psi_0}, \quad (22)$$

where we used that $E=O(t)$ and that with the required accuracy we can neglect $O(t^3)$ term in the right-hand side and use orthonormality to replace $\langle\psi_0'^{(1)}|\psi_0^{(1)}\rangle$ by δ_{ψ_0',ψ_0}. It is clear that the content of the brackets in Eq. (22) plays the role of an effective second-order Hamiltonian

$$\mathcal{H}_{eff}^{(2)}\equiv T_0-T_{-1}T_1. \quad (23)$$

Writing this result in terms of second-quantized operators and recalling that $J=4t^2/U$ in the second term, one recovers

the *t-J* Hamiltonian with correlated hopping. Again, for future reference, we write

$$(T_0-T_{-1}T_1)|\psi_0^{(1)}\rangle=E|\psi_0^{(1)}\rangle. \quad (24)$$

Contrary to the nondegenerate perturbation theory, the states in the $m=0$ subspace change as we improve the approximation. There is a link between the states at various order as will be discussed in more detail in Sec. IV F below.

C. Transformation of operators in the *t-J* model

Let us pause momentarily to develop transformation rules for the operators that should be used at this level of approximation. Consider, as an example, an operator O_{-1} that decreases the number of doubly-occupied states by one. Naively, one would expect that it has zero expectation in the case of the *t-J* model that is defined in the singly-occupied subspace. The correct way to proceed is to notice that the matrix elements of O_{-1} in the basis of first-order eigenstates Eq. (17) are given by

$$\langle\psi'^{(1)}|O_{-1}|\psi^{(1)}\rangle=\langle\psi_0'^{(1)}|-O_{-1}T_1|\psi_0^{(1)}\rangle. \quad (25)$$

Since the above expression is valid for any eigenstate, to first order the effective operator

$$O_{-1}^{(1)}=-O_{-1}T_1 \quad (26)$$

should be used to compute any matrix element of the original operator solely in terms of projected eigenstates $|\psi_0\rangle$. Both the Hamiltonian Eq. (23) and the operator Eq. (26) coincide with the CT result.

D. Third order

There are new technical issues that appear in orders higher than second. The first problem is that since $\langle\psi'^{(2)}|\psi^{(2)}\rangle=\langle\psi_0'^{(2)}|1+T_{-1}T_1|\psi_0^{(2)}\rangle+O(t^3)$, the second-order eigenvectors in the singly occupied subspace $|\psi_0^{(2)}\rangle$ in Eq. (18) do not form an orthonormal set to order t^2. This issue is easily resolved. To obtain an eigenvalue problem in standard form we define the orthonormal basis $|\varphi_0^{(2)}\rangle$ by

$$|\psi_0^{(2)}\rangle=(1+T_{-1}T_1)^{-1/2}|\varphi_0^{(2)}\rangle, \quad (27)$$

where the square root needs to be expanded to order t^2 to give

$$|\psi^{(2)}\rangle=\left(1-T_1-(E-T_0)T_1-\frac{1}{2}T_{-1}T_1\right)|\varphi_0^{(2)}\rangle. \quad (28)$$

This second-order eigenvector $|\psi^{(2)}\rangle$ should be used to obtain the third-order effective Hamiltonian. This is where one encounters the second difficulty. It concerns E-dependent terms that have to be treated carefully.

Suppose $|\psi^{(2)}\rangle$ in Eq. (28) is an eigenstate with energy E. Since the order of the E-dependent term should match the t^2-order of the eigenstate $|\psi^{(2)}\rangle$, E should be expanded in t. Clearly, we can replace E appearing in Eq. (28) by its first-order term in powers of t. To this end we write

$$E|\varphi_0^{(2)}\rangle=\mathcal{H}_{eff}^{(3)}|\varphi_0^{(2)}\rangle. \quad (29)$$

