

# Ground-state energy of the Hubbard model at half filling

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A recently proposed projection operator technique based on the introduction of cumulants is used to investigate the ground-state energy of the Hubbard model at half filling on a square lattice in two dimensions, in the antiferromagnetic phase. Our results in the intermediate and large regime of the ratio  $U/t$  are below those of variational Monte Carlo calculations, which set an upper bound for the energy. By including the most dominant spin-fluctuation processes, the present calculation also obeys the correct infinite  $U/t$  limit, where the Hubbard model at half filling reduces to the Heisenberg antiferromagnet. The relation of our approach to recent coupled-cluster calculations for the Hubbard model is also discussed. [S0163-1829(96)06327-8]

## I. INTRODUCTION

The cumulant approach<sup>1,2</sup> has proved to be a powerful technique in quantum many-body theory. It has been applied to a wide range of static as well as dynamical ground-state properties of both strongly and weakly correlated systems. Among the main advantages of the method is that it automatically preserves the property of size consistency. The energy is a size extensive quantity, i.e., the energy of two well-separated, but otherwise identical, systems equals twice the value of a single system. Approximations which are applied within the cumulant approach preserve this property. The method starts from a decomposition of a many-particle Hamiltonian  $H$  into an unperturbed part  $H_0$  and a perturbation  $H_1$ , i.e.,  $H = H_0 + H_1$ . The eigenvalue problem of  $H_0$  is supposed to be known. It was shown<sup>1,2</sup> that the ground-state energy  $E_g$  of the full Hamiltonian  $H$  can be written in terms of the following cumulant expression:

$$E_g = \langle H \Omega \rangle_0^c = \epsilon_0 + \langle H_1 \Omega \rangle_0^c. \quad (1)$$

Here, the brackets  $\langle \dots \rangle_0^c$  denote cumulant expectation values formed with the ground-state  $|\phi_0\rangle$  (with energy  $\epsilon_0$ ) of the unperturbed Hamiltonian  $H_0$ , i.e.,  $H_0|\phi_0\rangle = \epsilon_0|\phi_0\rangle$ .

For operator products of  $A_1, A_2, A_3, \dots$  the low order cumulants are defined as

$$\langle A_1 \rangle_0^c = \langle A_1 \rangle_0,$$

$$\langle A_1 A_2 \rangle_0^c = \langle A_1 A_2 \rangle_0 - \langle A_1 \rangle_0 \langle A_2 \rangle_0,$$

$$\begin{aligned} \langle A_1 A_2 A_3 \rangle_0^c &= \langle A_1 A_2 A_3 \rangle_0 - \langle A_1 \rangle_0 \langle A_2 A_3 \rangle_0^c - \langle A_2 \rangle_0 \langle A_1 A_3 \rangle_0^c \\ &\quad - \langle A_3 \rangle_0 \langle A_1 A_2 \rangle_0^c - \langle A_1 \rangle_0 \langle A_2 \rangle_0 \langle A_3 \rangle_0, \end{aligned} \quad (2)$$

etc. For a comprehensive discussion of cumulants see, e.g., Kubo's paper.<sup>3</sup> The quantity  $\Omega$  in (1) is defined by

$$\Omega = 1 + \lim_{x \rightarrow 0} \frac{1}{x - L_0 - H_1} H_1. \quad (3)$$

It can be considered as wave operator (or Moeller operator used in scattering theory) which transforms the unperturbed ground state  $|\phi_0\rangle$  into the exact ground state of the full

Hamiltonian  $H$ . The quantity  $L_0$  denotes the Liouville operator. It acts on the usual operators  $A$  of the unitary space as  $L_0 A = [H_0, A]_-$ .

The above expression for  $E_g$  is quite general and was used for strongly but also for weakly correlated systems. For a detailed discussion of Eq. (1) see previous publications.<sup>2</sup> In handling cumulant expectation values one must distinguish between prime and composite operators. A prime operator, such as  $H_1$  or  $L_0$  in Eqs. (1) and (3), is treated as a single entity in the cumulant ordering procedure. Expanding  $\Omega$ , the resulting products of  $L_0$  and  $H_1$  are composite operators in the cumulant formation. As is also obvious from Eqs. (1) and (3) the cumulant expression for  $E_g$  is well suited for applying the projection technique and can therefore be expanded into a continued fraction. However, due to the appearance of higher order cumulants, in practice it is often difficult to go beyond a finite order of the continued fraction expansion. For this reason, instead, an exponential ansatz for  $\Omega$  was proposed:<sup>4</sup>

$$\Omega = \exp \left( \sum_{\nu} \lambda_{\nu} A_{\nu} \right). \quad (4)$$

The set of relevant operators  $\{A_{\nu}\}$  entering (4) has to be chosen in such a way that  $\exp(\sum_{\nu} \lambda_{\nu} A_{\nu})|\phi_0\rangle$  (with appropriate parameters  $\lambda_{\nu}$  to be determined) represents a good approximation for the exact ground state. Following Schork and Fulde,<sup>4</sup> we obtain a set of coupled equations for  $E_g$  and  $\lambda_{\nu}$ :

$$E_g = \left\langle H \exp \left( \sum_{\nu} \lambda_{\nu} A_{\nu} \right) \right\rangle_0^c, \quad (5)$$

$$0 = \left\langle A_{\mu}^{\dagger} H \exp \left( \sum_{\nu} \lambda_{\nu} A_{\nu} \right) \right\rangle_0^c. \quad (6)$$

The coefficients  $\lambda_{\nu}$  are determined by (6). Note that the relation  $0 = \langle A^{\dagger} H \Omega \rangle_0^c$  holds for any operator  $A$ .

