Self-consistent random phase approximation: Application to the Hubbard model for finite number of sites

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(Received 8 July 2004; revised manuscript received 16 November 2004; published 22 February 2005)

Within the one-dimensional Hubbard model linear closed chains with various numbers of sites are considered in the self-consistent random phase approximation (SCRPA). Excellent results with a minimal numerical effort are obtained for $(2+4n)$-site cases, confirming earlier results with this theory for other models. However, the $4n$-site cases need further consideration. The SCRPA solves the two-site problem exactly. It therefore contains the two-electron and high-density Fermi gas limits correctly.

I. INTRODUCTION

The standard random phase approximation (s-RPA) is one of the most popular many-body approaches known. It was invented in condensed matter physics (see, e.g., Ref. 1) and has subsequently spread to almost all branches of physics, including atomic physics,[2] molecular physics,[3] plasma physics,[4] relativistic field theory,[5] nuclear physics,[6] and many more. The definition of the s-RPA is not uniform, depending on whether exchange is included or not. We understand it—e.g., as in nuclear physics[6]—as the small-amplitude limit of time-dependent Hartree-Fock (TDHF) theory and therfore with exchange. Its popularity probably stems from its conceptual simplicity, its numerical tractability (in spite of some serious problems in finite-size systems), and most of all its well-behaved properties concerning fulfillment of conservation laws (Ward identies), Goldstone theorem, and restoration of spontaneously broken symmetries. Though there exist respectable general theories (see, e.g., Refs. 7 and 8), any practical attempt to go beyond this basic HF-RPA scheme conserving these properties turned out to be technically extremely demanding and no well-accepted general and practical extension has emerged so far. Nevertheless, the standard RPA has also quite serious shortcomings and it is desirable to overcome them. One of the most prominent is its violation of the Pauli principle, often paraphrased as the "quasiboson approximation." It is most critical for only moderately collective modes or when the self-interaction of the gas of quantum fluctuations becomes important as in ultrasmall finite quantum systems. Since a couple of years two of the present authors and collaborators have been working on a nonlinear extension of the RPA (Ref. 9) which has shown surprisingly accurate results in a number of nontrivial models.[10] It is called the self-consistent RPA (SCRPA) and can be obtained from minimizing an energy-weighted sum rule. Therefore the s-RPA which is perturbative in the sense that it sums a certain class of diagrams (the bubbles) is upgraded in the SCRPA to a nonperturbative variational theory though it is in general not of the Raleigh-Ritz type. A strong bonus of this extension of the s-RPA is that it generally preserves its positive features as conservation laws and restoration of symmetries as well as numerical tractability, since it leads to equations of the Schrödinger type.[11] In this paper we want to apply this theory to the Hubbard model for strongly correlated electrons. Because of its necessarily increased numerical complexity over the s-RPA, we first want to consider finite clusters in reduced dimensions. Before going into the details, let us very briefly repeat the main ideas of the SCRPA.

One way of presentation is to outline its strong analogy with the Hartree-Fock-Bgoliubov (HFB) approach to interacting boson fields $b^\dagger$ and b. The HFB canonical transformation reads

$$q_\nu^\dagger = \sum_i u_{i,\nu} b_i^\dagger - v_{i,\nu} b_i. \tag{1}$$

The amplitudes u and v can be determined[12] from minimizing the following mean energy (energy-weighted sum rule):

$$\omega_\nu = \frac{\langle 0|[q_\nu,[H,q_\nu^\dagger]]|0\rangle}{\langle 0|[q_\nu,q_\nu^\dagger]|0\rangle}, \quad (2)$$

where H is the usual many-body Hamiltonian with two-body interactions and the ground state $|0\rangle$ is supposed to be the vacuum to the quasiboson operators q_ν—i.e.,

$$q_\nu|0\rangle = 0. \quad (3)$$

With this scheme and the usual orthonormalization conditions for the amplitudes u and v, which allows the inversion of Eq. (1), one derives standard HFB theory[6] with no need to construct $|0\rangle$ explicitly. Of course, in this way the fact that the HFB theory is a Raleigh-Ritz variational theory is not manifest but the scheme has the advantage to be physically transparent and to lead to the final equations with a minimum of mathematical effort.

For the SCRPA we follow exactly the same route. We replace in Eq. (1) the ideal boson operators by fermion pair operators of the particle-hole (ph) type and form an ansatz for a general transformation of ph-fermion pairs:

$$Q_\nu^\dagger = \sum_{ph} (\mathcal{X}_{ph}^\nu a_p^\dagger a_h - \mathcal{Y}_{ph}^\nu a_h^\dagger a_p), \quad (4)$$

with $|\nu\rangle = Q_\nu^\dagger|0\rangle$ an excited state of the spectrum. In analogy with Eq. (2) we minimize a mean excitation energy

$$\Omega_\nu = \frac{\langle 0|[Q_\nu,[H,Q_\nu^\dagger]]|0\rangle}{\langle 0|[Q_\nu,Q_\nu^\dagger]|0\rangle}, \quad (5)$$

with $|0\rangle$, in analogy with Eq. (3), the vacuum to the operators Q_ν, i.e.,

$$Q_\nu|0\rangle = 0, \quad (6)$$

and arrive at equations of the usual RPA type:[6]

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B}^* & -\mathcal{A}^* \end{pmatrix}\begin{pmatrix} \mathcal{X}^\nu \\ \mathcal{Y}^\nu \end{pmatrix} = \Omega_\nu \begin{pmatrix} \mathcal{X}^\nu \\ \mathcal{Y}^\nu \end{pmatrix}, \quad (7)$$

with

$$\mathcal{A}_{ph,p'h'} = \frac{\langle 0|[a_h^\dagger a_p,[H,a_{p'}^\dagger a_{h'}]]|0\rangle}{\sqrt{n_h - n_p}\sqrt{n_{h'} - n_{p'}}},$$

$$\mathcal{B}_{ph,p'h'} = -\frac{\langle 0|[a_h^\dagger a_p,[H,a_{h'}^\dagger a_{p'}]]|0\rangle}{\sqrt{n_h - n_p}\sqrt{n_{h'} - n_{p'}}}. \quad (8)$$

Here we supposed to work in a single-particle basis which diagonalizes the density matrix (natural orbits),

$$\langle 0|a_k^\dagger a_{k'}|0\rangle \equiv n_k \delta_{kk'}, \quad (9)$$

and therefore the n_k's are the occupation numbers. For H with a two-body interaction, Eqs. (8) only contain correlation functions of the $\langle a^\dagger a\rangle$ and $\langle a^\dagger a a^\dagger a\rangle$ types and, since Eq. (6) admits the usual RPA orthonormalization relations for the amplitudes $\mathcal{X}$ and $\mathcal{Y}$,[6] the relation (4) can be inverted and with Eq. (6) the correlation functions in Eq. (8) be expressed by $\mathcal{X}$ and $\mathcal{Y}$.

However, to be complete, occupation numbers $n_k = \langle 0|a_k^\dagger a_k|0\rangle$ and two-body correlation functions with other

index combinations than two-times particle and two-times hole need extra considerations. That will be done in the main text. This is, in short, the SCRPA scheme which, as HFB theory, is obviously non-linear, since the elements $\mathcal{A}$ and $\mathcal{B}$ in Eq. (7) become functionals of the $\mathcal{X}$ and $\mathcal{Y}$ amplitudes. We want to point out that no bosonization of fermion pairs is operated at any stage of the theory.

We want to apply this scheme to the Hubbard model of strongly correlated electrons which is one of the most wide-spread models to investigate strong electron correlations and high-T_c superconductivity. Its Hamiltonian is given by

$$H = -t\sum_{\langle ij\rangle\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, \quad (10)$$

where $c_{i\sigma}^\dagger$ and $c_{j\sigma}$ are the electron creation and destruction operators at site i and the $\hat{n}_{i\sigma} = c_{i\sigma}^+ c_{i\sigma}$ are the number operators for electrons at site i with spin projection σ. As usual t is the nearest-neighbor hopping integral and U the on-site Coulomb matrix element. In this exploratory work, we will limit ourselves to the simplest cases possible; i.e., we will consider closed chains in one dimension (1D) with an increasing number of sites at half filling, starting with the two-site problem. It will turn out that the next case of four sites is a configuration with degeneracies which cause problems in the SCRPA, as do all $4n(n=1,2,3,\dots)$ configurations in 1D. We therefore will postpone the treatment of these cases to future work and directly jump to the case of six-sites and only shortly outline at the end why the four-site case is unfavorable and how the problem can eventually be cured. In this work we will stop with the six-site case, considering it as sufficiently general to be able to extrapolate to the more-electron case. In this way one may hope to approach the thermodynamic limit in increasing the number of sites as much as possible. Let us mention that an earlier attempt to solve the SCRPA in 1D in the thermodynamic limit in a strongly simplified version of the SCRPA, the so-called renormalized RPA (r-RPA), produced interesting results.[13]

In detail our paper is organized as follows: in Sec. II we present the two-site case with its exact solution. In Sec. III we outline the six-site case with a detailed discussion of the results, and in Sec. IV we present the difficulties encountered in the four-site case and how, eventually, one can overcome them. Finally in Sec. V we give our conclusions together with some perspectives of this work.

II. TWO-SITE PROBLEM

In this section we will apply the general formalism of the SCRPA outlined in the Introduction to the two-site problem at half filling—i.e., two electrons with periodic boundary conditions. This case may seem trivial; the fact, however, is that such popular many-body approximations as the s-RPA, GW,[14] Gutzwiller wave function,[15] the two-particle self-consistent (TPSC) approach by Vilk, Chen, and Tremblay,[16] etc., do not yield very convincing results in this study case, whereas it has recently been shown that the SCRPA solves two-body problems exactly.[10,11,17] We again will briefly demonstrate this here for the two-site problem.

First we will transform Eq. (10) into momentum space. With the usual transformation to plane waves, $c_{j,\sigma}$

$=(1/\sqrt{N})\Sigma_{\mathbf{k}}a_{\tilde{\mathbf{k}},\sigma}e^{-i\tilde{\mathbf{k}}\cdot\tilde{\mathbf{x}}_j}$, this leads to the standard expression for a zero-range two-body interaction:

$$H = \sum_{\tilde{\mathbf{k}},\sigma}(\epsilon_k - \mu)\hat{n}_{\tilde{\mathbf{k}},\sigma} + \frac{U}{2N}\sum_{\tilde{\mathbf{k}},\tilde{\mathbf{p}},\tilde{\mathbf{q}},\sigma}a_{\tilde{\mathbf{k}},\sigma}^{\dagger}a_{\tilde{\mathbf{k}+\tilde{\mathbf{q}}},\sigma}a_{\tilde{\mathbf{p}},-\sigma}^{\dagger}a_{\tilde{\mathbf{p}-\tilde{\mathbf{q}}},-\sigma},$$

$$(11)$$

where $\hat{n}_{\tilde{\mathbf{k}},\sigma}=a_{\tilde{\mathbf{k}},\sigma}^{\dagger}a_{\tilde{\mathbf{k}},\sigma}$ is the occupation number operator of the mode $(\tilde{\mathbf{k}},\sigma)$ and the single-particle energies are given by $\epsilon_{\tilde{\mathbf{k}}}=-2t\Sigma_{d=1}^{D}\cos(k_d)$ with the lattice spacing set to unity.