Since we can anticipate $\mathcal{H}_{eff}^{(3)}$ to have the form

$$\mathcal{H}_{eff}^{(3)} = T_0 - T_{-1}T_1 + O(t^3), \qquad (30)$$

we can use $E|\varphi_0^{(2)}\rangle = T_0|\varphi_0^{(2)}\rangle + O(t^2)$. This is an iterative procedure and it can always be justified by the consistency of the result with the initial expectation outlined in Eq. (30). The replacement $E|\varphi_0^{(2)}\rangle = T_0|\varphi_0^{(2)}\rangle$ is valid for any of the eigenvectors $|\varphi_0^{(2)}\rangle$ of the effective Hamiltonian. After making this change in Eq. (28), the second-order eigenstate reads

$$|\psi^{(2)}\rangle = \left(1 - T_1 - T_1T_0 + T_0T_1 - \frac{1}{2}T_{-1}T_1\right)|\varphi_0^{(2)}\rangle. \quad (31)$$

This procedure allows us to find a Hamiltonian matrix. We will show in Sec. IV F that there is a relation between eigenvectors and eigenvalues at different orders. With the above state $|\psi^{(2)}\rangle$, the eigenvalue problem takes the form

$$\langle\psi'^{(2)}|H|\psi^{(2)}\rangle = \langle\varphi_0'^{(2)}|T_0 - T_{-1}T_1 - \frac{1}{2}T_{-1}T_1T_0 + T_{-1}T_0T_1$$

$$- \frac{1}{2}T_0T_{-1}T_1|\varphi_0^{(2)}\rangle = E\delta_{\varphi_0',\varphi_0}, \qquad (32)$$

which is clearly consistent with our expectation for the eigenvalue E expressed in Eq. (30). As in the lower orders, the effective low-energy Hamiltonian can be directly read off this equation. Thus, up to order $O(t^3)$, the effective Hamiltonian is given by

$$\mathcal{H}_{eff}^{(3)} = T_0 - T_{-1}T_1 - \frac{1}{2}T_{-1}T_1T_0 + T_{-1}T_0T_1 - \frac{1}{2}T_0T_{-1}T_1, \qquad (33)$$

which agrees with the CT approach to this order (see Sec. III).

The last equation, when taken out of context, may suggest that it contains terms that are not allowed within BW perturbation theory. Indeed, the general expression with projected wave function Eq. (14) shows that one cannot come back to the singly occupied state in any intermediate state. The series should contain only "proper" terms. So, terms like $T_{-1}T_1T_0$ in the above expression leave the impression that they should be forbidden since T_0 does not change the double occupancy. However, our derivation clearly shows that these terms come from expanding E using lower order results. Hence they are in fact perfectly acceptable.

The matrix elements of any operator to second order should be computed with the state $|\psi^{(2)}\rangle$ from Eq. (31). For the operator O_1, which increases the number of doubly-occupied sites by one, we obtain

$$\langle\psi'^{(2)}|O_1|\psi^{(2)}\rangle = \langle\varphi_0'^{(2)}| - T_{-1}O_1 + (T_{-1}T_0 - T_0T_{-1})O_1|\varphi_0^{(2)}\rangle, \qquad (34)$$

that also coincides with the CT result for the transformed operator, as discussed in Sec. III.

E. Fourth order

To obtain the effective Hamiltonian valid to the order t^4 one needs again (i) to orthonormalize the states $|\psi_0^{(3)}\rangle$, Eq.

(19) and (ii) to transform the E-dependent terms to equivalent operator expressions found in the previous steps. The procedure outlined for the second-order $|\psi^{(2)}\rangle$ should be followed here. From the normalization condition of $|\psi^{(3)}\rangle$ in Eq. (19), one finds that $|\psi_0^{(3)}\rangle$ should be orthonormalized with the help of

$$|\psi_0^{(3)}\rangle = (1 + T_{-1}T_1 - 2T_{-1}T_0T_1 + 2T_{-1}T_1E)^{-1/2}|\varphi_0^{(3)}\rangle. \qquad (35)$$

