Symmetry-adapted BCS-type trial wave functions for mesoscopic rings

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(Received 21 December 2000; published 27 March 2001)

In mesoscopic systems, the symmetry of the wave function cannot be broken and must be considered. We construct symmetry-adapted trial wave functions of the Bardeen-Cooper-Schrieffer-type for mesoscopic rings described by an extended-Hubbard model at half-filling. The comparison with exact numerical (Lanczos) diagonalization in small rings indicates that this variational approach is reasonably accurate. Within this approach, we demonstrate a crossover from a weak-correlation regime to a strong correlation one. Particularly interesting is the behavior of the lowest-excitation energy, which switches from a highest-occupied-molecular-orbital–lowest-unoccupied-molecular-orbital gap to a splitting energy related to a collective tunneling of electrons.

DOI: 10.1103/PhysRevB.63.155308 PACS number(s): 73.40.Gk, 71.45.Lr, 73.23.−b

I. INTRODUCTION

In condensed matter physics, variational approaches based on, e.g., BCS-type trial wave functions turned out to be very useful for describing various ordered phases like superconductivity or excitonic insulators.[1] These approaches are transparent physically but approximate. To test their validity for nontrivial models, the comparison with exact (or almost exact) results obtained by numerical methods [quantum Monte Carlo, exact diagonalization, density matrix renormalization group (DMRG)] is necessary.[2,3] Usually, the interest of such numerical studies on strong correlations was in *infinite* systems. Although inherently carried out in finite systems, they investigated the size (N) dependence only to deduce, via finite-size scaling analysis, results for $N\rightarrow\infty$. In view of recent advances in the fields of nanostructures and synthesis of larger molecules, the N dependence can also be considered a problem of interest by itself. This was confirmed by the results of several recent studies on mesoscopic Peierls rings.[4,5]

Besides exact numerical methods, *controlled* approximate treatments are useful for mesoscopic systems as well. Computer storage problems impose severe (disc space and/or computation time) limitations on the largest size in quantum Monte Carlo and exact diagonalization calculations ($N\sim 10-50$). Larger systems ($N\sim 100$) can be studied within DMRG, but mesoscopic rings are difficult to study, since convergence problems arise when applying periodic boundary conditions.[3] On the other side, it is unlikely to expect predictions in a certain field without the understanding in terms of simple physical concepts.

For mesoscopic systems, it is impossible to employ directly trial functions used for infinite systems, since they describe ordered states with *broken* symmetry. A certain type of ordering could develop in the ground state of a finite system, but this should occur *without symmetry breaking*. A concrete situation of this kind is encountered in mesoscopic Peierls rings and has been discussed recently.[5] In this paper, we shall demonstrate the importance of incorporating the correct symmetry in the wave function of mesoscopic systems of strongly correlated electrons. Moreover, we show that these systems can be described reasonably well within a variational treatment based on trial functions appropriately constructed. To illustrate this, we shall consider here finite rings described by an extended-Hubbard model at half-filling. Various Hubbard models have been often used to examine strongly correlated electrons in numerous low-dimensional compounds ranging from conducting polymers to cuprates. The one-dimensional extended-Hubbard model is interesting because its ground state displays various types of orderings. Out of these, charge- and spin-density-waves (CDW, SDW) are most relevant phases for quasi-one-dimensional compounds.

II. MODEL AND GENERAL PROPERTIES

Let us consider N electrons on N sites (half-filling case) described by an extended-Hubbard Hamiltonian,

$$H=-t\sum_{j=1}^{N}\sum_{\sigma=\uparrow,\downarrow}\left(c_{j,\sigma}^{\dagger}c_{j+1,\sigma}+c_{j+1,\sigma}^{\dagger}c_{j,\sigma}\right)+\sum_{j=1}^{N}\left(Un_{j,\uparrow}n_{j,\downarrow}+Vn_jn_{j+1}\right). \quad (1)$$

Here, c ($c^{\dagger}$) denotes creation (annihilation) operators for electrons, $n_{j,\sigma}\equiv c_{j,\sigma}^{\dagger}c_{j,\sigma}$, $n_j\equiv n_{j,\uparrow}+n_{j,\downarrow}$, t is the hopping integral between nearest neighbors (unless otherwise specified, set throughout to unity), U and V are on-site and nearest-neighbor potentials, respectively. Numerous methods (including mean field, quantum Monte Carlo exact numerical diagonalization, DMRG) have been employed previously to study the phase diagram of the model (1), but they were ultimately applied to the limit $N\rightarrow\infty$.[6–9]

In a sense, finite (mesoscopic) systems are more interesting than infinite systems. Besides the model parameters (t, U, V) characterizing the latter, the size N represents an extra parameter that can modify the physical properties of the former.