For our further considerations it is convenient to transform Eq. (11) to HF quasiparticle operators via (we switch to 1D)

$$a_{h,\sigma} = b_{h,\sigma}^{\dagger}, \quad a_{p,\sigma} = b_{p,\sigma}, \quad (12)$$

where h and p are momenta below and above the Fermi momentum, respectively, so that $b_{k,\sigma}|\text{HF}\rangle=0$ for all k where $|\text{HF}\rangle$ is the Hartree-Fock ground state in the plane-wave basis. For the two-site problem with periodic boundary conditions we then write, after normal ordering, the Hamiltonian (11) in the following way:

$$H = H_{HF} + H_{q=0} + H_{q=\pi}, \quad (13)$$

with

$$H_{HF} = E_{HF} + \sum_{\sigma}[-\epsilon_1\tilde{n}_{k_1,\sigma} + \epsilon_2\tilde{n}_{k_2,\sigma}],$$

$$\epsilon_1 = -t + \frac{U}{2}, \quad \epsilon_2 = t + \frac{U}{2}, \quad (14)$$

$$H_{q=0} = \frac{U}{2}(\tilde{n}_{k_2,\uparrow} - \tilde{n}_{k_1,\uparrow})(\tilde{n}_{k_2,\downarrow} - \tilde{n}_{k_1,\downarrow}), \quad (15)$$

$$H_{q=\pi} = -\frac{U}{2}(J_{\uparrow}^{-} + J_{\uparrow}^{+})(J_{\downarrow}^{-} + J_{\downarrow}^{+}), \quad (16)$$

and $J_{\sigma}^{-}=b_{1,\sigma}b_{2,\sigma}$, $J_{\sigma}^{+}=(J_{\sigma}^{-})^{+}$, and $\tilde{n}_{k_i,\sigma}=b_{i,\sigma}^{\dagger}b_{i,\sigma}$, where we introduced the abbreviation "1" and "2" for the two momenta $k_1=0$ and $k_2=-\pi$ of the system, respectively. The HF ground state is $|\text{HF}\rangle=b_{1,\uparrow}b_{1,\downarrow}|\text{vac}\rangle$ and the corresponding energy is given by

$$E_0^{HF} = \langle\text{HF}|H|\text{HF}\rangle = -2t + \frac{U}{2}. \quad (17)$$

The RPA excitation operator corresponding to Eq. (4) can, because of rotational invariance in spin-space, be separated according to spin-singlet ($S=0$, charge) and spin-triplet ($S=1$) excitations. The latter still can be divided into spin-longitudinal ($S=1, m_s=0$) and spin-transverse ($S=1, m_s=\pm1$) excitations. Let us first consider the charge- and spin-longitudinal sectors. For later convenience we will not separate them and write, for the corresponding RPA operator,

$$Q_{\nu}^{\dagger} = \mathcal{X}_{\uparrow}^{\nu}K_{\uparrow}^{+} + \mathcal{X}_{\downarrow}^{\nu}K_{\downarrow}^{+} - \mathcal{Y}_{\uparrow}^{\nu}K_{\uparrow}^{-} - \mathcal{Y}_{\downarrow}^{\nu}K_{\downarrow}^{-}, \quad (18)$$

where $K_{\sigma}^{\pm}=J_{\sigma}^{\pm}/\sqrt{1-\langle M_{\sigma}\rangle}$, $M_{\sigma}=\tilde{n}_{1\sigma}+\tilde{n}_{2\sigma}$, and the mean values $\langle\cdots\rangle$ are always taken with respect to the RPA vacuum:

$$Q_{\nu}|\text{RPA}\rangle = 0. \quad (19)$$

Because of the orthonormality relations

$$\sum_{\sigma}(\mathcal{X}_{\sigma}^{\nu}\mathcal{X}_{\sigma}^{\nu'} - \mathcal{Y}_{\sigma}^{\nu}\mathcal{Y}_{\sigma}^{\nu'}) = \delta_{\nu\nu'},$$

$$\sum_{\sigma}(\mathcal{X}_{\sigma}^{\nu}\mathcal{Y}_{\sigma}^{\nu'} - \mathcal{Y}_{\sigma}^{\nu}\mathcal{X}_{\sigma}^{\nu'}) = 0,$$

$$\sum_{\nu}(\mathcal{X}_{\sigma}^{\nu}\mathcal{X}_{\sigma'}^{\nu} - \mathcal{Y}_{\sigma}^{\nu}\mathcal{Y}_{\sigma'}^{\nu}) = \delta_{\sigma\sigma'},$$

$$\sum_{\nu}(\mathcal{X}_{\sigma}^{\nu}\mathcal{Y}_{\sigma'}^{\nu} - \mathcal{Y}_{\sigma}^{\nu}\mathcal{X}_{\sigma'}^{\nu}) = 0, \quad (20)$$

one can invert Eq. (18) to obtain

$$J_{\sigma}^{-} = \sqrt{1-\langle M_{\sigma}\rangle}\sum_{\nu}(\mathcal{X}_{\sigma}^{\nu}Q_{\nu} + \mathcal{Y}_{\sigma}^{\nu}Q_{\nu}^{\dagger}),$$

$$J_{\sigma}^{+} = (J_{\sigma}^{-})^{\dagger}. \quad (21)$$

The operators $J_{\sigma}^{\pm}$ and $1-M_{\sigma}$ form a $SU(2)$ algebra of spin-$\frac{1}{2}$ operators and, therefore, using the Casimir relation we obtain

$$M_{\sigma} = 2J_{\sigma}^{+}J_{\sigma}^{-}. \quad (22)$$

In this way we can calculate with Eq. (19) the following expectation values:

$$\langle J_{\sigma'}^{+}J_{\sigma}^{-}\rangle = \sqrt{\langle 1-M_{\sigma'}\rangle\langle 1-M_{\sigma}\rangle}\sum_{\nu}\mathcal{Y}_{\sigma'}^{\nu}\mathcal{Y}_{\sigma}^{\nu},$$

$$\langle J_{\sigma'}^{-}J_{\sigma}^{+}\rangle = \sqrt{\langle 1-M_{\sigma'}\rangle\langle 1-M_{\sigma}\rangle}\sum_{\nu}\mathcal{X}_{\sigma'}^{\nu}\mathcal{X}_{\sigma}^{\nu},$$

$$\langle J_{\sigma'}^{+}J_{\sigma}^{+}\rangle = \sqrt{\langle 1-M_{\sigma'}\rangle\langle 1-M_{\sigma}\rangle}\sum_{\nu}\mathcal{Y}_{\sigma'}^{\nu}\mathcal{X}_{\sigma}^{\nu},$$

$$\langle J_{\sigma'}^{-}J_{\sigma}^{-}\rangle = \sqrt{\langle 1-M_{\sigma'}\rangle\langle 1-M_{\sigma}\rangle}\sum_{\nu}\mathcal{X}_{\sigma'}^{\nu}\mathcal{Y}_{\sigma}^{\nu}, \quad (23)$$

with

$$\langle M_{\sigma}\rangle = \frac{2\sum_{\nu}|\mathcal{Y}_{\sigma}^{\nu}|^2}{1+2\sum_{\nu}|\mathcal{Y}_{\sigma}^{\nu}|^2}. \quad (24)$$

We will see that in order to close the system of SCRPA equations, expectation values $\langle M_{\sigma}M_{\sigma'}\rangle$ will also be needed. It is easy to see that we have

$$M_{\sigma}M_{\sigma} = 2M_{\sigma} \quad (25)$$

and

$$M_{\sigma}M_{\sigma'} = 4J_{\sigma}^{\dagger}J_{\sigma'}^{\dagger}J_{\sigma'}J_{\sigma} \quad (\sigma \neq \sigma'). \quad (26)$$

With Eq. (21) the expectation value of Eq. (26) gives

$$\langle M_\sigma M_{\sigma'}\rangle = 4(1-\langle M_\sigma\rangle)(1-\langle M_{\sigma'}\rangle)\sum_{\nu\nu'}\sum_{\nu_1\nu_2}\mathcal{Y}^\nu_\nu \mathcal{Y}^{\nu'}_{\nu'} Y^{\nu_1}_\sigma \mathcal{Y}^{\nu_2}_{\sigma'}$$

$$\times \langle Q_\nu Q_{\nu_1} Q^\dagger_{\nu_2} Q^\dagger_{\nu'}\rangle. \tag{27}$$

For the calculation of the correlation functions which appear on the right-hand side of Eq. (27) one commutes the destructors Q_ν to the right and uses Eq. (6), yielding again correlation functions $\langle M_\sigma M_{\sigma'}\rangle$. One then obtains a closed linear system of equations for the latter. Details are given in Appendix A.

The SCRPA matrix elements can be expressed in the following way:

$$\mathcal{A}_{\uparrow,\uparrow} = \langle [K^-_\uparrow,[H,K^+_\uparrow]]\rangle = 2t + \mathcal{B}_{\uparrow,\uparrow},$$

$$\mathcal{A}_{\downarrow,\downarrow} = \langle [K^-_\downarrow,[H,K^+_\downarrow]]\rangle = 2t + \mathcal{B}_{\downarrow,\downarrow},$$

$$\mathcal{A}_{\uparrow,\downarrow} = \langle [K^-_\uparrow,[H,K^+_\downarrow]]\rangle = \mathcal{B}_{\uparrow,\downarrow},$$

$$\mathcal{A}_{\downarrow,\uparrow} = \langle [K^-_\downarrow,[H,K^+_\uparrow]]\rangle = \mathcal{B}_{\downarrow,\uparrow}, \tag{28}$$

$$\mathcal{B}_{\uparrow,\uparrow} = -\langle [K^-_\uparrow,[H,K^-_\uparrow]]\rangle = U\sqrt{\frac{1-\langle M_\downarrow\rangle}{1-\langle M_\uparrow\rangle}}\sum_\nu (\mathcal{X}^\nu_\uparrow \mathcal{Y}^\nu_\downarrow + \mathcal{X}^\nu_\uparrow \mathcal{X}^\nu_\uparrow),$$

$$\mathcal{B}_{\downarrow,\downarrow} = -\langle [K^-_\downarrow,[H,K^-_\downarrow]]\rangle = U\sqrt{\frac{1-\langle M_\uparrow\rangle}{1-\langle M_\downarrow\rangle}}\sum_\nu (\mathcal{X}^\nu_\uparrow \mathcal{Y}^\nu_\downarrow + \mathcal{Y}^\nu_\uparrow \mathcal{Y}^\nu_\downarrow),$$

$$\mathcal{B}_{\uparrow,\downarrow} = -\langle [K^-_\uparrow,[H,K^-_\downarrow]]\rangle = -\frac{U}{2}\frac{\langle (1-M_\uparrow)(1-M_\downarrow)\rangle}{\sqrt{(1-\langle M_\uparrow\rangle)(1-\langle M_\downarrow\rangle)}},$$

$$\mathcal{B}_{\downarrow,\uparrow} = -\langle [K^-_\downarrow,[H,K^-_\uparrow]]\rangle = \mathcal{B}_{\uparrow,\downarrow}. \tag{29}$$

With our previous relations (23), (24), and (27) we can entirely express the elements of Eqs. (28) and (29) by the RPA
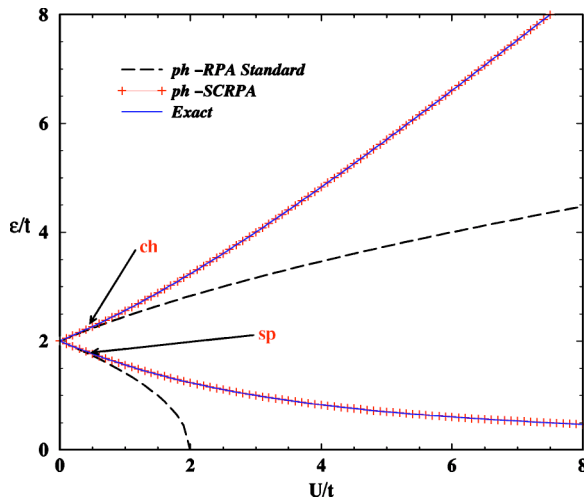

FIG. 1. Excitation energies of the standard RPA (dashed lines), SCRPA (crosses), and exact solution (solid lines) as a function of U in the channels of charge (*ch*) and longitudinal spin (*sp*) for the two-site case.

amplitudes and therefore we have a completely closed system of equation for the amplitudes $\mathcal{X}$, $\mathcal{Y}$. With the orthonormality relations (20) we furthermore have

$$\mathcal{A}_{\uparrow,\uparrow} = \mathcal{A}_{\downarrow,\downarrow} = A, \quad \mathcal{A}_{\uparrow,\downarrow} = \mathcal{A}_{\downarrow,\uparrow} = A',$$

$$\mathcal{B}_{\uparrow,\uparrow} = \mathcal{B}_{\downarrow,\downarrow} = B, \quad \mathcal{B}_{\uparrow,\downarrow} = \mathcal{B}_{\downarrow,\uparrow} = B', \tag{30}$$

and, therefore, the SCRPA equation can be written in the following form:

$$\begin{pmatrix} A & A' & B & B' \\ A' & A & B' & B \\ -B & -B' & -A & -A' \\ -B' & -B & -A' & -A \end{pmatrix} \begin{pmatrix} \mathcal{X}^\nu_\uparrow \\ \mathcal{X}^\nu_\downarrow \\ \mathcal{Y}^\nu_\uparrow \\ \mathcal{Y}^\nu_\downarrow \end{pmatrix} = \mathcal{E}_\nu \begin{pmatrix} \mathcal{X}^\nu_\uparrow \\ \mathcal{X}^\nu_\downarrow \\ \mathcal{Y}^\nu_\uparrow \\ \mathcal{Y}^\nu_\downarrow \end{pmatrix}. \tag{31}$$