The subsequent expansion of the square root to order t^3 is needed. The resulting expression for the eigenstate $|\psi^{(3)}\rangle$ will contain a term $-T_1E$. One has to to replace $E|\varphi_0^{(3)}\rangle$ with $(T_0 - T_{-1}T_1)|\varphi_0^{(3)}\rangle$, which gives E to second order in t when $|\varphi_0^{(3)}\rangle$ is an eigenstate. This leads to the second- and third-order terms.[27] In all other E-dependent terms in Eqs. (19) and (35) we can use $E|\varphi_0^{(3)}\rangle = T_0|\varphi_0^{(3)}\rangle$ as before since this already produces the terms of order t^3. Straightforward algebra finally leads to

$$|\psi^{(3)}\rangle = \left(1 - T_1 + T_0T_1 - T_1T_0 + \frac{1}{2}T_1^2 - \frac{1}{2}T_{-1}T_1 - \frac{1}{2}T_{-1}T_1^2\right.$$

$$- T_1T_0^2 - T_0^2T_1 + 2T_0T_1T_0 - \frac{1}{2}T_1T_0T_1 + \frac{3}{4}T_1^2T_0$$

$$\left. - \frac{1}{4}T_0T_1^2 + T_{-1}T_0T_1 - T_{-1}T_1T_0 + \frac{3}{2}T_1T_{-1}T_1\right)|\varphi_0^{(3)}\rangle, \qquad (36)$$

where $|\varphi_0^{(3)}\rangle$ is the orthonormal set of the $m=0$, singly-occupied eigenstates. With the help of this form of $|\psi^{(3)}\rangle$ the third-order expressions for the matrix element of an operator $\langle O_1\rangle$ can be obtained [see Appendix, Eq. (A2)].

Rather cumbersome, but still straightforward calculations for the eigenvalue problem with $|\psi^{(3)}\rangle$ yield the fourth-order effective Hamiltonian

$$\mathcal{H}_{eff}^{(4)} = \mathcal{H}_{eff}^{(4),CT_2} \qquad (37)$$

that is *identical* to the one obtained by the consecutive CT method, Eqs. (7). This effective Hamiltonian, within a unitary transformation in the singly occupied subspace, is the t-J model with ring exchange and various correlated hoppings.[6]

F. Connection between eigenstates at different orders

There is a connection between eigenvectors in the $m=0$ subspace at different orders in t. For definiteness, let us consider the eigenvalue problem defined by $\mathcal{H}_{eff}^{(3)}$ in Eq. (33). If $|\varphi_0^{(2)}\rangle$ is an eigenstate of $\mathcal{H}_{eff}^{(3)}$, then the corresponding energy to order t^3 is given by

$$(T_0 - T_{-1}T_1 + O(t^3))|\varphi_0^{(2)}\rangle = E|\varphi_0^{(2)}\rangle. \qquad (38)$$

We wish to rewrite this equation as

$$(T_0 - T_{-1}T_1)|\varphi_0^{(2)}\rangle = (E - O(t^3))|\varphi_0^{(2)}\rangle. \qquad (39)$$

Note that the left-hand side of this expression contains $T_0 - T_{-1}T_1 = \mathcal{H}_{eff}^{(2)}$, the effective Hamiltonian at the previous or-

der. The eigenvalue problem for $\mathcal{H}_{eff}^{(2)}$ gives eigenstates at the previous order, $|\varphi_0^{(1)}\rangle$ [$\equiv|\psi_0^{(1)}\rangle$ in Eq. (17)]. Taking the Hermitian product of Eq. (39) with an eigenstate $\langle\varphi_0'^{(1)}|$ we have, by applying $T_0-T_{-1}T_1$ on the bra,

$$\langle\varphi_0'^{(1)}|(T_0-T_{-1}T_1)|\varphi_0^{(2)}\rangle = E'\langle\varphi_0'^{(1)}|\varphi_0^{(2)}\rangle$$
$$= (E-O(t^3))\langle\varphi_0'^{(1)}|\varphi_0^{(2)}\rangle. \quad (40)$$