Relation (6) leads to a system of coupled nonlinear equations for the coefficients  $\lambda_{\nu}$ . Its solution provides an infinite continued fraction expression for the energy. This is readily demonstrated in a simple example, by taking only a single operator  $A$  in the exponential of ansatz (4), i.e.,

$\Omega = \exp(\lambda A)$ . The operator  $A$  is chosen as that part of the perturbation  $H_1$  which couples to the unperturbed ground state  $|\phi_0\rangle$ , i.e.,  $A|\phi_0\rangle = H_1|\phi_0\rangle$ , and thereby creates fluctuations in the unperturbed ground state  $|\phi_0\rangle$ . By expanding  $\exp(\lambda A)$  in (5) and (6) one easily realizes that the series terminate after the second and third term, respectively. The reason is that ground-state fluctuations of high power, generated by  $A$ , cannot be remedied by  $A^\dagger$  or  $H_1$ . One finds

$$E_g = \langle H \rangle_0 + \lambda \langle H_1 A \rangle_0^c, \quad (7)$$

$$0 = \langle A^\dagger H_1 \rangle_0^c + \lambda \langle A^\dagger H_0 A \rangle_0^c + \frac{1}{2} \lambda^2 \langle A^\dagger H_1 A^2 \rangle_0^c. \quad (8)$$

The solution for  $\lambda$  from (8) may implicitly be written as

$$\lambda = - \frac{\langle A^\dagger H_1 \rangle_0^c}{\langle A^\dagger H_0 A \rangle_0^c + \frac{1}{2} \lambda \langle A^\dagger H_1 A^2 \rangle_0^c}. \quad (9)$$

Due to the appearance of  $\lambda$  in the denominator of the right-hand side, expression (7) for  $E_g$  can easily be expanded into an infinite continued fraction.

In the original paper<sup>4</sup> the fluctuation operators  $\{A_\nu\}$  of ansatz (4) were restricted to prime operators, each one being an entity in the cumulant ordering. Here we propose two modifications.

(i) The operators  $\{A_\nu\}$  may also represent composite operators, i.e., *products* of operators, each of which is an entity in the cumulant ordering.

(ii) Noting that the wave operator  $\Omega$ , defined in Eq. (3), obeys the integral equation

$$\Omega = 1 + \lim_{x \rightarrow 0} \frac{1}{x - L_0} H_1 \Omega, \quad (10)$$

we may replace Eqs. (5) and (6) by

$$E_g = \langle H \rangle_0 + \lim_{x \rightarrow 0} \left\langle H_1 \frac{1}{x - L_0} H_1 \exp \left( \sum \lambda_\nu A_\nu \right) \right\rangle_0^c, \quad (11)$$

$$0 = \langle A_\mu^\dagger H_1 \rangle_0^c + \left\langle A_\mu^\dagger H_0 \exp \left( \sum \lambda_\nu A_\nu \right) \right\rangle_0^c + \lim_{x \rightarrow 0} \left\langle A_\mu^\dagger H_1 \frac{1}{x - L_0} H_1 \exp \left( \sum \lambda_\nu A_\nu \right) \right\rangle_0^c. \quad (12)$$

The advantage of recasting (1) and (3) into the new form (11) and (12) is the appearance of the term  $H_1 [1/(x - L_0)] H_1$  on the right-hand sides. This term may be interpreted as an *effective Hamiltonian* as obtained by second order perturbation theory. As mentioned above, it is understood that the operators  $A_\nu$  in (11) and (12) may also represent products of operators. A different way to obtain size-consistent results for the ground-state energy is provided by the coupled-cluster method which was originally invented by Coester and Kümmel for studies in nuclear physics.<sup>5,6</sup> A detailed account of this method was recently given by Bishop.<sup>7</sup> As was shown,<sup>4</sup> there is a close relationship between the cumulant formalism and the coupled-cluster treatment. By starting from the cumulant expressions (1) and (3) it was

shown that the coupled-cluster equations can be derived. Whether also the cumulant approach can be justified from the coupled-cluster equations is not clear at present. We believe that the cumulant approach is the more powerful scheme. It may serve as a basis for a variety of different types of self-consistent approximations. In this paper we use the modified version of the cumulant approach, Eqs. (11) and (12). It will turn out that the strong correlation limit for the ground-state energy of the Hubbard model at half filling (which is the Heisenberg model) is also correctly described by the cumulant approach. This is obtained by inclusion of the most dominant spin-fluctuation operators. The coupled-cluster method, when applied directly to the Heisenberg model,<sup>8</sup> gives a result in close agreement with ours, due to inclusion of similar spin-fluctuation processes. In the large  $U$  limit, our results are better than those obtained in a recent treatment of the Hubbard model, based also on the coupled-cluster method,<sup>9-11</sup> which has not yet taken into account all spin-fluctuation operators included in Ref. 8.

## II. GROUND-STATE ENERGY OF THE HUBBARD MODEL FOR $U \gg t$

We now turn to the application of this method and calculate the ground-state energy of the Hubbard model at half filling on a two-dimensional square lattice with  $N$  sites. The Hubbard model is given by

$$H = H_0 + H_1, \quad (13)$$

$$H_0 = U \sum_{i=1}^N n_{i\uparrow} n_{i\downarrow}, \quad (14)$$

$$H_1 = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}). \quad (15)$$

Here,  $U$  is the Coulomb repulsion between electrons on the same site.  $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$  is the occupation-number operator for electrons with spin  $\sigma$  on site  $i$ . The symbol  $\langle ij \rangle$  denotes pairs of nearest neighbors. In the case of strong electronic correlations,  $U \gg t$ , the above Hamiltonian is used as a model system for the electronic degrees of freedom of the  $\text{CuO}_2$  planes in high  $T_c$  superconductors. In this limit, double occupation with two electrons on the same site is strongly suppressed. Then, the Hubbard model can be transformed into the  $t$ - $J$  Hamiltonian which acts only in the unitary subspace where double occupancy is excluded:

$$H_{t-J} = H_J + H_t, \quad (16)$$

$$H_J = J \sum_{\langle ij \rangle} \left[ \vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \hat{n}_i \hat{n}_j \right], \quad (17)$$

$$H_t = -t \sum_{\langle ij \rangle \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.}). \quad (18)$$

The first part of  $H_J$  is the antiferromagnetic Heisenberg exchange with  $J \equiv 4t^2/U$ .  $H_t$  is the so-called conditional hopping term since the hopping of electrons is only allowed to a site which was empty before. We have also introduced  $\hat{n}_i = \sum_\sigma \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$  and  $\hat{c}_{i\sigma}^\dagger \equiv c_{i\sigma}^\dagger (1 - n_{i-\sigma})$ . For later reference we

define  $\hat{c}_{i\sigma}^\dagger \equiv c_{i\sigma}^\dagger n_{i-\sigma}$ . Note that  $\hat{c}_{i\sigma}^\dagger$  describes transitions from empty to singly occupied sites, whereas  $\hat{c}_{i\sigma}^\dagger$  describes transitions from singly to doubly occupied sites. At half filling, with one electron at each site, the  $t$ - $J$  model reduces to the Heisenberg Hamiltonian since in that case the restricted hopping term  $H_t$  cannot act.