Physical insight into the model (1) can be gained by examining the (classical) limit $t\rightarrow 0$. Then, for $0<U<2V$, there are two equivalent multielectronic configurations $|CDW_{1,2}\rangle$ for which the energy is the lowest, corresponding

TABLE I. Symmetries of the ideal-ordered states characterizing the CDW and SDW orderings in closed- and open-shell systems.

State	$N=4n+2$ (PBC)	$N=4n$ (ABC)	$N=4n$ (PBC)	$N=4n+2$ (ABC)
CDW_+	$T^+R^+C^+F^-$	$T^+R^+C^+F^+$	$T^+R^+C^+F^+$	$T^+R^+C^+F^-$
CDW_-	$T^-R^+C^-F^-$	$T^-R^+C^-F^+$	$T^-R^+C^-F^+$	$T^-R^+C^-F^-$
SDW_+	$T^-R^+C^-F^+$	$T^+R^+C^+F^+$	$T^-R^-C^+F^+$	$T^+R^-C^-F^+$
SDW_-	$T^+R^+C^+F^-$	$T^-R^+C^-F^-$	$T^+R^-C^-F^-$	$T^-R^-C^+F^-$

to doubly occupied sites and unoccupied sites alternating periodically (the bipolaronic limit of a CDW). In occupation number representation, they are expressed as $|CDW_1\rangle = |\ldots 0202\ldots\rangle$ and $|CDW_2\rangle = |\ldots 2020\ldots\rangle$. For $0<2V<U$, the lowest energy is obtained if each site is occupied exactly by one electron with either up or down spin; two possible states are those where the spin orientations alternate between adjacent sites, i.e., $|SDW_1\rangle = |\cdots\uparrow\downarrow\uparrow\downarrow\cdots\rangle$ and $|SDW_2\rangle = |\cdots\downarrow\uparrow\downarrow\uparrow\cdots\rangle$ (the antiferromagnetic limit of an SDW). The critical point ($U=2V$) of the CDW-SDW transition expected within this oversimplified analysis is not very far from what quantum calculations[7–9] predict for infinite systems ($U\lesssim 2V$).

The limiting configurations $|CDW_{1,2}\rangle$ and $|SDW_{1,2}\rangle$ represent dimerized states, i.e. states of broken symmetry. This is possible only in infinite systems. In finite ones, when the exact ground state is nondegenerate—a fact confirmed by our results for small rings studied by exact (Lanczos) diagonalization—it should preserve the symmetry of the Hamiltonian. The N-site ring described by Eq. (1) is invariant under the following symmetry transformations: $c_{j,\sigma}\rightarrow c_{j+1,\sigma}$ (elementary translation $\hat{T}$), $c_{j,\sigma}\rightarrow c_{N-j,\sigma}$ (space inversion $\hat{R}$), $c_{j,\sigma}\rightarrow(-1)^j c^\dagger_{j,\sigma}$ (charge conjugation $\hat{C}$) and $c_{j,\sigma}\rightarrow c_{j,-\sigma}$ (spin flip $\hat{F}$). Under the aforementioned transformations, the nondegenerate eigenstates $|\Psi_\mu\rangle$ of (1) should be either of even or of odd parity ($|\Psi_\mu\rangle\rightarrow\pm|\Psi_\mu\rangle$). We shall use, e.g., $C^\pm$ to denote an eigenstate that is symmetric (antisymmetric) with respect to charge conjugation. Out of the above multielectronic configurations that are classically equivalent, one can construct the following states compatible with the original symmetry: $|DW_\pm\rangle\propto|DW_1\rangle\pm|DW_2\rangle$ (DW is either CDW or SDW). Their symmetries are indicated in Table I for systems with $N=4n+2$ and $N=4n$, both for periodic (PBC) and antiperiodic (ABC) boundary conditions.