From this, one concludes that to order t^2,

$$(E-E')\langle\varphi_0'^{(1)}|\varphi_0^{(2)}\rangle = 0. \quad (41)$$

Hence, to that order, either $\langle\varphi_0'^{(1)}|\varphi_0^{(2)}\rangle=0$ or $E'=E$ or both. The generalization of this result means that an eigenvector in the low-energy subspace can have a nonzero overlap to order t^n with an eigenvector of the order t^{n-1} theory if and only if the energies agree to order t^{n-1}. Note, by the way, that the diagonalization of $\mathcal{H}_{eff}^{(n)}$ will in general give us energies that contain all powers of t. Nevertheless, E will be valid only to order t^n since the higher orders can be modified when the matrix elements of $\mathcal{H}_{eff}$ are calculated to higher order. A degeneracy that exists at a given order in t can be lifted at the next order. Energy levels of different symmetry can cross when evaluated at different orders in t so that the ground state of, for example, the t-J model with correlated hopping can be different from that of the model that includes ring exchange.

V. RESOLVENT METHOD

Another approach to deriving the low-energy effective theory is the resolvent method. It is based on an iterative execution of a procedure known as Lowdin downfolding.[24] It bears a lot of similarity with BW perturbation theory but works more directly with the Hamiltonian matrix rather than with the eigenstates. Of all the approaches considered in this paper the resolvent method requires the least amount of algebra.

We start by defining the projection operators P_m, $m=0,1,2$ and $P_>$. Operator P_m projects on a subspace with m doubly occupied sites. Operator $P_>$ projects on a subspace with more than two doubly-occupied sites

$$P_> = 1 - \sum_{m=0}^{2} P_m. \quad (42)$$

For our purposes it is convenient to rewrite Eq. (2) as

$$|\psi\rangle = |\psi_0\rangle + |\psi_1\rangle + |\psi_2\rangle + |\psi_>\rangle,$$

$$P_i|\psi_j\rangle = \delta_{ij}|\psi_j\rangle, \quad (43)$$

where i, $j=0,1,2$, and ">." The eigenvector equation can then be written in the following block form

$$\begin{pmatrix} T_0 & T_{-1} & & \\ T_1 & 1+T_0 & T_{-1} & \\ & T_1 & 2+T_0 & T_{-1} \\ & & T_1 & \mathcal{H}_> \end{pmatrix}\begin{pmatrix} |\psi_0\rangle \\ |\psi_1\rangle \\ |\psi_2\rangle \\ |\psi_>\rangle \end{pmatrix} = E\begin{pmatrix} |\psi_0\rangle \\ |\psi_1\rangle \\ |\psi_2\rangle \\ |\psi_>\rangle \end{pmatrix}, \quad (44)$$

where $\mathcal{H}_>=P_>\mathcal{H}P_>$. Similarly to Eq. (15) in the BW formalism one needs to keep only terms up to $|\psi_2\rangle$ to derive the effective theory to order t^4. Thus, Eq. (44) should suffice for our goals. It is convenient to rewrite this equation by components

$$E|\psi_0\rangle = T_0|\psi_0\rangle + T_{-1}|\psi_1\rangle, \quad (45)$$

$$E|\psi_1\rangle = (1+T_0)|\psi_1\rangle + T_1|\psi_0\rangle + T_{-1}|\psi_2\rangle, \quad (46)$$

$$E|\psi_2\rangle = (2+T_0)|\psi_2\rangle + T_1|\psi_1\rangle + T_{-1}|\psi_>\rangle, \quad (47)$$

$$E|\psi_>\rangle = \mathcal{H}_>|\psi_>\rangle + T_1|\psi_2\rangle. \quad (48)$$

Now we eliminate all components of $|\psi\rangle$ one by one, starting with $|\psi_>\rangle$ until only $|\psi_0\rangle$ is left. From Eq. (48) we obtain

$$|\psi_>\rangle = (E-\mathcal{H}_>)^{-1}T_1|\psi_2\rangle = O(t)|\psi_2\rangle,$$

where we take into account the fact that the operator in brackets is nonsingular and is $O(1)$. This expression for $|\psi_>\rangle$ is substituted in Eq. (47) for $|\psi_2\rangle$ to give

$$|\psi_2\rangle = (E-2-T_0-O(t))^{-1}T_1|\psi_1\rangle = \left(-\frac{1}{2}T_1+O(t^2)\right)|\psi_1\rangle, \quad (49)$$