Already the ground-state energy of the antiferromagnetic Heisenberg exchange (17) (with  $\hat{n}_i = \hat{n}_j = 1$  at half filling) is not exactly known. For a perturbative solution one may start by splitting  $H_J$  into an unperturbed “Ising” part, with the Néel state as its ground state, and a spin-fluctuation part which we shall consider as a perturbation:<sup>12,13</sup>

$$H_J = -\frac{NJ}{2} + H_{\text{Ising}} + H_{\text{SF}}, \quad (19)$$

$$H_{\text{Ising}} = J \sum_{\langle ij \rangle} S_i^z S_j^z, \quad (20)$$

$$H_{\text{SF}} = \frac{J}{2} \sum_{\langle ij \rangle} [S_i^+ S_j^- + S_i^- S_j^+]. \quad (21)$$

The contribution to the ground-state energy  $E_g$  from  $H_{\text{Ising}}$  is  $-(1/4)2NJ$ . Second order perturbation with respect to  $H_{\text{SF}}$  gives a further lowering of this energy by  $(1/6)NJ$ , so that the sum is  $-(1/3)2NJ$ . (The factor 6 comes from the fact that one pair of flipped spins frustrates the Néel order of six neighboring bonds.) Including the trivial contribution  $-NJ/2$  in (19), the ground-state energy of  $H_J$  so far is  $-(7/6)NJ$ . Higher order terms in the perturbation series change this result only slightly. Supported by numerical methods,<sup>14</sup> there is quite general agreement that the correct value is close to  $-1.17NJ$ .

We now apply our method to calculate the ground-state energy of the Hubbard model at half filling in the same limit  $U \gg t$ . We expect to arrive at the same value as for the Heisenberg model, as just explained. From the above discussion it is evident that in the large  $U$  limit only spin fluctuations reduce the ground-state energy relative to the energy of the Néel state. Charge fluctuations, induced by hopping operators, are unimportant since sites with double occupancy (unavoidable at half filling) are quite costly. (For decreasing values of  $U/t$ , however, charge fluctuations have to be considered.) Hence, in the exponent of ansatz (4) for  $\Omega$  we may restrict ourselves to spin-fluctuation operators only,

$$\Omega = \exp \left[ \sum_{\nu=1}^4 \sigma_\nu S_\nu \right]. \quad (22)$$

Here, the coefficients  $\sigma_\nu$  replace the coefficients  $\lambda_\nu$  from the former ansatz (4). They indicate that spin-fluctuation operators only are introduced in (22). We shall use four spin-fluctuation operators, denoted by  $S_\nu$ . They are best found from a perturbative treatment of the Heisenberg model (for instance by use of projection technique) up to fourth order:

$$S_1 = \begin{bmatrix} \uparrow_i & \downarrow_j \\ \downarrow_k & \uparrow_l \end{bmatrix}, \quad (23)$$

$$S_2 = (S_1)^2, \quad (24)$$

$$S_3 = \begin{bmatrix} \uparrow_i & \downarrow_j \\ \downarrow_k & \uparrow_l \end{bmatrix}, \quad (25)$$

$$S_4 = \begin{bmatrix} \uparrow_i & \downarrow_j & \uparrow_k & \downarrow_l \end{bmatrix}. \quad (26)$$

The up and down arrows with double lines indicate spins which are flipped relative to their original orientation in the Néel state. For instance, the first spin-fluctuation operator  $S_1$  is formed by two successive hoppings from site  $i$  to a neighboring site  $j$  and back, combined with flipping of the transferred spin. Explicitly,  $S_1$  is written as

$$S_1 = \sum_{\langle ij \rangle} c_{j\downarrow}^\dagger c_{i\downarrow} c_{i\uparrow}^\dagger c_{j\uparrow} = - \sum_{\langle ij \rangle} S_j^- S_i^+, \quad j \in \text{sublattice} \uparrow. \quad (27)$$

The sum runs over all pairs of neighboring sites  $i, j$ . In (27) we have again introduced the spin raising and lowering operators  $S_i^\sigma = c_{i\sigma}^\dagger c_{i-\sigma}$  ( $\sigma = \pm 1$ ). The remaining operators  $S_2$ ,  $S_3$ , and  $S_4$  are formed by four successive hopping processes.  $S_2$  is the first example for an operator which is *not prime*, but rather a composite operator. It appears here only due to the introduction of cumulants. Applying  $S_2$  is equivalent to applying  $S_1$  twice, and its main contribution comes from two spin-flip processes with overlapping sites.  $S_3$  creates a  $2 \times 2$  square of flipped spins. Finally,  $S_4$  creates all other four-site spin-flip configurations connected to each other.

Inserting (22) into (11) and (12) we obtain the following set of equations for the ground-state energy  $E_g$  and the coefficients  $\sigma_\nu$ :

$$E_g = \lim_{x \rightarrow 0} \left\langle H_1 \frac{1}{x - L_0} H_1 [1 + \sigma_1 S_1] \right\rangle_0^c, \quad (28)$$

$$0 = \sigma_1 \langle S_1^\dagger H_0 S_1 \rangle_0^c + \lim_{x \rightarrow 0} \left\langle S_1^\dagger H_1 \frac{1}{x - L_0} H_1 [1 + \sigma_1 S_1 + \tilde{\sigma}_2 S_2 + \sigma_3 S_3] \right\rangle_0^c, \quad (29)$$

$$\begin{aligned} 0 &= \langle S_2^\dagger H_0 [\tilde{\sigma}_2 S_2 + \sigma_3 S_3 + \sigma_4 S_4] \rangle_0^c + \lim_{x \rightarrow 0} \\ &\times \left\langle S_2^\dagger H_1 \frac{1}{x - L_0} H_1 [\sigma_1 S_1 + \tilde{\sigma}_2 S_2 + \sigma_3 S_3 + \sigma_4 S_4] \right\rangle_0^c \\ &+ \lim_{x \rightarrow 0} \left\langle S_2^\dagger H_1 \frac{1}{x - L_0} H_1 \left[ \sigma_1 \left( \tilde{\sigma}_2 - \frac{1}{3} \sigma_1^2 \right) \right. \right. \\ &\times S_1 S_2 + \sigma_1 \sigma_3 S_1 S_3 + \sigma_1 \sigma_4 S_1 S_4 \left. \left. \right] \right\rangle_0^c, \end{aligned} \quad (30)$$