Several previous studies on weakly correlated systems like cyclic polyenes (annulenes)[10] and finite Peierls rings[4,5] demonstrated that closed and open shell systems behave quite differently. By definition, a closed (open) shell system possesses a nondegenerate (degenerate) ground state in the absence of interaction. Rephrasing, the so-called highest-occupied-molecular-orbital–lowest-unoccupied-molecular-orbital (HOMO-LUMO) gap (i.e., the energy difference between the lowest-unoccupied orbital and the highest-occupied orbital) is finite for closed shells, but vanishes for open shells. Our results obtained by means of the exact numerical diagonalization for small size systems described by the Hamiltonian (1) confirm that notable differences between closed ($N=4n+2$ with PBC and $N=4n$ with ABC) and open ($N=4n$ with PBC and $N=4n+2$ with ABC) shells also exist in the presence of strong correlations. Therefore, we shall discuss closed and open shells separately. Since the approach proposed in this paper is particularly suitable for closed shells, we shall mainly examine this case and consider for specificity $N=4n+2$ and PBC. Open shells will be analyzed in Sec. VI.

For $N=4n+2$ and PBC, a straightforward analysis reveals that both states $|CDW_+\rangle$ and $|SDW_-\rangle$ are of symmetry $T^+R^+C^+F^-$. For small rings, we have computed the exact ground state $|\Psi_0\rangle$ by numerical (Lanczos) diagonalization. It turns out that $|\Psi_0\rangle$ contains, besides the terms entering $|CDW_+\rangle$ and $|SDW_-\rangle$, other contributions, but its symmetry is the same $T^+R^+C^+F^-$ in the whole $(U/t,V/t)$ plane. This is why $|\Psi_0\rangle$ can change gradually from a CDW-type state to an SDW-type one, e.g., by decreasing V at fixed U and t. The smoothness of the CDW-SDW transition in periodic $(4n+2)$-site rings is illustrated in Fig. 1(a) by exact (Lanczos) diagonalization results for the ground state CDW correlation function K_c,

$$K_c \equiv -\sum_{j=1}^{N}(-1)^j\langle n_j n_1\rangle. \tag{2}$$

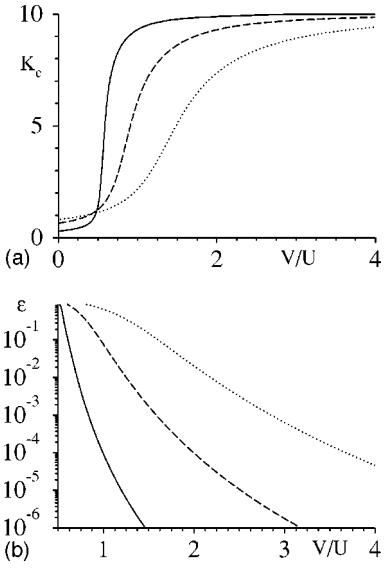

FIG. 1. Results obtained by exact (Lanczos) diagonalization for ten site periodic rings and $t/U=0.2;0.5;1$ (solid, dashed, and dotted lines, respectively). (a) The CDW correlation functions K_c reveal a smooth CDW-SDW transition. (b) The energy ε of the lowest excitation.

The inspection of the curves in Fig. 1(a) reveals the influence of quantum fluctuations on the CDW-SDW transition. With increasing t at fixed U, the transition occurs at values of $2V/U$ substantially larger than in infinite systems ($2V/U \gtrsim 1$); the transition is significantly pushed towards the CDW region. The larger the quantum fluctuations (t), the broader is the transition region.

For $V/U \gg 1$ and $V/t \gg 1$, $|\Psi_0\rangle$ tends to the symmetric superposition $|CDW_+\rangle$. This demonstrates that the classically equivalent configurations $|CDW_{1,2}\rangle$ contribute to the exact ground state and there exists a tunneling involving all electrons between them. To our knowledge, such a *collective quantum electron tunneling* has not been discussed by previous investigators. If so, an eigenstate $|\Psi_1\rangle$ tending to the antisymmetric superposition $|CDW_-\rangle$ in the same limit should also exist. This expectation is confirmed by calculations that show that $|\Psi_1\rangle$ has the symmetry $T^- R^+ C^- F^-$, in agreement with Table I. The tunneling splitting $\varepsilon \equiv \langle\Psi_1|H|\Psi_1\rangle - \langle\Psi_0|H|\Psi_0\rangle$ becomes vanishingly small, e.g., by increasing V at fixed U and t [cf. Fig. 1(b)].