where we expanded the denominator and kept terms of order t since the higher order terms do not contribute to the theory of the required t^4 order. This latter equation is used to eliminate $|\psi_2\rangle$ from Eq. (46). Thus we have

$$|\psi_1\rangle = \left(-T_1-(E-T_0)T_1-\frac{1}{2}T_{-1}T_1^2-(E-T_0)^2T_1+O(t^4)\right) \times|\psi_0\rangle, \quad (50)$$

where again the expansion of a denominator has been performed to the required order. Finally, we obtain an equation for $|\psi_0\rangle$

$$E|\psi_0\rangle = \left(T_0-T_{-1}T_1-T_{-1}ET_1+T_{-1}T_0T_1-\frac{1}{2}T_{-1}^2T_1^2-T_{-1}E^2T_1 \right.$$
$$\left. -T_{-1}T_0^2T_1+2ET_{-1}T_0T_1+O(t^5)\right)|\psi_0\rangle. \quad (51)$$

This is not the "true" eigenvalue equation since it contains E-dependent terms in the right-hand side, similar to the BW case. We rewrite it then by transferring E-dependent terms to the left as

$$E(1 + T_{-1}T_1 + ET_{-1}T_1 - 2T_{-1}T_0T_1)|\psi_0\rangle$$

$$= \left(T_0 - T_{-1}T_1 + T_{-1}T_0T_1 - \frac{1}{2}T_{-1}^2T_1^2 - T_{-1}T_0^2T_1 \right)|\psi_0\rangle, \tag{52}$$

where we omitted t^5-order terms. Below we will assume that operator expression accuracy is up to $O(t^4)$.

The derived equation for $|\psi_0\rangle$ still does not have the form of the Schrödinger equation $E|\psi\rangle = \mathcal{H}|\psi\rangle$. To transform Eq. (52) into a Schrödinger equation an orthogonalization procedure similar to the one we used in BW calculations must be performed. We introduce $|\chi_0\rangle$ such as

$$|\psi_0\rangle = \alpha|\chi_0\rangle \equiv (1 + T_{-1}T_1 + ET_{-1}T_1 - 2T_{-1}T_0T_1)^{-1/2}|\chi_0\rangle.$$

Substituting in Eq. (52), left multiplying by α and then expanding the square root keeping third order terms, the left-hand side is $E|\chi_0\rangle$ and the right-hand side still has some E-dependent terms. Transferring them to the left we find that $|\chi_0\rangle$ satisfies

$$E\left(1 + \frac{1}{2}(T_{-1}T_1T_0 + T_0T_{-1}T_1)\right)|\chi_0\rangle$$

$$= \left(T_0 - T_{-1}T_1 - \frac{1}{2}T_{-1}T_1T_0 - \frac{1}{2}T_0T_{-1}T_1 + T_{-1}T_0T_1 \right.$$

$$+ T_{-1}T_0T_1T_0 + T_0T_{-1}T_0T_1 + (T_{-1}T_1)^2$$

$$\left. - \frac{1}{2}T_{-1}^2T_1^2 - T_{-1}T_0^2T_1 \right)|\chi_0\rangle. \tag{53}$$

The left-hand side of this equation still does not have the desired form. An extra orthogonality transformation analogous to that performed with α above is required

$$|\chi_0\rangle = \left(1 + \frac{1}{2}T_{-1}T_1T_0 + \frac{1}{2}T_0T_{-1}T_1\right)^{-1/2}|\varphi_0\rangle,$$

with the subsequent square root expansion. The resulting eigenvalue equation for $|\varphi_0\rangle$ by the resolvent method finally takes the Schrödinger equation form $E|\varphi_0\rangle = \mathcal{H}_{eff}^{(4)R}|\varphi_0\rangle$ with the effective Hamiltonian given, to fourth order, by

$$\mathcal{H}_{eff}^{(4)R} = \mathcal{H}_{eff}^{(4)CT_1} + \frac{1}{4}(T_{-1}T_1T_0^2 + T_0^2T_{-1}T_1) - \frac{1}{2}T_0T_{-1}T_1T_0. \tag{54}$$

This effective Hamiltonian does not coincide with the other forms of $\mathcal{H}_{eff}^{(4)}$ we have obtained so far, namely Eqs. (6), (7), and (37). It is however unitarily related to all others through the transformation Eqs. (8) and (10). For example, the "angle of rotation" $\gamma = 1/4$ transforms Eq. (54) back to $\mathcal{H}_{eff}^{(4),CT_1}$ in Eq. (6).