$$\begin{aligned}
0 = & \langle S_3^\dagger H_0 [\tilde{\sigma}_2 S_2 + \sigma_3 S_3] \rangle_0^c + \lim_{x \rightarrow 0} \\
& \times \left\langle S_3^\dagger H_1 \frac{1}{x - L_0} H_1 [\sigma_1 S_1 + \tilde{\sigma}_2 S_2 + \sigma_3 S_3 + \sigma_4 S_4] \right\rangle_0^c \\
& + \lim_{x \rightarrow 0} \left\langle S_3^\dagger H_1 \frac{1}{x - L_0} H_1 \left[ \sigma_1 \left( \tilde{\sigma}_2 - \frac{1}{3} \sigma_1^2 \right) S_1 S_2 \right. \right. \\
& \left. \left. + \sigma_1 \sigma_3 S_1 S_3 + \sigma_1 \sigma_4 S_1 S_4 \right] \right\rangle_0^c, \quad (31)
\end{aligned}$$

where  $\tilde{\sigma}_2$  is defined by  $\tilde{\sigma}_2 \equiv \sigma_2 + (1/2)\sigma_1^2$ . An additional equation must be added which is obtained from (31) by interchanging indices  $3 \leftrightarrow 4$ . Next, all cumulant expectation values in (28) to (31) have to be evaluated. From this, a set of nonlinear equations for the coefficients  $\sigma_\nu$  is obtained. It can be reduced to a quartic equation for  $\sigma_1$ . The values for the coefficients are found to be  $\sigma_1 = 0.1756$ ,  $\sigma_2 = (-)2.32 \times 10^{-3}$ ,  $\sigma_3 = 3.04 \times 10^{-2}$ , and  $\sigma_4 = 8.85 \times 10^{-3}$ . The final value for the ground-state energy  $E_g$  for the Hubbard model at half filling and  $U \gg t$  is obtained from (28):

$$E_g = -1.1756 \times N \frac{4t^2}{U}, \quad U \gg t. \quad (32)$$

It agrees well with that of the Heisenberg model. Note that the coefficients  $\sigma_2$ ,  $\sigma_3$ , and  $\sigma_4$  are smaller by at least one order of magnitude than  $\sigma_1$ . This shows a tendency for rapid convergence when operators for multiple hoppings are added to the ansatz.

### III. GROUND-STATE ENERGY FOR GENERAL VALUES OF $U/t$

Next, let us consider the ground-state energy for smaller values of  $U/t$ . To see how the energy varies when  $U/t$  decreases, we have to add charge fluctuations to the ansatz (22) for  $\Omega$ , which will produce states with empty and doubly occupied sites. The simplest possible operator is

$$A_1 = \sum_{\langle ij \rangle \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma}, \quad j \in \text{sublattice } \sigma. \quad (33)$$

The quantity  $\hat{c}_{i\sigma}^\dagger$  has been defined already below Eq. (18). It describes the creation of an electron with spin  $\sigma$  on a site  $i$  where an electron with spin  $-\sigma$  is already present there. The operator  $A_1$  is written symbolically as

$$A_1 = \boxed{\uparrow \downarrow_i \bigcirc_j}. \quad (34)$$

The circle denotes a hole. The opposite-directed arrows indicate two opposite electron spins at the same site. We will also include two operators of second order in the hopping Hamiltonian  $H_t$ :

$$A_2 = (A_1)^2, \quad (35)$$

$$A_3 = \sum_{\langle ijk \rangle \sigma} \hat{c}_{i-\sigma}^\dagger \hat{c}_{j-\sigma} \hat{c}_{j\sigma}^\dagger \hat{c}_{k\sigma}, \quad k \in \text{sublattice } \sigma. \quad (36)$$

When evaluated with their respective Hermitian conjugates they are the only second order operators to yield nonzero expectation values. In other words, only those hopping operators of second order are included in the set  $A_\nu$  which represent *connected diagram* contributions to the energy. In symbols, a typical term in  $A_3$  would be

$$A_3 = \boxed{\uparrow \downarrow_i \uparrow_j \bigcirc_k} \quad (37)$$

where sites  $i$  and  $k$  ( $i \neq k$ ) are nearest neighbors of site  $j$ .

The resulting new ansatz for  $\Omega$  therefore reads

$$\Omega = \exp \left\{ \left[ \sum_{\nu=1}^4 \sigma_\nu S_\nu \right] + \left[ \sum_{\nu=1}^3 \alpha_\nu A_\nu \right] \right\}. \quad (38)$$

Equation (38) is valid for both large and moderate values of  $U/t$ . For the sake of simplicity, instead of using Eq. (12) we prefer in the following to evaluate the new coefficients  $\alpha_\nu$  from the original relation (6). We can do that because the *effective Hamiltonian*  $H_1[1/(x-L_0)]H_1$  in Eq. (12) was primarily devised to describe effective spin fluctuations for large values of the ratio  $U/t$ . Using (38), the following equations for  $\alpha_\nu$  are obtained from (6):

$$\begin{aligned}
0 = & \langle A_1^\dagger H_1 \rangle_0^c + \alpha_1 \langle A_1^\dagger H_0 A_1 \rangle_0^c + \sigma_1 \langle A_1^\dagger H_0 S_1 \rangle_0^c \\
& + \tilde{\alpha}_2 \langle A_1^\dagger H_0 A_2 \rangle_0^c + \alpha_3 \langle A_1^\dagger H_0 A_3 \rangle_0^c, \quad (39)
\end{aligned}$$

$$\begin{aligned}
0 = & \alpha_1 \langle A_2^\dagger H_1 A_1 \rangle_0^c + \tilde{\alpha}_2 \langle A_2^\dagger H_0 A_2 \rangle_0^c + \alpha_1 \sigma_1 \langle A_2^\dagger H_1 A_1 S_1 \rangle_0^c \\
& + \alpha_1 \left( \tilde{\alpha}_2 - \frac{1}{3} \alpha_1^2 \right) \langle A_2^\dagger H_1 A_1 A_2 \rangle_0^c + \alpha_1 \alpha_3 \langle A_2^\dagger H_1 A_1 A_3 \rangle_0^c, \quad (40)
\end{aligned}$$

$$\begin{aligned}
0 = & \alpha_1 \langle A_3^\dagger H_1 A_1 \rangle_0^c + \alpha_3 \langle A_3^\dagger H_0 A_3 \rangle_0^c + \alpha_1 \sigma_1 \langle A_3^\dagger H_1 A_1 S_1 \rangle_0^c \\
& + \alpha_1 \alpha_3 \langle A_3^\dagger H_1 A_1 A_3 \rangle_0^c. \quad (41)
\end{aligned}$$