The system (31) has the two positive roots $\mathcal{E}_1 = \sqrt{(A-A')^2-(B-B')^2}$ and $\mathcal{E}_2 = \sqrt{(A+A')^2-(B+B')^2}$. The SCRPA equation (31) can be solved numerically by iteration, leading, as expected, to the exact result. This latter fact can also be seen analytically in noticing that, by symmetry,

$$\mathcal{X}^1_\uparrow = -\mathcal{X}^1_\downarrow \equiv \mathcal{X}_{sp}, \quad \mathcal{Y}^1_\uparrow = -\mathcal{Y}^1_\downarrow \equiv \mathcal{Y}_{sp},$$

$$\mathcal{X}^2_\uparrow = \mathcal{X}^2_\downarrow \equiv \mathcal{X}_{ch}, \quad \mathcal{Y}^2_\uparrow = \mathcal{Y}^2_\downarrow \equiv \mathcal{Y}_{ch}. \tag{32}$$

Therefore the 4×4 equation (31) decouples into two 2×2 equations corresponding to charge (*ch*) and spin (*sp*). Then we see that the exact ground-state wave function which contains only up to 2p-2h excitations

$$|0\rangle \propto (1+dJ^+_\uparrow J^+_\downarrow)|\text{HF}\rangle \tag{33}$$

is the exact vacuum to the RPA operators—i.e., $Q_{ch(sp)}|\text{RPA}\rangle=0$—under the condition that

$$d = \left(\frac{\mathcal{Y}}{\mathcal{X}}\right)_{ch(sp)} \equiv \tan(\phi). \tag{34}$$

We therfore can express the SCRPA equations by the single parameter ϕ and obtain the solution analytically (up to the solution a nonlinear equation for ϕ). The solution agrees for all quantities with the exact result. For example the ground-state energy is given by

$$E^{SCRPA}_0 = -2t\cos(2\phi) + \frac{U}{2}[1-\sin(2\phi)]. \tag{35}$$

This expression can either be derived directly from $\langle H\rangle$ using Eq. (33) and (34) or one uses a generalization of the standard RPA expression for the ground-state energy:[6]

$$E^{SCRPA}_0 = E_{HF} - \frac{1}{2}\sum_\sigma (1-\langle M_\sigma\rangle)[\mathcal{E}_2|\mathcal{Y}_{ch}|^2 + \mathcal{E}_1|\mathcal{Y}_{sp}|^2]. \tag{36}$$

It is straightforward to verify that expressions (35) and (36) are identical.

The standard RPA expression are recovered from Eq. (31) in replacing in all expectation values the RPA ground state by the uncorrelated HF determinant. In Fig. 1 we compare
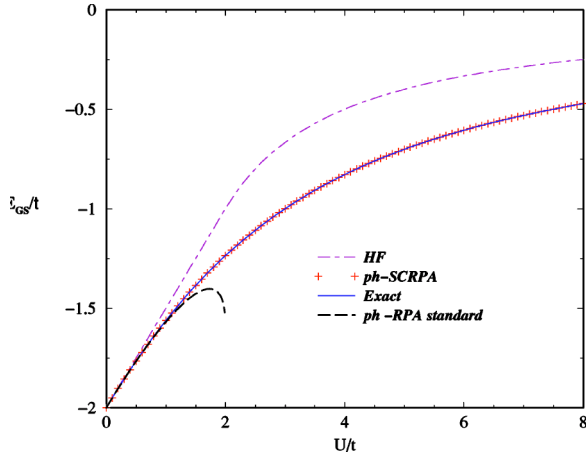
FIG. 2. Ground-state energy in HF (dot-dashed line), standard RPA (dashed line), SCRPA (crosses), and exact solution (solid line) as a function of U in the charge and longitudinal spin responses for the two-site case.

the standard RPA with the SCRPA and exact results for the excitation energies and in Fig. 2 the corresponding ground-state energies together with the HF values are shown. From these figures one should especially appreciate the long way the SCRPA has gone from the s-RPA to recover the exact result. For instance it is clearly seen that the instability of the s-RPA at $U=2$ is, as expected for such a small system, an artifact and is completely washed out by the self-consistent treatment of quantum fluctuations contained in the SCRPA approach.

Without explicit demonstration let us also mention that the SCRPA in the spin-transverse channel with $Q_\nu^\dagger = \mathcal{X}_{1\downarrow 2\uparrow}^\nu b_{2\uparrow}^\dagger b_{1\downarrow} + \mathcal{X}_{1\uparrow 2\downarrow}^\nu b_{2\downarrow}^\dagger b_{1\uparrow} - \mathcal{Y}_{1\downarrow 2\uparrow}^\nu b_{1\downarrow} b_{2\uparrow} - \mathcal{Y}_{1\uparrow 2\downarrow}^\nu b_{1\uparrow} b_{2\downarrow}$ as well as in the particle-particle channel with $Q^\dagger = \mathcal{X} b_{2\uparrow}^\dagger b_{2\downarrow}^\dagger - \mathcal{Y} b_{1\downarrow} b_{1\uparrow}$ also gives the exact solution for the two-site problem. How the pp-SCRPA works can be seen in Ref. 10 where for the pairing problem the two-particle problem is also solved exactly.

The fact that the SCRPA solves the two-site problem exactly is nontrivial, since other well-known many-body approaches,[14–16] as already mentioned, so far failed to obtain this limit correctly.

III. SIX-SITE PROBLEM

After this positive experience with the two-site problem we next will consider the one-dimensional six-sites case, as for the four-site case problems appear needing particular considerations to be outlined in Sec. IV. We again consider the plane-wave transformation explained in Sec. II with the corresponding Hamiltonian in momentum space (11). In the first Brillouin zone $-\pi \leqslant k < \pi$ we have for $N=6$ the following wave numbers:

$$k_1 = 0, \quad k_2 = \frac{\pi}{3}, \quad k_3 = -\frac{\pi}{3},$$

$$k_4 = \frac{2\pi}{3}, \quad k_5 = -\frac{2\pi}{3}, \quad k_6 = -\pi. \qquad (37)$$

With the HF transformation

$$a_{h,\sigma} = b_{h,\sigma}^\dagger, \quad a_{p,\sigma} = b_{p,\sigma}, \qquad (38)$$

such that $b_{k,\sigma}|\text{HF}\rangle = 0$ for all k, we can write the Hamiltonian in the following way (normal order with respect to $b^\dagger$, b):

$$H = H_{HF} + H_{|q|=0} + H_{|q|=\pi/3} + H_{|q|=2\pi/3} + H_{|q|=\pi}, \qquad (39)$$

where

$$H_{HF} = E_0^{HF} + \sum_\sigma (\epsilon_4 \tilde{n}_{4,\sigma} + \epsilon_5 \tilde{n}_{5,\sigma} + \epsilon_6 \tilde{n}_{6,\sigma} - \epsilon_1 \tilde{n}_{1,\sigma}$$
$$- \epsilon_2 \tilde{n}_{2,\sigma} - \epsilon_3 \tilde{n}_{3,\sigma}), \qquad (40\text{a})$$

$$H_{|q|=0} = G \sum_{i=1}^3 (\tilde{n}_{p_i,\uparrow} - \tilde{n}_{h_i,\uparrow}) \sum_{j=1}^3 (\tilde{n}_{p_j,\downarrow} - \tilde{n}_{h_j,\downarrow}), \qquad (40\text{b})$$

$$H_{|q|=\pi/3} = G\{\{[(S_{4\uparrow,6\uparrow}^- + S_{6\uparrow,5\uparrow}^+) - (S_{2\uparrow,1\uparrow}^+ + S_{1\uparrow,3\uparrow}^-)$$
$$+ (J_{2\uparrow,4\uparrow}^- + J_{5\uparrow,3\uparrow}^+)][(S_{6\downarrow,4\downarrow}^+ + S_{5\downarrow,6\downarrow}^-) - (S_{1\downarrow,2\downarrow}^- + S_{1\downarrow,3\downarrow}^-)$$
$$+ (J_{4\downarrow,2\downarrow}^+ + J_{3\downarrow,5\downarrow}^-)]\} + \text{c.c.}\}, \qquad (40\text{c})$$

$$H_{|q|=2\pi/3} = G\{\{[(S_{5\uparrow,4\uparrow}^+ - S_{3\uparrow,2\uparrow}^+) + (J_{1\uparrow,5\uparrow}^- + J_{4\uparrow,1\uparrow}^+ + J_{3\uparrow,6\uparrow}^-$$
$$+ J_{6\uparrow,2\uparrow}^+)][(S_{4\downarrow,5\downarrow}^- - S_{2\downarrow,3\downarrow}^-) + (J_{5\downarrow,1\downarrow}^+ + J_{1\downarrow,4\downarrow}^- + J_{6\downarrow,3\downarrow}^+$$
$$+ J_{2\downarrow,6\downarrow}^-)]\} + \text{c.c.}\}, \qquad (40\text{d})$$

$$H_{|q|=\pi} = G[(J_{1\uparrow,6\uparrow}^- + J_{2\uparrow,5\uparrow}^- + J_{3\uparrow,4\uparrow}^-) + \text{c.c.}][(J_{1\downarrow,6\downarrow}^- + J_{2\downarrow,5\downarrow}^-$$
$$+ J_{3\downarrow,4\downarrow}^-) + \text{c.c.}], \qquad (40\text{e})$$

with the definition of operators

$$\tilde{n}_{k,\sigma} = b_{k,\sigma}^\dagger b_{k,\sigma},$$

$$J_{ph,\sigma}^- = b_{h,\sigma} b_{p,\sigma}, \quad J_{ph,\sigma}^+ = (J_{ph,\sigma}^-)^\dagger$$

$$S_{ll',\sigma}^+ = b_{l,\sigma}^\dagger b_{l',\sigma}, \quad \text{with} \quad l > l' \;\; S_{l'l,\sigma}^- = (S_{ll',\sigma}^+)^\dagger, \qquad (41)$$

and

$$E_{HF} = -8t + \frac{3}{4}U,$$

$$\epsilon_1 = -2t + \frac{U}{2}, \quad \epsilon_2 = \epsilon_3 = -t + \frac{U}{2},$$

$$\epsilon_4 = \epsilon_5 = t + \frac{U}{2}, \quad \epsilon_6 = 2t + \frac{U}{2},$$

$$G = \frac{U}{6}. \qquad (42)$$

The level scheme is shown in Fig. 3. The hole states are labeled $h = \{1, 2, 3\}$ and the particle states $p = \{4, 5, 6\}$. The HF ground state is

$$|\text{HF}\rangle = a_{1,\uparrow}^\dagger a_{1,\downarrow}^\dagger a_{2,\uparrow}^\dagger a_{2,\downarrow}^\dagger a_{3,\uparrow}^\dagger a_{3,\downarrow}^\dagger |-\rangle. \qquad (43)$$

We see that the Hamiltonian for six sites has largely the same structure as the one for two sites. It is only augmented
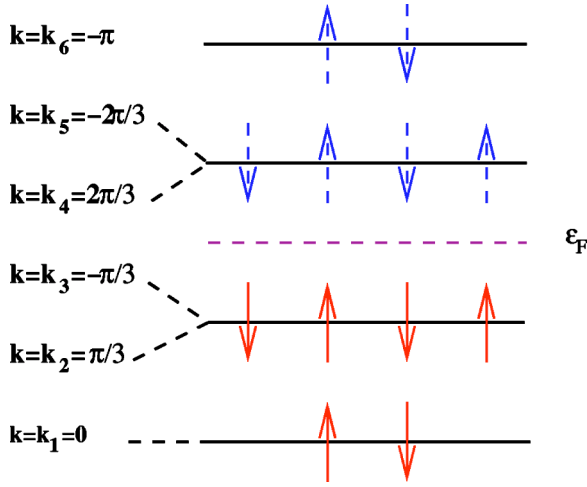
FIG. 3. Excitation spectrum of the HF ground state $U=0$ for the chain with six sites at half filling and projection of spin $m_s=0$. The occupied states are represented by the solid arrows and those not occupied are represented by the dashed arrows.

by $H_{|q|=\pi/3}+H_{|q|=2\pi/3}$ which contains the S operators on which we will comment below.