Unlike $|CDW_+\rangle$, the superposition $|SDW_-\rangle$ can *never* exhaust the expansion of the exact ground state, although there are parameter regions where $|SDW_-\rangle$ gives the largest contribution to $|\Psi_0\rangle$. This can be understood both classically and quantum mechanically. As discussed above, for $t \to 0$ and $0 < 2V < U$, the lowest energy is obtained if each site is occupied exactly by one electron with either up or down spin. $|SDW_{1,2}\rangle$ are only two states out of $\binom{N}{N/2}$ such configurations. On the other side, the total spin is a good quantum number for model (1), but (unlike $|CDW_\pm\rangle$) $|SDW_\pm\rangle$ are not eigenstates of the total spin operator $\mathbf{S}^2$. This suggests that, in the SDW regime, the significant contributions to $|\Psi_0\rangle$ should be more numerous and, hence, a more complicated-variational ansatz than that used employed below would be necessary. Therefore, we shall focus our attention in this paper only on the CDW part of the phase diagram.

III. SYMMETRY ADAPTED BCS-TRIAL FUNCTIONS FOR MESOSCOPIC RINGS IN THE CDW REGIME

Within a mean-field picture, a CDW is represented by a nonvanishing site-independent average $(-1)^j \langle n_j - 1\rangle$. This means that the charge excess at each even-numbered site is equal to the charge deficit at each odd-numbered site. As noted, there also exists another equivalent configuration (obtained by interchanging the words even and odd above). To describe such states, one could choose a BCS-type trial wave functions of the form [$\kappa \equiv (N-2)/4$, $|0\rangle$—vacuum state]

$$|\varphi_{1,2}\rangle = \prod_{\sigma} \prod_{p=-\kappa}^{\kappa} (a^\dagger_{p,\sigma} \cos\theta_{p,\sigma} \pm b^\dagger_{p,\sigma} \sin\theta_{p,\sigma})|0\rangle, \quad (3)$$

where a certain ordering of the factors should be adopted (e.g., p increases by 1 from right to left), $\theta_{p,\sigma}$ are adjustable (real) parameters and $a^\dagger_{p,\sigma}$ ($b^\dagger_{p,\sigma}$) are creation operators of right- (left-) moving electrons,

$$c_{j,\sigma} = N^{-1/2} \sum_{p=-\kappa}^{\kappa} [a_{p,\sigma} \exp(2\pi i j p/N) + (-1)^j b_{p,\sigma} \exp(2\pi i j p/N)]. \quad (4)$$

A straightforward analysis reveals that, by imposing,

$$\theta_{p,\sigma} = \theta_{p,-\sigma} = \theta_p, \quad (5)$$

the functions $|\varphi_1\rangle$ and $|\varphi_2\rangle$ are eigenstates of the total spin $\mathbf{S}^2$ ($S=0$) and their symmetry under spin flip F^- coincides to that of the states $|\Psi_{0,1}\rangle$ and $|CDW_\pm\rangle$. However, both $|\varphi_1\rangle$ and $|\varphi_2\rangle$ correspond to states with broken $\hat{T}$, $\hat{R}$, and $\hat{C}$ symmetries. They cannot describe directly CDW ordering in mesoscopic systems, but can be used to construct trial functions whose symmetry is correct. The linear combinations $|\varphi_1\rangle \pm |\varphi_2\rangle$ are eigenstates of $\hat{T}$ and $\hat{C}$, but their transformation $\hat{R}$ is still incorrect. This last drawback can be eliminated by using the following functions:[11]

$$|\Psi_{A,B}\rangle \equiv \mathcal{C}^{-1/2}_{A,B} [|\varphi_1\rangle + |\psi_1\rangle \pm |\varphi_2\rangle \pm |\psi_2\rangle], \quad (6)$$

where the functions $|\psi_{1,2}\rangle$ are obtained replacing the quantities $\theta_{p,\sigma}$ by $\theta_{-p,\sigma}$ in the expressions (3) for $|\varphi_{1,2}\rangle$. The normalization constant is expressed by

$$\mathcal{C}_{A,B} \equiv 4\left[1 \pm \prod_{p=-\kappa}^{\kappa} \cos^2 2\theta_p + \prod_{p=-\kappa}^{\kappa} \cos^2(\theta_p - \theta_{-p}) \pm \prod_{p=-n}^{n} \cos^2(\theta_p + \theta_{-p})\right]. \quad (7)$$