We have defined  $\tilde{\alpha}_2 \equiv \alpha_2 + (1/2)\alpha_1^2$ . Note, also Eqs. (28)–(31) will be modified since the spin-fluctuation operators couple also to the new hopping operators  $A_\nu$ . The modified equation for the energy reads

$$E_g = \lim_{x \rightarrow 0} \left\langle H_1 \frac{1}{x - L_0} H_1 [1 + \sigma_1 S_1 + \alpha_2 A_2 + \alpha_3 A_3] \right\rangle_0^c. \quad (42)$$

However, to keep the calculation in the analytic realm we choose to leave Eqs. (29)–(31) for the spin-flip parameters  $\sigma_\mu$  unchanged. Their renormalisation by charge fluctuations is assumed to be small. (In the large  $U$  limit the  $\sigma_\mu$ 's must tend to the values found in the previous section, so the approximation is justified for large and moderate values of  $U$ ; as  $U$  tends to zero this approximation will break down.) In consequence, for smaller values of  $U$  the variation of the energy is mainly due to the new hopping operators just added. The coefficients  $\alpha_\nu$  are found after calculating the cumulants in (39)–(41). Keeping  $\sigma_1$  constant, with the value found above, again a system of nonlinear equations has to be solved. It reduces again to a single quartic equation. Finally, the solution for the coefficients  $\alpha_\nu$  is to be inserted into Eq. (42) for the energy.

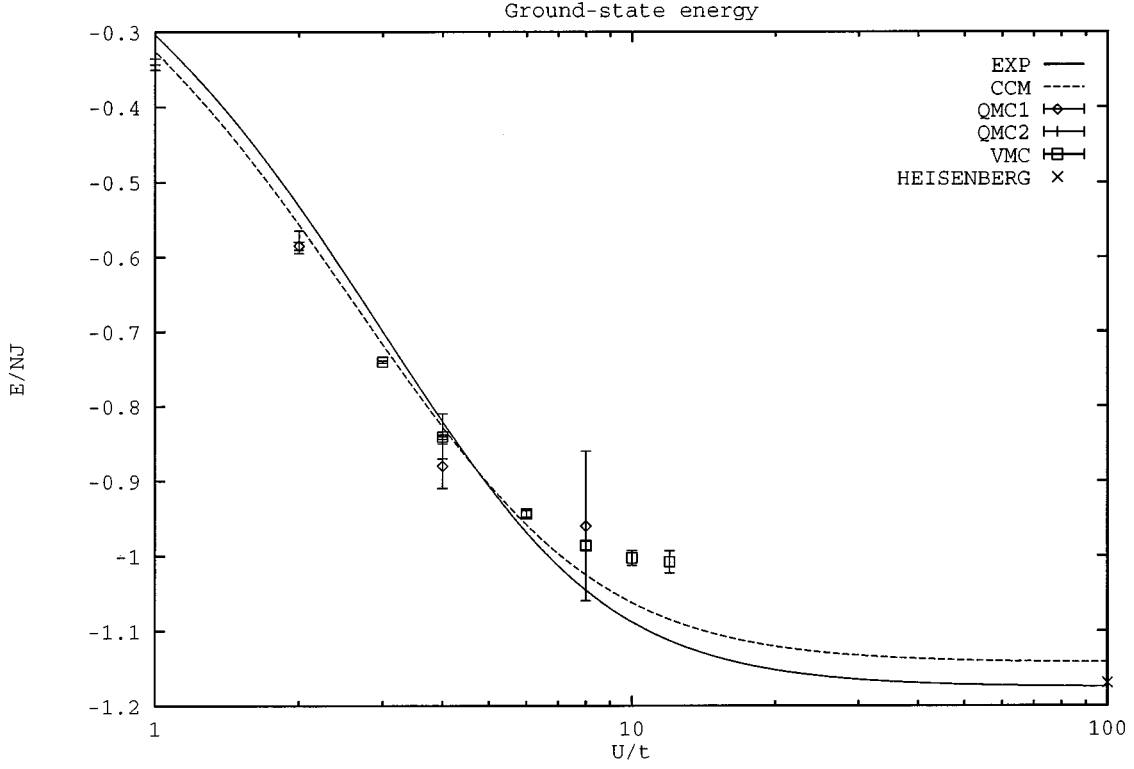


FIG. 1. Ground-state energy of the two-dimensional Hubbard model at half filling. The solid line is the result of the exponential (EXP) ansatz in its new formulation. The dotted line is the result of the couple-cluster method (CCM). Quantum Monte Carlo (QMC) and variational Monte Carlo (VMC) data are shown as well. The Heisenberg limit is indicated by a cross.

#### IV. RESULTS AND DISCUSSION

The result for  $E_g$  (in units of  $J=4t^2/U$ ) is plotted in Fig. 1 as function of  $U/t$  (full line). Quantum Monte Carlo (QMC) results<sup>15</sup> are available only in the weak and intermediate coupling regime, up to  $U/t=8$ . The variational Monte Carlo (VMC) method<sup>16</sup> provided results in the strong correlation regime too. Both QMC and VMC data points are shown in Fig. 1. The QMC and VMC results agree well where both are available. However, in the strong coupling regime the VMC results can only set an upper bound for the ground-state energy. The authors themselves recognized<sup>16</sup> that in this regime they failed to take fully into account the strong spin fluctuations which should further reduce the energy (as well as the staggered magnetization). It is to be noted that our results for the energy lie below the VMC results; at the same time, our results tend monotonically to the correct value at the infinite  $U$  limit. The infinite  $U$  value, indicated by a cross on the figure, is the QMC result<sup>14</sup> for the Heisenberg antiferromagnet. This improvement, then, can be attributed to the spin-fluctuation operators included in our exponential ansatz in its new formulation. Due to our approximations (leaving the coefficients  $\sigma_\mu$  unchanged from their values at large  $U$ ), our results are less accurate than those of Refs. 9–11 for  $U < 4t$ , as evidenced in the figure.