There are three different absolute values of momentum transfers as shown in Table I. Since the momentum transfer $|q|$ is a good quantum number, the RPA equations are block diagonal and can be written down for each $|q|$ value separately. For example, for $|q|=\pi/3$ we have the following RPA operator for charge and longitudinal spin excitations:

$$Q^\dagger_{|q|=\pi/3,\nu} = \mathcal{X}^\nu_{2\uparrow,4\uparrow}K^+_{4\uparrow,2\uparrow} + \mathcal{X}^\nu_{2\downarrow,4\downarrow}K^+_{4\downarrow,2\downarrow} + \mathcal{X}^\nu_{3\uparrow,5\uparrow}K^+_{5\uparrow,3\uparrow}$$
$$+ \mathcal{X}^\nu_{3\downarrow,5\downarrow}K^+_{5\downarrow,3\downarrow} - \mathcal{Y}^\nu_{2\uparrow,4\uparrow}K^-_{2\uparrow,4\uparrow} - \mathcal{Y}^\nu_{2\downarrow,4\downarrow}K^-_{2\downarrow,4\downarrow}$$
$$- \mathcal{Y}^\nu_{3\uparrow,5\uparrow}K^-_{5\uparrow,3\uparrow} - \mathcal{Y}^\nu_{3\downarrow,5\downarrow}K^-_{3\downarrow,5\downarrow}, \qquad (44)$$

where

$$K^\pm_{p\sigma,h\sigma} = \frac{J^\pm_{p\sigma,h\sigma}}{\sqrt{1 - \langle M_{p\sigma,h\sigma}\rangle}} \qquad (45)$$

and

$$M_{p\sigma,h\sigma} = \tilde{n}_{p,\sigma} + \tilde{n}_{h,\sigma}. \qquad (46)$$

We write this RPA operator in shorthand notation as

TABLE I. The various momentum transfers in the six-site case.

$|q|=\dfrac{2\pi}{3}$	$|q|=\pi$	$|q|=\dfrac{\pi}{3}$
$51 \rightarrow q_{51}=-2\pi/3$	$61 \rightarrow q_{61}=-\pi$	$42 \rightarrow q_{42}=+\pi/3$
$41 \rightarrow q_{41}=+2\pi/3$	$52 \rightarrow q_{52}=-\pi$	$53 \rightarrow q_{53}=-\pi/3$
$62 \rightarrow q_{62}=+2\pi/3$	$43 \rightarrow q_{43}=+\pi$	
$63 \rightarrow q_{63}=-2\pi/3$		

$$Q^\dagger_\nu = \sum_{i=1}^4 \frac{1}{\sqrt{1-\langle M_i\rangle}}(\mathcal{X}^\nu_i J^+_i - \mathcal{Y}^\nu_i J^-_i), \qquad (47)$$

again with the properties

$$|\nu\rangle = Q^\dagger_\nu|0\rangle, \qquad (48a)$$

$$Q_\nu|0\rangle = 0. \qquad (48b)$$

The matrix elements in the SCRPA equation

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B}^* & -\mathcal{A}^* \end{pmatrix}\begin{pmatrix} \mathcal{X}^\nu \\ \mathcal{Y}^\nu \end{pmatrix} = \mathcal{E}_\nu \begin{pmatrix} \mathcal{X}^\nu \\ \mathcal{Y}^\nu \end{pmatrix}$$

are then of the form

$$\mathcal{A}_{i,i'} = \frac{\langle[J^-_{i'}[H,J^+_i]]\rangle}{\sqrt{(1-\langle M_{i'}\rangle)(1-\langle M_i\rangle)}}, \qquad (49a)$$

$$\mathcal{B}_{i,i'} = \frac{\langle[J^-_{i'}[H,J^-_i]]\rangle}{\sqrt{(1-\langle M_{i'}\rangle)(1-\langle M_i\rangle)}}. \qquad (49b)$$

Since the SCRPA equations have the same mathematical structure as the standard RPA, one also has equivalent orthonormality relations $\Sigma_i(\mathcal{X}^\nu_i\mathcal{X}^{\nu'}_i - \mathcal{Y}^\nu_i\mathcal{Y}^{\nu'}_i)=\delta_{\nu\nu'}$, etc., in analogy to Eqs. (20) of the two-site case. This allows us to invert Eq. (47) and to calculate the expectation values which will appear in Eqs. (49a) and (49b) in complete analogy to Eq. (23).

The missing expectation values $\langle M_i\rangle$ can be expressed by the $\mathcal{X}$ and $\mathcal{Y}$ amplitudes in observing that $J^\pm_i$ and $J^0_i =\frac{1}{2}(M_i-1)$ form, as in the two-site case, an $SU(2)$ Lie algebra for spin-$\frac{1}{2}$ particles. Using the Casimir relation one again obtains $M_i=2J^+_iJ^-_i$ and thus

$$\langle M_i\rangle = \frac{2\sum_\nu|\mathcal{Y}^\nu_i|^2}{1+2\sum_\nu|\mathcal{Y}^\nu_i|^2}. \qquad (50)$$

We also will need expectation values of

$$M_iM_j = 4J^+_iJ^-_iJ^+_jJ^-_j \quad \text{for } i \neq j$$

[for $M_iM_i=2M_i$ we can use Eq. (50)]. Those can again be calculated following the same procedure as outlined in Eq. (27) and Appendix A.

In order to solve the SCRPA equations we now practically have prepared all we need. Nonetheless, at this point we have to discuss a limitation of our RPA ansatz (44) which is not absolutely necessary but which turned out to be convenient for numerical reasons. The fact is that our RPA ansatz is restricted to ph and hp configurations, as this is also the case in standard RPA. In the latter case this is a strict consequence of the use of HF occupation numbers n^0_p and n^0_h with values zero or one, respectively. In the SCRPA case with a correlated ground state the occupation numbers are different from zero and one and *a priori* there is no formal reason not to include into the RPA operator also pp and hh configurations of the form $a^\dagger_p a_{p'} \equiv b^\dagger_p b_{p'}$ and $a^\dagger_h a_{h'} \equiv -b^\dagger_{h'} b_h$. Such terms are usually called scattering or anomalous terms.[19] With rounded occupation numbers the SCRPA equations (at $T=0$) are for-

mally and mathematically equivalent to standard RPA equations at finite temperature where also pp and hh components are to be included, in principle.[18] The inclusion of those scattering terms[18,19] [the S terms in Eq. (39)] usually is of little quantitative consequence,[11] but entails, however, the important formal property that, as for the standard RPA, the energy-weighted sum rule is fulfilled exactly.[11,19] In spite of this desirable feature, we had to refrain from the inclusion of the scattering configurations in this work because the factors $\sqrt{1-\langle M_i\rangle}$ by which the SCRPA matrix is divided [see Eqs. (49a) and (49b)] can become very small in these cases and this perturbed the convergence process of the iterative solution of the SCRPA equations. Though we do not exclude that a more adequate numerical procedure could be found to stabilize the iteration cycle, we decided to postpone such an investigation, because, as already mentioned and as will be shown later, the influence of the scattering terms is, as found already in other studies,[11] very small. We will shortly come back to this discussion when presenting the results for the energy-weighted sum rule below. As a consequence and for consistency we then also will have to disregard the S terms of the Hamiltonian (remember that also in standard RPA these terms do not contribute). Under these conditions we then obtain a completely closed systemof SCRPA equations. For completeness we give some examples of SCRPA matrix elements which correspond to the ansatz (44) for $|q|=\pi/3$:

$$\mathcal{A}_{1,1} = \frac{\langle[J^-_{2\uparrow,4\uparrow}[H,J^+_{4\uparrow,2\uparrow}]]\rangle}{(1-\langle M_{24,\uparrow}\rangle)}$$

$$= \epsilon_4 - \epsilon_2 - G\{2\langle J^-_{2\uparrow,4\uparrow}(J^-_{3\downarrow,5\downarrow}+J^+_{4\downarrow,2\downarrow})\rangle$$
$$+ \langle(J^-_{1\uparrow,4\uparrow}+J^-_{2\uparrow,6\uparrow})(J^-_{1\downarrow,5\downarrow}+J^-_{3\downarrow,6\downarrow}+J^+_{4\downarrow,1\downarrow}+J^+_{6\downarrow,2\downarrow})\rangle$$
$$+ \langle(J^-_{3\uparrow,4\uparrow}+J^-_{2\uparrow,5\uparrow})[(J^-_{1\downarrow,6\downarrow}+J^-_{2\downarrow,5\downarrow}+J^-_{3\downarrow,4\downarrow})$$
$$+ \text{c.c.}]\rangle\}(1-\langle M_{24,\uparrow}\rangle)^{-1}, \qquad (51a)$$

$$\mathcal{A}_{2,1} = \frac{\langle[J^-_{2\downarrow,4\downarrow}[H,J^+_{4\uparrow,2\uparrow}]]\rangle}{\sqrt{(1-\langle M_{24,\downarrow}\rangle)(1-\langle M_{24,\uparrow}\rangle)}}$$

$$= G\{\langle(1-M_{24,\uparrow})(1-M_{24,\downarrow})\rangle$$
$$+ \langle(J^+_{4\uparrow,1\uparrow}-J^+_{6\uparrow,2\uparrow})(J^-_{1\downarrow,4\downarrow}-J^-_{2\downarrow,6\downarrow})\rangle$$
$$+ \langle(J^+_{4\uparrow,3\uparrow}-J^+_{5\uparrow,2\uparrow})(J^-_{3\downarrow,4\downarrow}-J^-_{2\downarrow,5\downarrow})\rangle\}$$
$$\times\{(1-\langle M_{24,\downarrow}\rangle)(1-\langle M_{24,\uparrow}\rangle)\}^{-1/2}$$

$$\vdots \qquad (51b)$$

The other matrix elements can be elaborated along the same lines. Of course in the approximation where the expectation values in Eqs. (51a) and (51b) are evaluated with the HF ground state the usual matrix elements of the standard RPA are recovered. We should also mention that in expressions (51a) and (51b) expectation values such as, for example, $\langle J^-_{1\uparrow,4\uparrow}J^+_{4\downarrow,1\downarrow}\rangle$ which involve momentum transfers other than the one under consideration ($|q_3|=\pi/3$ in the specific example) must be discarded. That this implicit channel coupling cannot be taken into account without deteriorating the quality of the SCRPA solutions is an empirical law which was established quite sometime ago.[20] It is part of the decou-

pling scheme and it is intuitively understandable that, since each channel is summing specific correlations, one cannot mix the channels implicitly without perturbing the balance of the minimization procedure which is done channel by channel. It can also be noticed that, neglecting the S terms in H, the channel coupling disappears.