We note that transformation of operators can also be devised within the resolvent approach in a manner similar to the BW calculations, Sec. IV, using the above relations between $|\varphi_0\rangle$ and the states with $m > 0$ doubly-occupied sites.

VI. BIG PICTURE: GENERAL TRANSFORMATION

Thus far, we have shown that while different methods of performing perturbation theory preserve the original energy spectrum of the Hubbard model, the effective Hamiltonians, Eqs. (6), and Eq. (54) differ from each other and from Eqs. (7) and (37) that agree with each other. The terms in question all arise at fourth order and are all reducible[11] with respect to the zero-double occupancy sector. That is, they contain hopping processes that do not originate from excitation to the doubly occupied subspace, $T_0T_{-1}T_1T_0$, nor terminate once an electron is returned to the singly occupied subspace, for example, $T_{-1}T_1T_{-1}T_1$. All such processes can be viewed as arising from a transformation[25] of the eigenstates in the low-energy sector. To lay plain how the effective Hamiltonian is unavoidably affected by this transformation, we now formulate a general method which makes it possible to derive all of the Hamiltonians presented thus far within a single computation scheme. Our starting point is BW integral equation, Eq. (14), whose solution we write symbolically as

$$|\psi\rangle = G(t,E)|\psi_0\rangle. \tag{55}$$

The exact expression for the energy-dependent operator $G(t,E)$ is obtained by iterating Eq. (14). Applying $P = 1 - Q$ (see Sec. IV) to the left-hand side of the Schrödinger equation, Eq. (12), we obtain

$$(E - T_0)|\psi_0\rangle - PT_{-1}Q|\psi\rangle = 0, \tag{56}$$

which can be recast as a nonlinear eigenvalue problem

$$E|\psi_0\rangle = (T_0 + PT_{-1}G(t,E))|\psi_0\rangle, \tag{57}$$

using Eq. (55). Taylor expansion of $G(t,E)$ results in a polynomial in the energy eigenvalue. Through fourth order we find that

$$E|\psi_0\rangle = \left(T_0 - T_{-1}T_1 + T_{-1}T_0T_1 - T_{-1}T_0^2T_1 - \frac{1}{2}T_{-1}^2T_1^2 \right.$$

$$\left. + (- ET_{-1}T_1 - E^2T_{-1}T_1 + 2ET_{-1}T_0T_1) \right)|\psi_0\rangle. \tag{58}$$

To eliminate the energy-dependence on the right-hand side of this equation, we substitute Eq. (57) for each occurrence of $E|\psi_0\rangle$ until all the energy dependence has disappeared. The result of this procedure is an eigenvalue problem

$$E|\psi_0\rangle = \left(T_0 - T_{-1}T_1 + T_{-1}T_0T_1 - T_{-1}T_0^2T_1 - \frac{1}{2}T_{-1}^2T_1^2 \right.$$

$$\left. - T_{-1}T_1(T_0 - T_{-1}T_1) + T_{-1}T_1T_0^2 + 2T_{-1}T_0T_1T_0 \right)|\psi_0\rangle$$

$$= \widetilde{H}|\psi_0\rangle, \tag{59}$$

with a non-Hermitian operator $\widetilde{H}$. All the terms in the second parenthesis arise explicitly from eliminating the energy dependence in Eq. (58) and as a consequence are products of the proper BW terms in the first parenthesis. It is in this sense that such terms are reducible with respect to the zero double occupancy sector. The lack of Hermiticity surfaces

because projection does not respect the mutual orthogonality of the eigenstates in any of the degenerate subspaces.