It was mentioned above that the coupled-cluster method is an alternative size-consistent many-body approach to ground-state properties. This method starts from the following ansatz for the exact ground state:

$$|\Psi_g\rangle = e^S |\phi_0\rangle. \quad (43)$$

The vector  $|\phi_0\rangle$  is a model state. The operator  $S$  is decomposed into  $S = \sum_\nu \eta_\nu S_\nu$ , where  $S_\nu$  are so-called multiconfigurational excitation operators with respect to  $|\phi_0\rangle$ . The equations for the ground-state energy  $E_g$  and the coefficients  $\eta_\nu$  are given within the coupled-cluster treatment by

$$E_g = \langle \phi_0 | e^{-S} H e^S | \phi_0 \rangle, \quad (44)$$

$$0 = \langle \phi_0 | S_\nu^\dagger e^{-S} H e^S | \phi_0 \rangle. \quad (45)$$

Note the similarity of these equations with the cumulant equations (5) and (6). The configurational excitation operators  $S_\nu$  correspond to the fluctuation operators  $A_\nu$  in the cumulant approach.

Applying the coupled-cluster treatment to the Hubbard model at half filling,<sup>9–11</sup> up to six configurational excitation variables  $S_\nu$  were used. In the large  $U$  limit they correspond to our variables  $A_1$ , Eq. (34), and  $S_1$  from Eq. (23). Recall that these operators produce charge and spin fluctuations when applied on the Néel state. The resulting ground-state energy is also shown in Fig. 1 as a function of  $U/t$  (dotted line). As can be seen, for large values of  $U/t$ , the coupled-cluster results deviate from our results, although they improve upon the variational Monte Carlo results. To trace back in more detail the reasons for these deviations, note that the coupled-cluster result for the ground-state energy of the Hubbard model is  $-(8/7)JN$  for large  $U$ , as compared to about  $-(7/6)JN$  for the Heisenberg antiferromagnet, within the framework of the same method.<sup>8</sup> The coupled-cluster result for the Hubbard model may be understood also within the cumulant approach based on Eqs. (5) and (6), which then

gives the same number: To show this, we use the same fluctuation operators  $A_1$  and  $S_1$  and find the following cumulant equations for the parameters  $\lambda_1$  and  $\sigma_1$  for  $U \gg t$ :

$$E_g = \langle H \rangle_0 + \lambda_1 \langle H_1 A_1 \rangle_0^c, \quad (46)$$

$$0 = \langle A_1^\dagger H_1 \rangle_0^c + \sigma_1 \langle A_1^\dagger H_1 S_1 \rangle_0^c + \lambda_1 \langle A_1^\dagger H_0 A_1 \rangle_0^c + \frac{\lambda_1^2}{2} \langle A_1^\dagger H_1 A_1^2 \rangle_0^c, \quad (47)$$

$$0 = \lambda_1 \langle S_1^\dagger H_1 A_1 \rangle_0^c + \sigma_1 \langle S_1^\dagger H_0 S \rangle_0^c + \lambda_1 \sigma_1 \langle S_1^\dagger H_1 A_1 S_1 \rangle_0^c. \quad (48)$$

It is easy to solve for the energy. For large  $U/t$  one obtains

$$E_g = - \frac{\langle A_1^\dagger H_1 \rangle_0^c \langle H_1 A_1 \rangle_0^c}{\langle A_1^\dagger H_0 A_1 \rangle_0^c} - \frac{\langle A_1^\dagger H_1 S_1 \rangle_0^c \langle S_1^\dagger H_1 A_1 \rangle_0^c \langle H_1 A_1 \rangle_0^c}{\langle A_1^\dagger H_0 A_1 \rangle_0^c \langle S_1^\dagger H_1 A_1 S_1 \rangle_0^c}. \quad (49)$$

As mentioned before this results in

$$E_g = -4Nt^2 \frac{1 + 1/7}{U} = -\frac{8}{7}JN. \quad (50)$$

If one compares with the ground-state energy of the Heisenberg antiferromagnet,  $H_J$ , one realizes that the first term in (49) corresponds to the Ising part, and the second one to the spin-fluctuation part of  $H_J$ . The number 7 in (50) is due to the following cumulant from Eq. (49):

$$\langle S_1^\dagger H_1 A_1 S_1 \rangle_0^c = \langle S_1^\dagger H_1 A_1 S_1 \rangle_0 - \langle S_1^\dagger S_1 \rangle_0 \langle H_1 A_1 \rangle_0 = 7 \times 4tN. \quad (51)$$

It describes all connected diagrams which combine spin and charge fluctuations, when applied to the Néel state  $|\phi_0\rangle$ . There are contributions from altogether *seven* bonds which are tied to a pair of two neighboring flipped spins.

By starting instead from the modified cumulant equations (11) and (12) the large  $U$  result for the ground-state energy is given by

$$E_g = \langle H^{\text{eff}} \rangle_0^c - \frac{\langle S_1^\dagger H^{\text{eff}} \rangle_0^c \langle H^{\text{eff}} S_1 \rangle_0^c}{\langle S_1^\dagger H^{\text{eff}} S_1 \rangle_0^c}. \quad (52)$$

Here

$$H^{\text{eff}} = \lim_{x \rightarrow 0} H_1 \frac{1}{x - L_0} H_1 \quad (53)$$

is the effective Hamiltonian of second order in the hopping term  $H_1 = H_t$ , introduced just below Eq. (12). The operators  $H_1$  and  $L_0$  are entities in the cumulant ordering. The result (52) agrees with that derived from the Heisenberg exchange (21). Depending on the respective cumulant expectation values,  $H^{\text{eff}}$  takes over the role of either the Ising part or the spin-fluctuation part of the Heisenberg antiferromagnet. The second term of Eq. (52) describes an effective spin-fluctuation contribution to the ground-state energy from second order in  $H_1$ . This leads to a further lowering by an amount of  $(1/6)NJ$ , as was already discussed below Eq. (21). The correct factor 6, instead of 7, is evaluated from the cumulant  $\langle S_1^\dagger H^{\text{eff}} S_1 \rangle_0^c$  in the dominator of (52). The factor 6 is due to the six frustrated Ising bonds surrounding a pair

of flipped spins. The bond connecting the two flipped spins is correctly excluded since it is not frustrated. This is not the case in (49) or in the coupled-cluster treatment of the Hubbard model.<sup>9-11</sup> Together with the effective Ising part, i.e., the first term of (52), this leads to the (almost) correct ground-state energy value of  $-(7/6)NJ$  for the Hubbard model at half filling and large  $U/t$ .

This result demonstrates the advantage of the present cumulant approach in the modified form (11) and (12) as compared to the original version (5) and (6). To improve upon the coupled-cluster approach to the Hubbard model<sup>9-11</sup> one should take into account more spin-fluctuation operators, like  $S_3$  and  $S_4$  of Eqs. (25) and (26), which were in fact used in the application of the coupled-cluster method to the Heisenberg model,<sup>8</sup> leading to an energy value close to  $-(7/6)NJ$ .