We here give for the transfer $|q|=\pi/3$ the totality of the elements of the matrix SCRPA, $\mathcal{A}$ and $\mathcal{B}$, just as was used in the numerical calculation. For others transfers there will be analogous expressions. Indeed with the abbreviations

$$i=1\equiv(2\uparrow,4\uparrow), \quad i=2\equiv(2\downarrow,4\downarrow),$$

$$i=3\equiv(3\uparrow,5\uparrow), \quad i=4\equiv(3\downarrow,5\downarrow),$$

the elements of matrices $\mathcal{A}$ and $\mathcal{B}$ are given by

$$\mathcal{A}_{1,1} = \epsilon_4 - \epsilon_2 - 2G\frac{\langle J^-_{2\uparrow,4\uparrow}(J^-_{3\downarrow,5\downarrow}+J^+_{4\downarrow,2\downarrow})\rangle}{1-\langle M_{24,\uparrow}\rangle},$$

$$\mathcal{A}_{2,1} = G\frac{\langle(1-M_{24,\uparrow})(1-M_{24,\downarrow})\rangle}{\sqrt{(1-\langle M_{24,\downarrow}\rangle)(1-\langle M_{24,\uparrow}\rangle)}},$$

$$\mathcal{A}_{3,1} = \mathcal{A}_{4,1} = \mathcal{A}_{3,2} = \mathcal{A}_{4,2} = 0,$$

$$\mathcal{A}_{2,2} = \epsilon_4 - \epsilon_2 - 2G\frac{\langle(J^-_{3\uparrow,5\uparrow}+J^+_{4\uparrow,2\uparrow})J^-_{2\downarrow,4\downarrow}\rangle}{1-\langle M_{24,\downarrow}\rangle},$$

$$\mathcal{A}_{3,3} = \epsilon_5 - \epsilon_3 - 2G\frac{\langle J^-_{3\uparrow,5\uparrow}(J^-_{2\downarrow,4\downarrow}+J^+_{5\downarrow,3\downarrow})\rangle}{1-\langle M_{35,\uparrow}\rangle},$$

$$\mathcal{A}_{4,3} = G\frac{\langle(1-M_{35,\uparrow})(1-M_{35,\downarrow})\rangle}{\sqrt{(1-\langle M_{35,\downarrow}\rangle)(1-\langle M_{35,\uparrow}\rangle)}},$$

$$\mathcal{A}_{4,4} = \epsilon_5 - \epsilon_3 - 2G\frac{\langle(J^-_{2\uparrow,4\uparrow}+J^+_{5\uparrow,3\uparrow})J^-_{3\downarrow,5\downarrow}\rangle}{1-\langle M_{35,\downarrow}\rangle}, \qquad (52a)$$

$$\mathcal{B}_{1,1} = -2G\frac{\langle J^-_{2\uparrow,4\uparrow}(J^-_{2\downarrow,4\downarrow}+J^+_{5\downarrow,3\downarrow})\rangle}{1-\langle M_{24,\uparrow}\rangle},$$

$$\mathcal{B}_{2,1} = \mathcal{B}_{3,1} = \mathcal{B}_{4,2} = \mathcal{B}_{4,3} = 0,$$

$$\mathcal{B}_{4,1} = G\frac{\langle(1-M_{24,\uparrow})(1-M_{35,\downarrow})\rangle}{\sqrt{(1-\langle M_{35,\downarrow}\rangle)(1-\langle M_{24,\uparrow}\rangle)}},$$

$$\mathcal{B}_{2,2} = -2G\frac{\langle(J^-_{2\uparrow,4\uparrow}+J^+_{5\uparrow,3\uparrow})J^-_{2\downarrow,4\downarrow}\rangle}{1-\langle M_{24,\downarrow}\rangle},$$

$$\mathcal{B}_{3,2} = G\frac{\langle(1-M_{35,\uparrow})(1-M_{24,\downarrow})\rangle}{\sqrt{(1-\langle M_{24,\downarrow}\rangle)(1-\langle M_{35,\uparrow}\rangle)}},$$

$$\mathcal{B}_{3,3} = -2G\frac{\langle J^-_{3\uparrow,5\uparrow}(J^-_{3\downarrow,5\downarrow}+J^+_{4\downarrow,2\downarrow})\rangle}{1-\langle M_{35,\uparrow}\rangle},$$
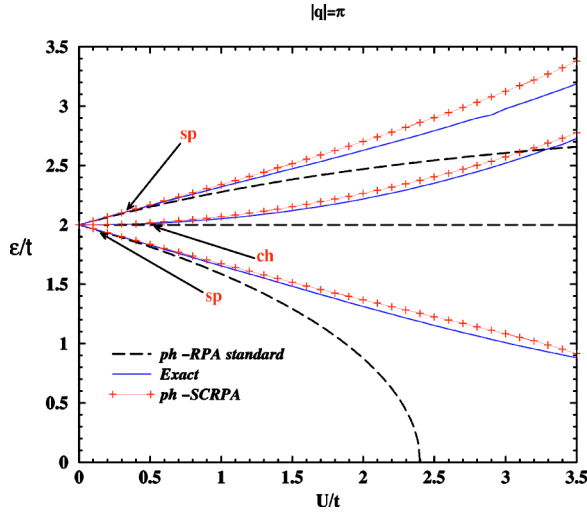
FIG. 4. Energies of excited states in the standard RPA, SCRPA, and exact cases as a function of U for six sites with spin projection $m_s=0$ and for $|q|=\pi$. States of the charge response and those of the longitudinal spin response are denoted by *ch* and *sp*, respectively.

$$\mathcal{B}_{4,4} = -2G\frac{\langle(J_{3\uparrow,5\uparrow}^- + J_{4\uparrow,2\uparrow}^+)J_{3\downarrow,5\downarrow}^-\rangle}{1-\langle M_{35,\downarrow}\rangle}. \tag{52b}$$

Let us add that the matrices $\mathcal{A}$ and $\mathcal{B}$ are symmetric and that the expectation values $\langle\cdots\rangle$ in Eqs. (52a) and (52b) can be expressed in an analogous way as the expectation values (23) and (27) by the amplitudes $\mathcal{X}, \mathcal{Y}$.

The structure of the self-consistent matrix elements (52a) and (52b) is also quite transparent: the bare interaction which survives in the limit of the standard RPA is renormalized—i.e., screened—by two-body correlation functions which are calculated self-consistently. The general structure of the scheme is in a way similar to the one proposed by Tremblay and co-workers;[16] however, the details of the expressions and the spirit of derivation are different. One can also interpret our theory as a mean-field theory of quantum fluctuations as this was done in Ref. 9.

Let us now come to the presentation of the results. In Figs. 4, 5, and 6 we display the excitation energies in the three channels $|q|=\pi$, $2\pi/3$, and $\pi/3$ as a function of U/t. The exact values are given by the solid lines, the SCRPA ones by crosses, and the ones corresponding to the standard RPA by the dashed lines. We see that in all three cases the SCRPA results are excellent and a strong improvement over the standard RPA. As expected, this is particularly important at the phase transition points where the lowest root of the standard RPA goes to zero, indicating the onset of a staggered magnetization on the mean-field level. It is particularly interesting that the SCRPA allows one to go beyond the mean-field instability point. However, contrary to the two-site case where the SCRPA, in the plane-wave basis, solved the model for all values of U, here at some values $U>U_{cr}$ the system "feels" the phase transition and the SCRPA stops to converge and also deteriorates in quality. Up to these values of U the SCRPA shows very good agreement with the exact solution and in particular it completely smears the
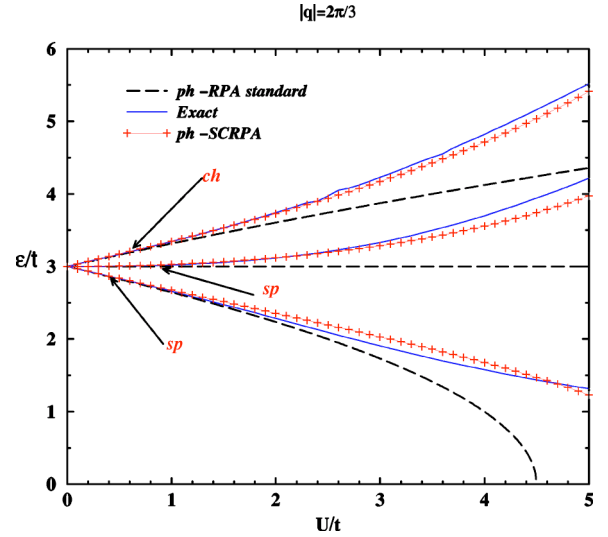
sharp phase transition point of the standard RPA which is an artifact of the linearization.

In Fig. 7 we show the ground-state energy [see Eq. (36)]

$$E_0^{SCRPA} = E_{HF} - \sum_\nu \mathcal{E}_\nu \sum_i (1-\langle M_i\rangle)|\mathcal{Y}_i^\nu|^2 \tag{53}$$

as a function of U. In addition to the exact, SCRPA, and s-RPA values we also show the HF energy. Again we see that the SCRPA is in excellent agreement with the exact solution. The standard RPA is also good for low values of U but strongly deteriorates close to the lowest phase transition point which occurs in the $|q|=\pi$ channel at $U=12t/5$. The HF energies, on the contrary, deviate quite strongly from the exact values.

The reader certainly has remarked that our RPA ansatz (44) has so far not separated charge and spin excitations. In the two-site problem this was automatically and exactly the
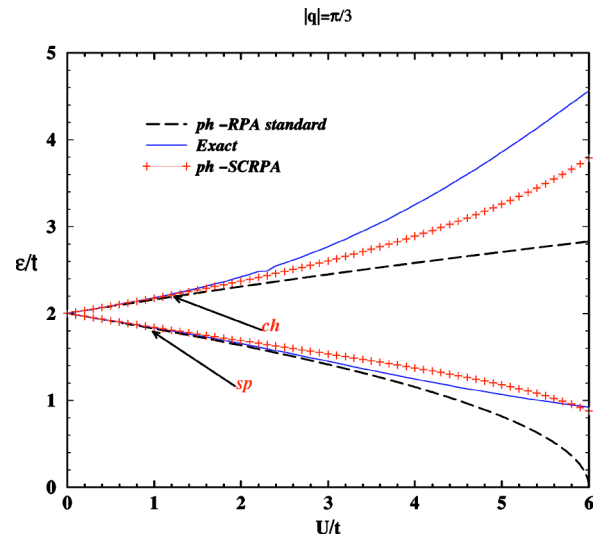

FIG. 5. Same as Fig. 4 but for $|q|=2\pi/3$.

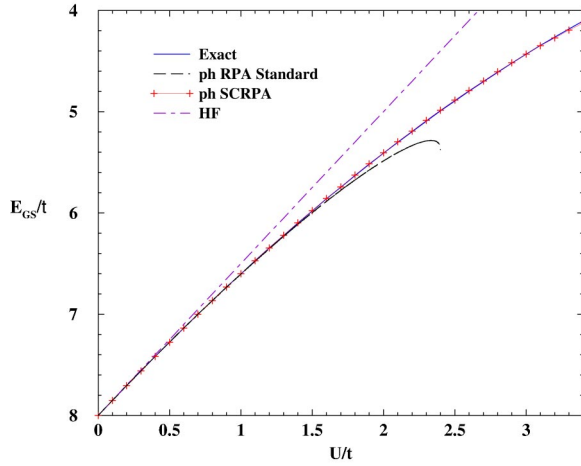FIG. 6. Same as Fig. 4 but for $|q|=\pi/3$.

FIG. 7. Energy of the ground state in the HF, standard RPA, SCRPA, and exact cases as a function of U for six sites with spin projection $m_s=0$.

case. However, here, since we did not consider the S operators in the Hamiltonian or the RPA operator, spin symmetry is violated. On the other hand, this permits us to evaluate the importance of the S operators. Normally the eigenvectors of the RPA matrix should be such that for charge (ch) excitations the operators $J^+_{ph\uparrow}+J^+_{ph\downarrow}$ and $J^-_{ph\uparrow}+J^-_{ph\downarrow}$ can be factored whereas for spin (sp) excitations the combinations $J^+_{ph\uparrow}-J^+_{ph\downarrow}$ and $J^-_{ph\uparrow}-J^-_{ph\downarrow}$ hold. Because of our violation of spin symmetry, this factorization is not exact. To have a measure of this violation we plot in Fig. 8 the ratio

$$r = \frac{|\mathcal{X}^\nu_{ph\uparrow}| - |\mathcal{X}^\nu_{ph\downarrow}|}{|\mathcal{X}^\nu_{ph\uparrow}| + |\mathcal{X}^\nu_{ph\downarrow}|}. \qquad (54)$$

For exact spin symmetry, r should be zero. From Fig. 8 we see that the violation is on the level of a fraction of 1%. This, therefore justifies, *a posteriori*, having neglected the scattering terms (S terms) in the Hamiltonian and RPA operator. A further indication that S terms are not important comes from the energy-weighted sum rule. We know that the sum rule
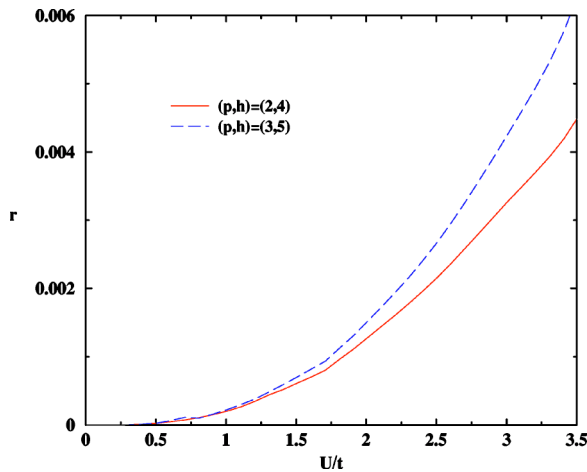