Hermiticity can be restored by a suitable global transformation of the eigenstates within each degeneracy subspace. To proceed, we consider the operator

$$Z = 1 + aT_{-1}T_1 + bT_{-1}T_1T_0 + cT_0T_{-1}T_1 + dT_{-1}T_0T_1,$$

which is explicitly not unitary. As such, it can be used to construct an effective Hamiltonian

$$\mathcal{H}_{eff} = Z^{-1}\tilde{H}Z \tag{60}$$

by placing appropriate conditions on the coefficients, a, b, c, and d so that $\mathcal{H}_{eff}$ is Hermitian. Through fourth order, Hermiticity is restored by demanding that

$$a = -\frac{1}{2},$$

$$b = \gamma - \frac{1}{2}, \tag{61}$$

$$c = -\gamma - \frac{1}{2},$$

$$d = 1.$$

The resultant effective Hamiltonian,

$$\mathcal{H}_{eff}^{(4)} = T_0 - T_{-1}T_1 + T_{-1}T_0T_1 - \frac{1}{2}(T_{-1}T_1T_0 + T_0T_{-1}T_1)$$

$$- T_{-1}T_0^2T_1 - \frac{1}{2}T_{-1}^2T_1^2 + T_{-1}T_0T_1T_0 + T_0T_{-1}T_0T_1$$

$$+ (T_{-1}T_1)^2 - \frac{1}{2}(T_{-1}T_1T_0^2 + T_0^2T_1T_{-1})$$

$$+ \gamma(2T_0T_{-1}T_1T_0 - T_{-1}T_1T_0^2 - T_0^2T_{-1}T_1) \tag{62}$$

contains three reducible terms whose magnitude is set by an arbitrary constant γ. These terms are given precisely by the "additional" canonical transformation in Eq. (10). Because all the terms controlled by the magnitude of γ are reducible, they provide no more than a transformation of the eigenstates within the degeneracy subspace with zero double occupancy. The multiplicity of Hamiltonians we have derived here all arise from different choices for γ. For example, within the canonical transformation method of Ref. 6, we have $\gamma=0$. Effective Hamiltonians within a sector with a fixed number of doubly occupied sites can only be determined up to an arbitrary rotation of the eigenstates within the degeneracy space. To understand what happens in the case of BW perturbation theory, we recall that, although one starts from a set of wave functions that are orthogonal in the full Hilbert space, the projection into a degeneracy subspace is a process that does not respect the orthogonality. To get a Hermitian Hamiltonian we have to perform a general transformation on the degeneracy subspace in such a way that the orthogonality of the projected components is restored. This is what the general nonunitary transformation defined by Eq. (60) is do-

ing. Canonical transformations, on the other hand, are by definition unitary and hence no additional orthogonalization transformations are necessary.[8,9]

VII. SOME COMMENTS ON EXPERIMENT

Several experimental groups[7] have pointed out that high-temperature superconductors show spectral weight rearrangements over the Mott scale.[31] Rearrangement of spectral weight over large energy scales is expected in strongly correlated systems simply because many of the eigenstates are localized or almost localized. Using the Lehman representation, one can easily see that the momentum eigenstates probed by photoemission or optical spectroscopy, for example, have nonvanishing projection on essentially all the true eigenstates of the interacting problem. When the Mott gap is closed, this means that spectral weight changes will occur over all the energy scales when doping or temperature is changed. When the Mott gap is opened, this will continue to be the case but, nevertheless, the spectral rearrangements over the lower Hubbard band will be describable to a high degree of accuracy using only the effective low-energy theory, *as long as one uses the operators that are appropriate for the low-energy sector*. These operators take into account rearrangements in the upper Hubbard band through virtual states. For example, upon doping by an amount x, exact calculations on the Hubbard model show that the spectral weight transfered from the upper to the lower Hubbard band exceeds $2x$, while $2x$ was argued to be the prediction of the t-J model by some early work.[32] Even at the level of the t-J model, however, there is a correction[8,9] to the low-energy spectral weight (LESW) from the transitions across the Hubbard gap that arise from transforming the electron operators. Through order $(t/U)^2$, the LESW agrees well with the exact diagonalization on small systems.