One should mention that nonlinear terms which appear in the equations for the parameters  $\lambda_1$  and  $\sigma_1$  make the result (52) for  $E_g$  somewhat worse again. This is the reason why we have included in Sec. III in the ansatz for  $\Omega$  the new variables  $S_2, S_3, S_4$ , and  $A_2, A_3$  for higher spin and charge fluctuations, respectively. They improve the result for  $E_g$  again. The new variables have to include composite quantities, i.e., products of entities in the cumulant ordering, since the nonlinear terms in the equations for  $\lambda_1$  and  $\sigma_1$  leading to (52) are composed of products of entities as well. For the extended ansatz the new equations (29) and (39) for  $\lambda_1$  and  $\sigma_1$  turn out to be linear again, with linear couplings to the new parameters  $\tilde{\lambda}_2, \tilde{\sigma}_2, \dots$ . Instead, the equations for the latter parameters contain nonlinear terms again. However, the final result for  $E_g$  changes now only slightly upon inclusion of these terms.

We remark here that the original cumulant formulation (5) and (6) of the exponential ansatz should also lead to the same result as with the new formulation (11) and (12) where an effective Hamiltonian appears. However, the sets of fluctuation operators must be much larger in this case, to account for the intermediate processes induced by the construction of the effective Hamiltonian in the new formulation. This will also be the case for the coupled-cluster method. Without these intermediate set of operators, there will be no coupling to the operators of higher orders in the hopping Hamiltonian.

In the next section we show that composite variables evolve quite naturally from the continued fraction expansion of the ground-state energy  $E_g$ . In fact, there is a close relationship between the continued fraction and the ansatz  $\exp(S)$  for the wave operator  $\Omega$  with properly chosen fluctuation variables including composite ones. This will be demonstrated in the next section.

## V. COMPARISON WITH PROJECTION TECHNIQUE

In this final section we compare our expression for the ground-state energy  $E_g$  with an expression which one obtains by applying the projection technique directly on Eqs. (1) and (3). By combining both equations,  $E_g$  can be put into the form

$$E_g = \langle H \rangle_0 + \lim_{x \rightarrow 0} \varphi(x), \quad (54)$$

$$\varphi(x) = \left( H_1 \left| \frac{1}{x - L_0 - H_1} H_1 \right. \right). \quad (55)$$

For convenience, we have defined a new metric

$$(A|B) = \langle A^\dagger B \rangle_0^c \quad (56)$$

which uses cumulant expectation values with respect to the unperturbed ground state  $|\phi_0\rangle$  of  $H_0$ . Expression (55) is convenient for evaluation by use of the projection operator technique. We start by decomposing  $H_1$  into a sum of operators which are eigenvectors of  $L_0$  to different eigenvalues  $\Delta_\nu$ , i.e.,

$$H_1 = \sum_\nu A_\nu, \quad (57)$$

$$L_0 A_\nu = [H_0, A_\nu]_- = \Delta_\nu A_\nu. \quad (58)$$

With (57) the quantity  $\varphi(x)$  can be decomposed into

$$\varphi(x) = \sum_{\mu, \nu} \varphi_{\mu\nu}(x), \quad (59)$$

$$\varphi_{\mu\nu}(z) = \left( A_\mu \left| \frac{1}{z - L_0 - H_1} A_\nu \right. \right). \quad (60)$$

By use of the well-known identity from projection formalism,<sup>17,18</sup> it can be shown that  $\varphi_{\mu\nu}(x)$  obeys the following set of linear equations:

$$\sum_{\eta} [x \chi_{\mu\nu} - \omega_{\mu\nu} - M_{\mu\nu}(x)] \chi_{\nu\eta}^{-1} \varphi_{\eta\mu'}(x) = \chi_{\mu\mu'}. \quad (61)$$

The new quantities  $\chi_{\mu\nu}$ ,  $\omega_{\mu\nu}$ , and  $M_{\mu\nu}$  are generalized susceptibility, frequency, and memory matrices. They are defined by

$$\chi_{\mu\nu} = (A_\mu | A_\nu), \quad (62)$$

$$\omega_{\mu\nu} = (A_\mu | [L_0 + H_1] A_\nu), \quad (63)$$

$$M_{\mu\nu}(x) = \left( H_1 A_\mu \left| Q \frac{1}{x - Q(L_0 + H_1)Q} Q H_1 A_\nu \right. \right). \quad (64)$$

In (64) the quantity  $Q$  is a projection operator. It projects onto the subspace perpendicular to that spanned by  $\{A_\nu\}$ , i.e.,

$$Q = 1 - P \text{ with } P = \sum_{\mu, \nu} |A_\mu\rangle \chi_{\mu\nu}^{-1} \langle A_\nu|. \quad (65)$$

Comparing the memory matrix (64) with the original quantity  $\varphi_{\mu\nu}(x)$ , Eq. (60), one finds that both have the same structure: Expression (64) is found from (60) by replacing  $L_0 + H_1$  by  $Q[L_0 + H_1]Q$  and  $A_\nu$  by  $QH_1 A_\nu$ . As above, we can decompose the latter quantity  $QH_1 A_\nu$  into new eigenvectors of  $QL_0Q$  and derive a new set of “equations of motion” for  $M_{\mu\nu}(x)$ . Repeating this procedure results in an infinite continued fraction expansion for the ground-state energy  $E_g$ .

Usually, continued fraction expansions have to be terminated after some steps due to the increasing effort necessary for evaluating the new coefficients of successive denomina-

tors. However, there is a close relationship between the expression for  $E_g$ , obtained from the exponential ansatz, and the continued fraction expansion. It may be shown that  $E_g$ , found from the exponential ansatz, coincides with the continued fraction expression up to a certain denominator depending on the chosen set of fluctuation operators. At the same time, the exponential ansatz represents an infinite (partial) summation of the continued fraction.