FIG. 8. The ratio r [Eq. (54)] as a function of the interaction U for the ph excitations (2, 4) and (3, 5) in the channel $|q|=\pi/3$.
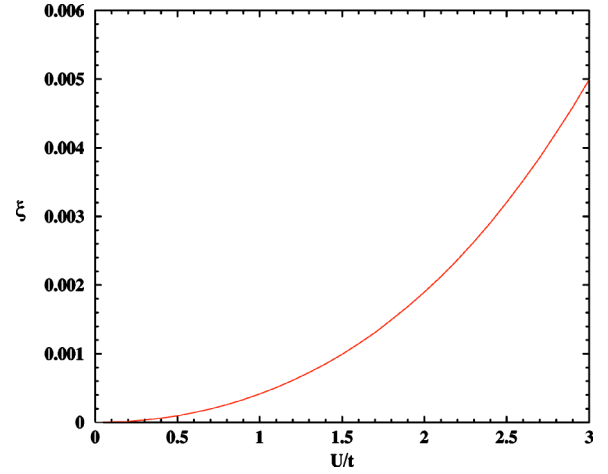
including the S terms is fulfilled in the SCRPA.[13,19] However, neglecting them gives a slight violation. Considering the exact relation

$$L = R, \qquad (55)$$

with

$$L = \sum_\nu (E_\nu - E_0)|\langle \nu|F|0\rangle|^2$$

$$= \sum_{\nu,|q|} (E_\nu - E_0)|\langle 0|Q_{|q|,\nu}F|0\rangle|^2$$

$$= \sum_{\nu,|q|} (E_\nu - E_0)|\langle 0|[Q_{|q|,\nu},F]|0\rangle|^2$$

$$= \sum_{\nu,|q|} (E_\nu - E_0)\left| \sum_{i(|q|)} \sqrt{1-M_i}(\mathcal{X}^\nu_i + \mathcal{Y}^\nu_i) \right|^2, \qquad (56a)$$

$$R = \frac{1}{2}\langle 0|[F,[H,F]]|0\rangle$$

$$= \sum_{i(|q|)} \sqrt{1-M_i} \sum_{i'(|q|)} \sqrt{1-M_{i'}}(\mathcal{A}_{i,i'} - \mathcal{B}_{i,i'}), \qquad (56b)$$

with

$$F = \sum_{i(|q|)} (J^+_i + \text{H.c.}), \qquad (57)$$

we trace in Fig. 9 the ratio $\xi=(R-L)/R$. Again we see that the violation is on the level of a fraction of 1%, confirming the very small influence of the scattering terms.

A further quantity which crucially tests the ground-state correlations is the occupation numbers. We have no direct access to them; however, we will use the so-called Catara approximation for their evaluation:[21]

$$n_{p\sigma} = \langle \hat{n}_{p\sigma}\rangle = \sum_h \langle J^+_{ph,\sigma}J_{ph,\sigma}\rangle = \sum_h (1 - \langle M_{ph\sigma}\rangle)\sum_\nu |\mathcal{Y}^\nu_{ph\sigma}|^2,$$

$$(58a)$$

FIG. 9. The ratio $\xi=(R-L)/R$ of the energy-weighted sum rule in the charge response for the six-site case.
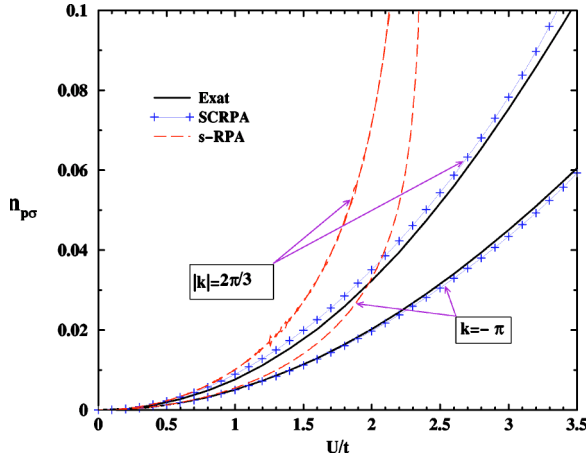
FIG. 10. Occupation numbers as function of the interaction U for various values of the momenta k for states above the Fermi level. For each approximation, s-RPA and SCRPA, the occupation numbers are represented in increasing order like k $(-\pi, -2\pi/3, 2\pi/3)$. Let us notice that the modes $k=2\pi/3$ and $k=-2\pi/3$ are degenerate.

$$n_{h\sigma} = \langle \hat{n}_{h\sigma} \rangle = \sum_{p} \langle J^{+}_{ph,\sigma} J^{-}_{ph,\sigma} \rangle = 1 - \sum_{p} (1 - \langle M_{ph\sigma} \rangle) \sum_{\nu} |\mathcal{Y}^{\nu}_{ph\sigma}|^{2}.$$
(58b)

We show these quantities in Figs. 10 and 11 in comparison with the exact values and the ones of the standard RPA. We again see the excellent performance of the SCRPA.

Concluding this section we can say that the expectation we had from the two-site case, with its exact solution, have very satisfactorily also been fulfilled in the six-site case. However, in spite of the very good performance of the SCRPA, there is the limitation that the SCRPA, in the symmetry conserving basis of plane waves used here, cannot be employed in the strong-U limit. One also may wonder how
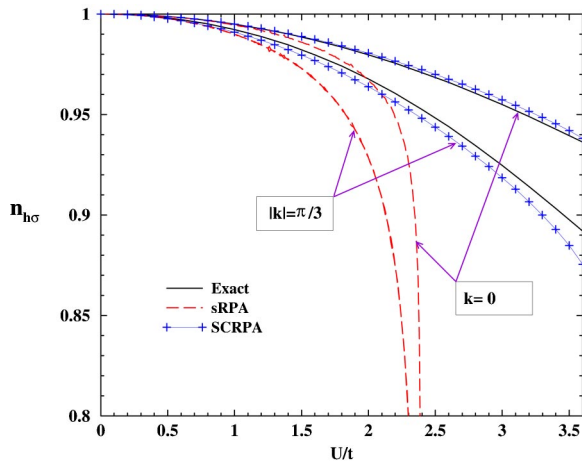

FIG. 11. Occupation numbers as a function of the interaction U for various values of the momenta k for the holes states. For each approximation, s-RPA and SCRPA and exact solution, the occupation numbers are represented like $k=0, \pi/3, -\pi/3$. Let us notice that the modes $k=\pi/3$ and $k=-\pi/3$ are degenerate.
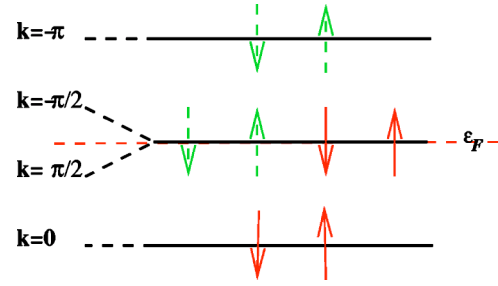

FIG. 12. Level spectrum for $U=0$ for the half-filled chain with four sites with spin projection $m_s=0$. The occupied states are represented by the solid arrows and those not occupied are represented by the dashed arrows.

the extension to cases with sites number $2+4n$ with $n>1$ works. For such cases it does not make sense anymore to elaborate the Hamiltonian in its detailed form as given in Eq. (40). This explicit expression was only given to make clear the detailed internal structure of the approach for a definite example. In the general case with many sites one would just take the form (11) of the Hamiltonian, calculate the double commutators as needed in Eqs. (8), and then express the resulting correlation functions by the $\mathcal{X}$ and $\mathcal{Y}$ amplitudes. That such a program is feasible in terms of analytic work and numerical execution was demonstrated in our earlier work on the multilevel pairing model[10] where cases up to 100 levels were treated. However, this number was not considered an upper limit. Though the present model is slightly more complicated, we think that a generalization to the case of many sites is perfectly possible. It needs, however, some investment which is planned for the future. This also concerns the $D=2$ case. Another question to ask is whether the degradation of the SCRPA results going from the $N=2$ to the $N=6$ case does not go on considering $N=10,14$, etc.? One again may cite the experience with the multilevel pairing model[10] where also the $N=2$ case turned out to be exact in the SCRPA but not the other cases. However, all $N>2$ cases showed more or less the same degrees of accuracy: excellent results of SCRPA up to the phase transition point and deterioration beyond. Since this behavior has also been found in simpler models,[12] we think that this is a generic feature of the SCRPA and that this behavior will also translate to the case of the present model.

Another problem for further work is how to continue the present theory into the strong-coupling regime. Of course, there exists the possibility to perform the SCRPA in the symmetry-broken basis, but details and how to match with the symmetry-unbroken phase must still be worked out. Also the inclusion of higher-order operators, as will shortly be discussed in the next section, may be an interesting direction in this respect.

IV. FOUR-SITE PROBLEM

A. Symmetry-unbroken case

The problem of the four-site case is easily located in regarding the level scheme of Fig. 12 (see also Ref. 22 dealing with the attractive Hubbard model in 1D). We see that the
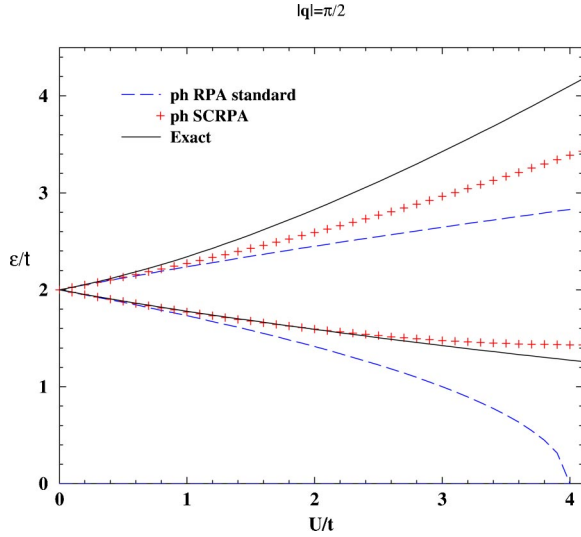
FIG. 13. Energies of excited states with the standard RPA, SCRPA, and exact solution for four sites with spin projection $m_s = 0$ and for $|q| = \pi/2$ in the symmetry-unbroken basis.
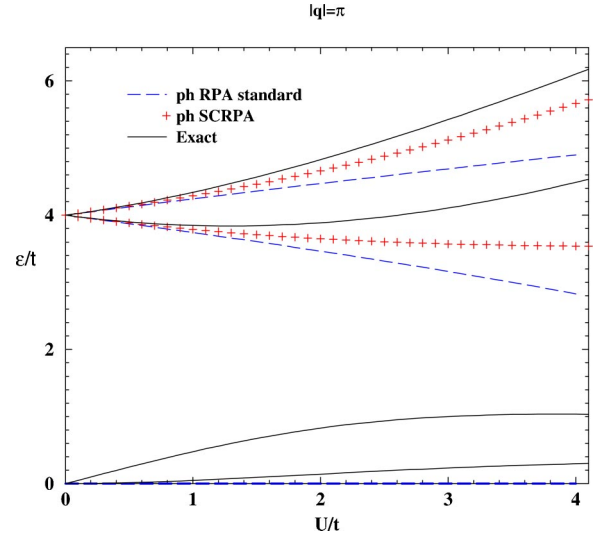

FIG. 14. Energies of excited states with the standard RPA, SCRPA, and exact solution for four sites with spin projection $m_s = 0$ and for $|q| = \pi$ in the symmetry-unbroken basis.