VIII. CONCLUSION

We have studied several methods for performing degenerate perturbation theory. We have shown that, to fourth order, they lead to low-energy effective theories that appear different but, in fact, are all related through a unitary transformation in the low-energy subspace, Eqs. (8) and (10). The necessity of a unitary transformation in the low-energy subspace to prove the equivalence of the theories does not normally occur in lower-order theories and thus is a rather unfamiliar property. The most systematic approaches are the two canonical transformation methods, the easiest algebraically are the general transformation (Sec. VI) and the resolvent method, while the Brillouin-Wigner method, modified in the manner of Rayleigh-Schrödinger, becomes rather cumbersome in higher orders. Nevertheless, the latter method gives some insight into the other approaches. In particular, it allows to understand the appearance of terms in intermediate states that appear, at first glance, to be in the low-energy subspace ("improper terms"). Also, it shows that in the low-energy subspace, eigenvectors at order t^n have nonzero projection on eigenvectors at order t^{n-1} only if the expansions of the corresponding energies agree to order t^{n-1}. The need to

orthogonalize and to keep track of the order of the energy expansion makes the BW approach in practice more delicate to carry out to high order. However, the existence of a small parameter makes it completely equivalent to the canonical transformation and resolvent approaches.

This work has laid plain how perturbation theory to all orders can be formulated unambiguously. Although the question of the accuracy of projected schemes in treating the full Hubbard model has not been addressed in the present work, it is generally assumed that such projected schemes should capture all the physics of the original Hubbard model to a given order in t/U. Note, however, that this presupposes that in the strong coupling limit all observables can be expanded in powers of t/U. For an infinite system, this may not always be true. Also, as is the case with any perturbation theory, such projected schemes obviously fail to adequately describe phase transitions. For example, at half-filling the interaction tuned Mott transition is beyond the domain of applicability of the projected theory. In the case of the doping-induced Mott transition, the projected theory cannot address the question of the chemical potential, which is of order U. Nonetheless, as long as the interaction U is much larger than the bandwidth, it is possible to write a unique (up to a unitary transformation in the target space) low-energy effective theory whose range of applicability is limited by the condition that physical observables have a well-defined expansion in t/U. We reiterate that consistency of such procedures requires that all operators be transformed as well. Although we presented the results within the Hubbard model, all methods are easily generalizable to other models.

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APPENDIX: MISCELLANEOUS ADDITIONAL RESULTS

The third-order CT generator S_3, version of Ref. 6, is given by

$$S_3 = \frac{2}{3}(T_{-1}^2 T_1 + T_1 T_{-1}^2 - T_{-1} T_1^2 - T_1^2 T_{-1} + 2 T_1 T_{-1} T_1$$
$$- 2 T_{-1} T_1 T_{-1}) + T_0^2 T_{-1} + T_{-1} T_0^2 - T_1 T_0^2 - T_0^2 T_1$$
$$- 2 T_0 T_1 T_0 + 2 T_0 T_{-1} T_0. \tag{A1}$$

The BW third-order expressions for the matrix element of an off-diagonal operator $\langle O_1 \rangle$ increasing the number of doubly-occupied sites by one is given by

$$\langle \psi'^{(3)} | O_1 | \psi^{(3)} \rangle$$
$$= \langle \varphi_0'^{(3)} | - T_{-1} O_1 + (T_{-1} T_0 - T_0 T_{-1}) O_1 + \frac{3}{2} T_{-1} T_1 T_{-1} O_1$$
$$- \frac{1}{2} T_{-1}^2 T_1 O_1 - T_0^2 T_{-1} O_1 - T_{-1} T_0^2 O_1 + 2 T_0 T_{-1} T_0 O_1$$
$$+ \frac{1}{2} T_{-1} O_1 T_{-1} T_1 - \frac{1}{2} T_{-1}^2 O_1 T_1 | \varphi_0^{(3)} \rangle. \tag{A2}$$

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