To show this, let us use the following ansatz for the wave operator:

$$\Omega = \exp \left[ \sum_{n=1}^{\infty} \left( \sum_{\nu} \lambda_n^{(\nu)} A_n^{(\nu)} \right) \right], \quad (66)$$

where the first sum runs over all powers  $n$  of  $H_1$ . The set of excitation operators  $\{A_n^{(\nu)}\}$  is found from a decomposition of  $(H_1)^n$  into eigenvectors of  $L_0$ . Most important, it includes both prime and composite operators. The composite operators of order  $n$  should include all possible products of lower order operators (either prime or composite). For instance, when  $n=2$ , the set of operators  $\{A_2^{(\nu)}\}$  must include all composite operators  $\{A_1^{(\nu')} \cdot A_1^{(\nu'')}\}$ . When applied to the unperturbed ground state  $|\phi_0\rangle$  we find

$$(H_1)^n |\phi_0\rangle = \sum_{\nu} A_n^{(\nu)} |\phi_0\rangle \quad (67)$$

with

$$L_0 A_n^{(\nu)} = \Delta_n^{(\nu)} A_n^{(\nu)}, \quad (68)$$

$$(A_m^{(\mu)} | A_n^{(\nu)}) = 0 \text{ for } m \neq n. \quad (69)$$

The orthogonality condition in (69) is used in order to simulate the role of the projection operator  $Q$  used in the projection method. When expanding the exponential ansatz (66), products of operators  $A_{n_1}^{(\nu_1)} \cdot A_{n_2}^{(\nu_2)} \cdot \dots \cdot A_{n_k}^{(\nu_k)}$  ( $n_1 + n_2 + \dots + n_k = n$ ) appear, which are already contained as composite operators  $A_n^{(\nu)}$  of order  $n$  in (66). Thus in the series expansion of (66) these quantities can be regrouped together with new coefficients  $\tilde{\lambda}_n^{(\nu)}$ . As an example, compare  $\tilde{\alpha}_2$  just below Eq. (41). Therefore, the wave operator reduces to the following linear form:

$$\Omega = 1 + \sum_{n=1}^{\infty} \left( \sum_{\nu} \tilde{\lambda}_n^{(\nu)} A_n^{(\nu)} \right). \quad (70)$$

The new coefficients  $\tilde{\lambda}_n^{(\nu)}$  are in general nonlinear combinations of the old coefficients  $\lambda_n^{(\nu)}$ . (Note, however, that  $\tilde{\lambda}_1^{(\nu)} = \lambda_1^{(\nu)}$ .) The resulting equations for  $\tilde{\lambda}_n^{(\nu)}$  are found from (6) and turn out to be linear:

$$\begin{aligned} 0 &= (A_1^{(\mu)} | H \Omega) \\ &= (A_1^{(\mu)} | H_1) + \sum_{\nu'} \tilde{\lambda}_n^{(\nu')} (A_1^{(\mu)} | H_0 A_1^{(\nu')}) \\ &\quad + \sum_{\nu''} \tilde{\lambda}_2^{(\nu'')} (A_1^{(\mu)} | H_1 A_2^{(\nu'')}), \end{aligned} \quad (71)$$

$$\begin{aligned}
0 &= (A_n^{(\mu)} | H \Omega) \\
&= \sum_{\nu} \tilde{\lambda}_{n-1}^{(\nu)} (A_n^{(\mu)} | H_1 A_{n-1}^{(\nu)}) + \sum_{\nu'} \tilde{\lambda}_n^{(\nu')} \\
&\quad \times (A_n^{(\mu)} | H_0 A_n^{(\nu')}) + \sum_{\nu''} \tilde{\lambda}_{n+1}^{(\nu'')} (A_n^{(\mu)} | H_1 A_{n+1}^{(\nu'')}), \quad n \geq 2.
\end{aligned} \tag{72}$$

All we need is to find the first coefficient  $\lambda_1^{(\nu)}$  since

$$E_g = \langle H \rangle_0 + \sum_{\nu} \lambda_1^{(\nu)} (H_1 | A_1^{(\nu)}). \tag{73}$$

With respect to the lower index  $n$  the above system of linear equations (71) and (72) for  $\tilde{\lambda}_n^{(\nu)}$  can be written in matrix form. However, each matrix element by itself corresponds to a block matrix. Its dimension depends on the upper indices  $\mu, \nu$ :

$$\sum_{n'} \mathcal{M}_{nn'} \tilde{\lambda}_{n'} = V_n. \tag{74}$$

Here and in the following we suppress the index indicating the elements inside a given block. All elements of the vector  $V_n$  are zero except for  $n=1$  where  $V_1^\mu = (A_1^{(\mu)} | H_1)$ . In block form,  $\mathcal{M}$  is tridiagonal:

$$\mathcal{M}_{nn'} = \begin{pmatrix} \mathcal{M}_{11} & \mathcal{M}_{12} & & & \\ \mathcal{M}_{12}^T & \mathcal{M}_{22} & \mathcal{M}_{23} & & \\ & \mathcal{M}_{23}^T & \mathcal{M}_{33} & \mathcal{M}_{34} & \\ & & \mathcal{M}_{34}^T & \mathcal{M}_{44} & \mathcal{M}_{45} \\ & & & \mathcal{M}_{45}^T & \ddots \end{pmatrix} \tag{75}$$

where we have defined

$$M_{nn}^{\nu\mu} = (A_n^{(\nu)} | H_0 A_n^{(\mu)}), \tag{76}$$

$$M_{nn+1}^{\nu\mu} = (A_n^{(\nu)} | H_1 A_{n+1}^{(\mu)}), \tag{77}$$

and  $T$  denotes the transposed matrix. The solution for  $\tilde{\lambda}_1$  is easily obtained recursively:

$$\tilde{\lambda}_1 = \mathcal{M}_{11}^{-1} \cdot V_1, \tag{78}$$

$$\mathcal{M}_{11}^{-1} = (\mathcal{M}_{11} - \mathcal{M}_{12} \cdot \mathcal{M}_{22}^{-1} \cdot \mathcal{M}_{12}^T)^{-1}, \tag{79}$$

$$\mathcal{M}_{22}^{-1} = (\mathcal{M}_{22} - \mathcal{M}_{23} \cdot \mathcal{M}_{33}^{-1} \cdot \mathcal{M}_{23}^T)^{-1}, \tag{80}$$

$$\mathcal{M}_{33}^{-1} = (\mathcal{M}_{33} - \mathcal{M}_{34} \cdot \mathcal{M}_{44}^{-1} \cdot \mathcal{M}_{34}^T)^{-1}, \tag{81}$$

etc. When inserted into Eq. (73) the solution for  $E_g$  is nothing but the continued fraction expansion obtained from projection technique. Note, when the ansatz (66) for  $\Omega$  contains only a *finite* number of fluctuation operators, it is impossible to arrive at the linearized form (70) for  $\Omega$ . This was already demonstrated for the simple example in Sec. I. The exponential ansatz (66) provides an infinite summation of the continued fraction.

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