Fermi energy coincides with the second level which is half filled. The uncorrelated ground state is therefore degenerate and excitations with momentum transfer $|q| = \pi$ cost no energy. On the other hand, for excitations with $|q| = \pi/2$ there is no problem. The corresponding RPA operator is given by

$$Q^\dagger_{|q|=\pi/2,\nu} = \mathcal{X}^\nu_{13,\uparrow} K^+_{31,\uparrow} + \mathcal{X}^\nu_{24,\uparrow} K^+_{42,\uparrow} + \mathcal{X}^\nu_{13,\downarrow} K^+_{31,\downarrow} + \mathcal{X}^\nu_{24,\downarrow} K^+_{42,\downarrow}$$
$$- \mathcal{Y}^\nu_{13,\uparrow} K^-_{13,\uparrow} - \mathcal{Y}^\nu_{24,\uparrow} K^-_{24,\uparrow} - \mathcal{Y}^\nu_{13,\downarrow} K^-_{13,\downarrow} - \mathcal{Y}^\nu_{24,\downarrow} K^-_{24,\downarrow}. \tag{59}$$

In Fig. 13 we show the results of the s-RPA and SCRPA, together with the exact solution. We see that the lower excitation is still very well reproduced by the SCRPA, whereas for the second excited state the SCRPA only reduces the difference of the s-RPA to exact by half. The real problem shows up for the transfer $|q| = \pi$. The corresponding operator is

$$Q^\dagger_{|q|=\pi,\nu} = \mathcal{X}^\nu_{14,\uparrow} K^+_{41,\uparrow} + \mathcal{X}^\nu_{14,\downarrow} K^+_{41,\downarrow} + \mathcal{X}^\nu_{23,\uparrow} K^+_{32,\uparrow} + \mathcal{X}^\nu_{23,\downarrow} K^+_{32,\downarrow}$$
$$- \mathcal{Y}^\nu_{14,\uparrow} K^-_{14,\uparrow} - \mathcal{Y}^\nu_{14,\downarrow} K^-_{14,\downarrow} - \mathcal{Y}^\nu_{23,\uparrow} K^-_{23,\uparrow} - \mathcal{Y}^\nu_{23,\downarrow} K^-_{23,\downarrow}. \tag{60}$$

The standard RPA produces a doubly degenerate zero mode independent of U as seen in Fig. 14. As compared with the exact solution, we see that these two zero modes approximate two very low-lying exact solutions. Unfortunately, because of these modes at low energy, the SCRPA could not be stabilized. The only possibility consisted in excluding the components $K^\pm_{32,\uparrow}$ and $K^\pm_{32,\downarrow}$ in the RPA operator. Then self-consistency was achieved without problem and the result is shown in Fig. 14. The result of the SCRPA is halfway between the s-RPA and the exact solution. On the other hand, because of the omission of the two lower states, the ground-state energy cannot correctly be calculated in the SCRPA. Therefore, for the four-site problem in the symmetry-

unbroken basis (plane waves), the SCRPA cannot fully account for the situation.

B. Symmetry-broken basis

An analysis of the HF solution shows that, as soon as $U \neq 0$, the plane-wave state becomes unstable and the system prefers a staggered magnetization. The general HF transformation can be written as

$$\begin{pmatrix} c^\dagger_{1,\uparrow} \\ c^\dagger_{2,\uparrow} \\ c^\dagger_{3,\uparrow} \\ c^\dagger_{4,\uparrow} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} v & -1 & 0 & u \\ u & 0 & -1 & -v \\ v & 1 & 0 & u \\ v & 0 & 1 & -v \end{pmatrix} \begin{pmatrix} a^\dagger_{1,\uparrow} \\ a^\dagger_{2,\uparrow} \\ a^\dagger_{3,\uparrow} \\ a^\dagger_{4,\uparrow} \end{pmatrix}, \tag{61a}$$

$$\begin{pmatrix} c^\dagger_{4,\downarrow} \\ c^\dagger_{3,\downarrow} \\ c^\dagger_{2,\downarrow} \\ c^\dagger_{1,\downarrow} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} v & -1 & 0 & u \\ u & 0 & -1 & -v \\ v & 1 & 0 & u \\ v & 0 & 1 & -v \end{pmatrix} \begin{pmatrix} a^\dagger_{1,\downarrow} \\ a^\dagger_{2,\downarrow} \\ a^\dagger_{3,\downarrow} \\ a^\dagger_{4,\downarrow} \end{pmatrix}, \tag{61b}$$

with $u = \cos(\vartheta)$ and $v = \sin(\vartheta)e^{i\varphi}$. The minimization of the ground-state energy, with

$$|\text{HF}\rangle = a^\dagger_{1,\uparrow} a^\dagger_{1,\downarrow} a^\dagger_{2,\uparrow} a^\dagger_{2,\downarrow} |-\rangle, \tag{62}$$

shows that $\varphi = 0$ for any value of U and the angle ϑ is obtained from

$$\tan^4(\vartheta) - \frac{U}{2t} \tan^3(\vartheta) - 1 = 0. \tag{63}$$

The occupation numbers are given by

$$n_{1,\uparrow} = n_{3,\uparrow} = n_{2,\downarrow} = n_{4,\downarrow} = \frac{1}{2}[1 + \sin^2(\vartheta)],$$
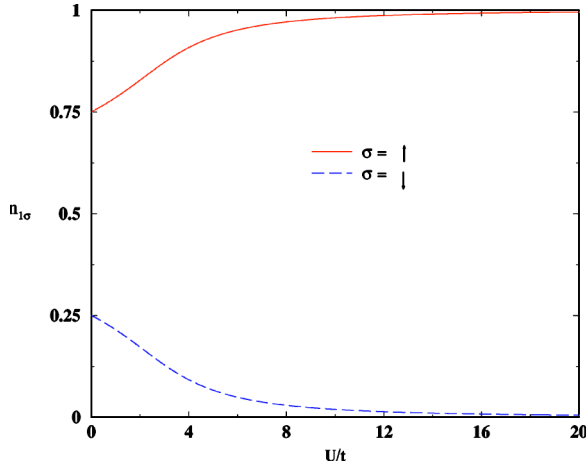
FIG. 15. Occupation numbers for site 1, $n_{1,\uparrow}$ et $n_{1,\downarrow}$, as a function of interaction U in the symmetry-broken basis.

$$n_{1,\downarrow} = n_{3,\downarrow} = n_{2,\uparrow} = n_{4,\uparrow} = \frac{1}{2}\cos^2(\vartheta), \qquad (64)$$

and shown in Fig. 15 which illustrates the spontaneous symmetry breaking for any value of U. For $U \rightarrow \infty$ we have a perfect antiferromagnet.

We can now perform a SCRPA calculation in the symmetry-broken basis. The RPA operators are given by

$$Q_{\sigma\nu}^{\dagger} = \mathcal{X}_{1\sigma,3\sigma}^{\nu} K_{3\sigma,1\sigma}^{+} + \mathcal{X}_{2-\sigma,4-\sigma}^{\nu} K_{4-\sigma,2-\sigma}^{+} - \mathcal{Y}_{1\sigma,3\sigma}^{\nu} K_{1\sigma,3\sigma}^{-}$$
$$- \mathcal{Y}_{2-\sigma,4-\sigma}^{\nu} K_{2-\sigma,4-\sigma}^{-}, \qquad (65)$$

with $\sigma = \pm\frac{1}{2}$. We also have two other excitation operators

$$Q_{1\nu}^{\dagger} = \mathcal{X}_{1\uparrow,4\uparrow}^{\nu} K_{4\uparrow,1\uparrow}^{+} + \mathcal{X}_{1\downarrow,4\downarrow}^{\nu} K_{4\downarrow,1\downarrow}^{+} - \mathcal{Y}_{1\uparrow,4\uparrow}^{\nu} K_{1\uparrow,4\uparrow}^{-} - \mathcal{Y}_{1\downarrow,4\downarrow}^{\nu} K_{1\downarrow,4\downarrow}^{-}$$
$$(66)$$

and

$$Q_{2\nu}^{\dagger} = \mathcal{X}_{2\uparrow,3\uparrow}^{\nu} K_{3\uparrow,2\uparrow}^{+} + \mathcal{X}_{2\downarrow,3\downarrow}^{\nu} K_{3\downarrow,2\downarrow}^{+} - \mathcal{Y}_{2\uparrow,3\uparrow}^{\nu} K_{2\uparrow,3\uparrow}^{-} - \mathcal{Y}_{2\downarrow,3\downarrow}^{\nu} K_{2\downarrow,3\downarrow}^{-}.$$
$$(67)$$

In Figs. 16 and 17 we give the results. The most striking feature is that the s-RPA and SCRPA are very close and that the error with respect to the exact solution does not become greater than 25% for any value of U. Though the improvement of the SCRPA over the s-RPA is very small in each channel, at the end in the ground-state energy this sums to a more substantial correction in the right direction for the ground-state energy. This is shown in Fig. 17 as a function of $a\tan(U/t)$. We see that the HF, s-RPA and SCRPA become exact for $U=0$ and $U \rightarrow \infty$. In between the SCRPA deviates, e.g., by 8% from the exact result at $U \simeq 6$ $[a\tan(U/t) \simeq 1.4]$ whereas this deviation is 20% for the s-RPA.

Concluding this section on the four-site case at half filling we can say that in the symmetry-unbroken basis the SCRPA is unable to account for some low-lying excitations and therefore fails to reproduce the ground-state energy as well. In the symmetry-broken basis the SCRPA gives very little correction over the s-RPA. However, the maximum error is not greater than 25% for all values of U for the excited states
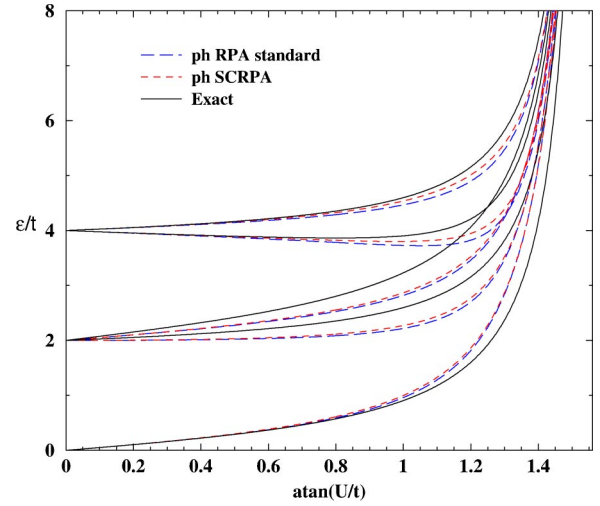

FIG. 16. Energies of excited states with the standard RPA, SCRPA, and exact solution as a function of U for four sites with spin projection $m_s=0$ in the symmetry-broken basis.

and the ground-state energy in the SCRPA whereas this is 30% for the standard RPA. This may be an interesting result in view of the importance of the so-called "plaquettes" (see, e.g., Ref. 23) in high-T_c superconductivity. Nevertheless, even though one plaquette (four sites) may reasonably be described, the present approach cannot account for the situation of many plaquettes in interaction which is the real situation in 2D. For the future it is therefore very interesting to develop an extension of the present SCRPA which not only gives an exact solution for the two-site case but equally for the four-site case. Such a generalization is possible in including into the RPA operator in addition to the fermion pair operators also quadruples of fermion operators. This is a general principle and it has already been demonstrated to hold true in the case of the simpler Lipkin model.[24] One could call such an extension a second SCRPA in analogy to the well-known standard second RPA which involves in addition to the ph configurations also 2p-2h ones. In the case of many
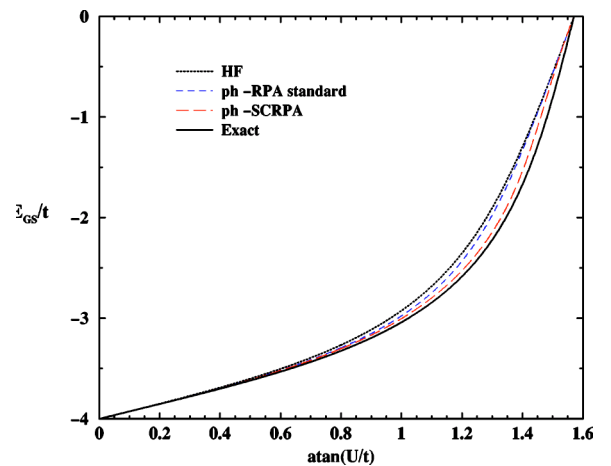

FIG. 17. Ground-state energies in the HF, standard RPA, SCRPA, and exact solution as a function of $a\tan(U/t)$ for four sites with spin projection $m_s=0$ in the symmetry-broken basis.

plaquettes this second SCRPA would then constitute a self-consistent mean-field theory for plaquettes.

V. DISCUSSION, CONCLUSIONS, AND OUTLOOK

In this work a many-body approach which was essentially developed in the nuclear physics context in recent years[9] has been applied to the Hubbard model for a finite number of sites. The theory is an extension of the standard RPA, called the self-consistent RPA, which aims to correct its well-known deficiencies such as the quasiboson approximation with its ensuing violation of the Pauli principle and its perturbation theoretical aspect. Of course the appealing features of the RPA, such as, for instance, fulfillment of sum rules, restoration of broken symmetries, Goldstone theorem, numerical practicability, and physical transparency, should be kept as much as possible. That this is indeed the case with the SCRPA has in the past been demonstrated with applications to several nontrivial models[10] such as, for instance, the many-level pairing (Richardson) model[10] and the three-level Lipkin model.[11] The SCRPA can be derived by minimizing an energy-weighted sum rule and it is therefore a nonperturbative variational approach though it is in general not of the Raleigh-Ritz type. The resulting equations are a nonlinear version of the RPA type which can be interpreted as the mean-field equations of interacting quantum fluctuations. Though the SCRPA equations are of the Schrödinger type, their nonlinearity nonetheless makes their numerical solution quite demanding. We therefore thought it indicated to begin with applications to the Hubbard model, restricting them to low-dimensional cases given by a finite number of sites where exact diagonalization can easily be obtained. We then logically started out considering the two-site case (with periodic boundary conditions), increasing the number of sites by steps of 2—i.e., $N=2,4,6,\ldots$ To our satisfaction the SCRPA solves the two-site problem exactly for any value of U. This, as a matter of fact, did not come entirely as a surprise, since the same happened already with the pairing problem for two fermions[10] and indeed it can be shown that the SCRPA solves a general two-body problem exactly.[17] It is nonetheless worth pointing out that other respectable many-body theories fail in the two-particle case, apart from the low-U limit.

In the four-site problem at half filling the SCRPA failed. This, as in all $4n$ ($n=1,2,3,\ldots$) cases, presents the particular problem that the system is unstable with respect to the formation of staggered magnetization for any finite value of U and this prevented the SCRPA solution from existing in the plane-wave basis for particular values of the momentum transfer $|q|$. At the end of the paper we indicated that extending the present RPA ansatz of ph pairs to include quadruples of fermion operators can solve not only the two-electron but also the four-electron case exactly. This is particularly interesting in view of the fact that the four-site case (plaquette) may be very important for the explanation of high-T_c superconductivity, in considering the many plaquette configurations in 2D.[23] In this work we jumped directly to the six-site problem which, as all $2+4n$ cases, causes no particular difficulties in the SCRPA, even in the symmetry-unbroken basis

of plane waves. Of course, in the case of six sites, the SCRPA is not exact anymore. However, it is shown that the results are still excellent for all quantities considered: excited states, ground state, and occupation numbers. Contrary to the two-site case, the SCRPA solutions in the plane-wave basis cannot be obtained for all values of U. Somewhere after the point where, as a function of U, the first mean-field instability shows up, the SCRPA also starts to deteriorate and in fact does not converge any longer. Often the mean-field critical value of U is by passed by 20% up to 50% in the SCRPA, still staying excellent. However, to go into the strong-U limit we have to introduce the above mentioned quadruple fermion operators or perform a SCRPA calculation in the symmetry-broken basis.[12] Such investigations shall be left for the future. We also gave arguments why we think that, going to the $N>6$ cases, the precision we found for $N=6$ will not deteriorate. We therefore think that our formalism will allow one to find precise results for system sizes where an exact diagonalization becomes prohibitive. Problems in 2D with closed-shell configurations probably also can and shall be considered with the present formalism. Also, as shown in Ref. 10, the extension to finite temperatures is possible.

We also should mention that in this work we neglected the so-called scattering terms of the form $a_p^\dagger a_{p'}$ or $a_h^\dagger a_{h'}$—that is, fermion ph operators where either both indices are above or both below the Fermi level. In the standard RPA those configurations automatically decouple from the ph and hp spaces. However, in the SCRPA with its rounded occupation numbers, there is formally no reason not to include them. As a matter of fact, as shown in earlier work,[11,19] to assure the fulfillment of the f sum rule and the restoration of broken symmetries, these scattering terms must be taken into account. In the present case, as well as in earlier studies, the scattering terms seem to be almost linearly dependent with the ordinary ph and hp configurations. This fact induced difficulties with the iteration procedure, since they correspond to very small eigenvalues of the norm matrix. Though we do not exclude the possibility that this difficulty could be mastered with a more refined numerical algorithm, we finally refrained from pursuing this effort, since we could show that the influence of the scattering terms on the results is only on the level of a fraction of percent and also the f sum rule is only violated on this order.

In short we showed that the SCRPA, as in previous models, performs excellently in the symmetry-unbroken regime of the Hubbard model. However, the high-U limit and the $4n$-site cases need further developements.

ACKNOWLEDGMENTS

APPENDIX A: PARTICLE-HOLE CORRELATION FUNCTIONS

We give the commutations rules which will be useful in the calculation of the correlations functions in the ph channel:

$$[Q_\nu, Q_{\nu'}^\dagger] = \sum_i (\mathcal{X}_i^\nu \mathcal{X}_i^{\nu'} - \mathcal{Y}_i^\nu \mathcal{Y}_i^{\nu'}) \frac{1 - M_i}{1 - \langle M_i \rangle},$$

$$[M_i, Q_\nu] = -2\mathcal{Y}_i^\nu \sum_{\nu_1} (\mathcal{X}_i^{\nu_1} Q_{\nu_1}^\dagger + \mathcal{Y}_i^{\nu_1} Q_{\nu_1}),$$

$$[M_i, Q_\nu^\dagger] = 2\mathcal{Y}_i^\nu \sum_{\nu_1} (\mathcal{Y}_i^{\nu_1} Q_{\nu_1}^\dagger + \mathcal{X}_i^{\nu_1} Q_{\nu_1}). \tag{A1}$$

$$[Q_\nu, Q_{\nu'}] = \sum_i (\mathcal{Y}_i^\nu \mathcal{X}_i^{\nu'} - \mathcal{X}_i^\nu \mathcal{Y}_i^{\nu'}) \frac{1 - M_i}{1 - \langle M_i \rangle},$$

Thus, the following average values can be calculated (commuting the Q's to the right):

$$\langle Q_{\nu_3} Q_{\nu_2}^\dagger Q_{\nu_1} Q_{\nu_0}^\dagger \rangle = \sum_{ij} \frac{(\mathcal{X}_i^{\nu_3} \mathcal{X}_i^{\nu_2} - \mathcal{Y}_i^{\nu_3} \mathcal{Y}_i^{\nu_2})}{(1 - \langle M_i \rangle)} \frac{(\mathcal{X}_j^{\nu_1} \mathcal{X}_j^{\nu_0} - \mathcal{Y}_j^{\nu_1} \mathcal{Y}_j^{\nu_0})}{(1 - \langle M_j \rangle)} \langle (1 - M_i)(1 - M_j) \rangle, \tag{A2}$$

$$\langle Q_{\nu_3} [Q_{\nu_1}, Q_{\nu_2}^\dagger] Q_{\nu_0}^\dagger \rangle = \sum_{ij} \frac{(\mathcal{X}_i^{\nu_3} \mathcal{X}_i^{\nu_0} - \mathcal{Y}_i^{\nu_3} \mathcal{Y}_i^{\nu_0})}{(1 - \langle M_i \rangle)} \frac{(\mathcal{X}_j^{\nu_1} \mathcal{X}_j^{\nu_2} - \mathcal{Y}_j^{\nu_1} \mathcal{Y}_j^{\nu_2})}{(1 - \langle M_j \rangle)} \langle (1 - M_i)(1 - M_j) \rangle - 2\sum_i \frac{\mathcal{X}_i^{\nu_3} \mathcal{X}_i^{\nu_2} \mathcal{X}_i^{\nu_1} \mathcal{X}_i^{\nu_0} - \mathcal{Y}_i^{\nu_3} \mathcal{Y}_i^{\nu_2} \mathcal{Y}_i^{\nu_1} \mathcal{Y}_i^{\nu_0}}{(1 - \langle M_i \rangle)}. \tag{A3}$$

Finally, one can express the correlation function according to the amplitudes RPA, $\langle M_i \rangle$ and of $\langle M_i M_j \rangle$ as

$$\langle Q_{\nu_3} Q_{\nu_1} Q_{\nu_2}^\dagger Q_{\nu_0}^\dagger \rangle = \langle Q_{\nu_3} [Q_{\nu_1}, Q_{\nu_2}^\dagger] Q_{\nu_0}^\dagger \rangle + \langle Q_{\nu_3} Q_{\nu_2}^\dagger Q_{\nu_1} Q_{\nu_0}^\dagger \rangle = 2\sum_{ij} \frac{(\mathcal{X}_i^{\nu_3} \mathcal{X}_i^{\nu_2} - \mathcal{Y}_i^{\nu_3} \mathcal{Y}_i^{\nu_2})}{(1 - \langle M_i \rangle)} \frac{(\mathcal{X}_j^{\nu_1} \mathcal{X}_j^{\nu_0} - \mathcal{Y}_j^{\nu_1} \mathcal{Y}_j^{\nu_0})}{(1 - \langle M_j \rangle)} \langle (1 - M_i)(1 - M_j) \rangle$$

$$+ \sum_{ij} \frac{(\mathcal{X}_i^{\nu_3} \mathcal{X}_i^{\nu_0} - \mathcal{Y}_i^{\nu_3} \mathcal{Y}_i^{\nu_0})}{(1 - \langle M_i \rangle)} \frac{(\mathcal{X}_j^{\nu_1} \mathcal{X}_j^{\nu_2} - \mathcal{Y}_j^{\nu_1} \mathcal{Y}_j^{\nu_2})}{(1 - \langle M_j \rangle)} \langle (1 - M_i)(1 - M_j) \rangle - 2\sum_i \frac{\mathcal{X}_i^{\nu_3} \mathcal{X}_i^{\nu_2} \mathcal{X}_i^{\nu_1} \mathcal{X}_i^{\nu_0} - \mathcal{Y}_i^{\nu_3} \mathcal{Y}_i^{\nu_2} \mathcal{Y}_i^{\nu_1} \mathcal{Y}_i^{\nu_0}}{(1 - \langle M_i \rangle)}. \tag{A4}$$

APPENDIX B: DENSITY-DENSITY CORRELATION FUNCTIONS

Given that this RPA formalism preserves the number of particles per spin, σ (owing to the fact that the transformation HF does not break the symmetry of spin), one has

$$\hat{N}_\sigma = N_\sigma + \sum_p \tilde{n}_{p\sigma} - \sum_h \tilde{n}_{h\sigma} \tag{B1}$$

and the average value $\langle \hat{N}_\sigma \rangle = N_\sigma = N/2$, which gives us

$$\sum_p \langle \tilde{n}_{p\sigma} \rangle = \sum_h \langle \tilde{n}_{h\sigma} \rangle. \tag{B2}$$

On the other hand, one also has

$$\hat{N}_\sigma \hat{N}_{\sigma'} = \left(N_\sigma + \sum_p \tilde{n}_{p\sigma} - \sum_h \tilde{n}_{h\sigma} \right) \left(N_{\sigma'} + \sum_{p'} \tilde{n}_{p'\sigma'} - \sum_{h'} \tilde{n}_{h'\sigma'} \right), \tag{B3}$$

with the average value $\langle \hat{N}_\sigma \hat{N}_{\sigma'} \rangle = N_\sigma + N_{\sigma'}$, which gives us

$$\left\langle \left(\sum_p \tilde{n}_{p\sigma} - \sum_h \tilde{n}_{h\sigma} \right) \left(\sum_{p'} \tilde{n}_{p'\sigma'} - \sum_{h'} \tilde{n}_{h'\sigma'} \right) \right\rangle$$

$$= N_{\sigma'} \left\langle \left(\sum_p \tilde{n}_{p\sigma} - \sum_h \tilde{n}_{h\sigma} \right) \right\rangle$$

$$+ N_\sigma \left\langle \left(\sum_{p'} \tilde{n}_{p'\sigma'} - \sum_{h'} \tilde{n}_{h'\sigma'} \right) \right\rangle. \tag{B4}$$

Thus, for our case, there is the relation

$$\left\langle \left(\sum_p \tilde{n}_{p\uparrow} - \sum_h \tilde{n}_{h\uparrow} \right) \left(\sum_{p'} \tilde{n}_{p'\downarrow} - \sum_{h'} \tilde{n}_{h'\downarrow} \right) \right\rangle$$

$$= 3 \left(\sum_{p\sigma} \langle \tilde{n}_{p\sigma} \rangle - \sum_{h\sigma} \langle \tilde{n}_{h\sigma} \rangle \right) = 0. \tag{B5}$$

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