One can show that these trial functions possess the symmetry properties of the exact eigenstates $|\Psi_{0,1}\rangle$ (cf. Sec. II): $|\Psi_A\rangle$ has the symmetries of $|\Psi_0\rangle$ ($T^+ R^+ C^+ F^-$), while $|\Psi_B\rangle$ has the symmetries of $|\Psi_1\rangle$ ($T^- R^+ C^- F^-$).[12]

The trial functions $|\Psi_{A,B}\rangle$ defined by Eq. (6) represent the starting point of the presently proposed variational approach for closed-shell systems. The essential difference from the case of infinite systems is that the trial functions used here are adapted to the symmetry of the mesoscopic systems. In order to compute physical properties of interest, one should determine $\{\theta_p\}$ ($N/2$ independent values for *each* state) by minimizing numerically the energy functionals $E_{A,B} \equiv \langle\Psi_{A,B}|H|\Psi_{A,B}\rangle$ obtained by combining Eqs. (1), (6), and (7). Because the expressions of $E_{A,B}$ are lengthy, they will be omitted.

IV. EXACT DIAGONALIZATION VERSUS SYMMETRY-ADAPTED BCS-TRIAL FUNCTIONS FOR SMALL RINGS

We have performed extensive computations on small rings by means of both exact numerical diagonalization and the trial functions defined in Sec. III. Some representative results are collected in Fig. 2. By inspecting the curves for the CDW and SDW correlation functions (K_c and K_s, respectively) of Figs. 2(a) and 2(b), one can conclude that the symmetry adapted trial functions $|\Psi_{A,B}\rangle$ are reasonably accurate. K_s is defined by replacing the operators $n_j \equiv n_{j,\uparrow}$

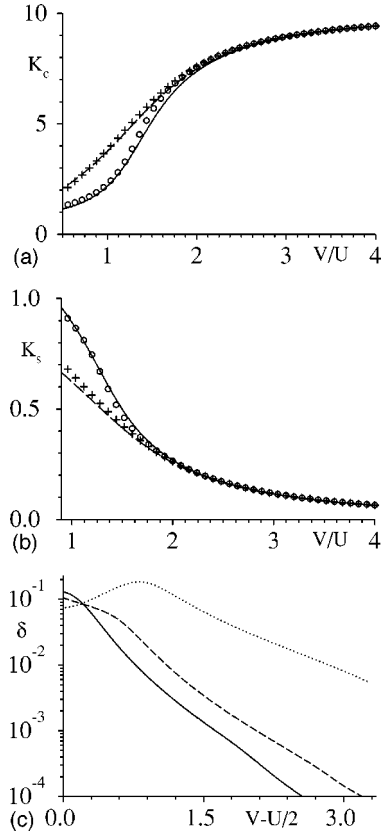

FIG. 2. Results for ten site periodic rings ($t=1$). (a),(b) CDW and SDW correlation functions $K_{c,s}$ obtained by means of the exact eigenstates $|\Psi_{0,1}\rangle$ (solid and dashed lines, respectively) and the symmetry-adapted trial functions $|\Psi_{A,B}\rangle$ (circles and crosses, respectively). (c) Absolute error in the ground state energy divided by the exact correlation energy $\delta \equiv (\langle\Psi_A|H|\Psi_A\rangle - \langle\Psi_0|H|\Psi_0\rangle)/(E_{HF} - \langle\Psi_0|H|\Psi_0\rangle)$ for $U=5;2.5;1$ (solid, dashed, and dotted lines, respectively).

$+n_{j,\downarrow}$ in the expression (2) of K_c by $n_{j,\uparrow}-n_{j,\downarrow}$ ($1\leqslant j\leqslant N$). One should note at this point that the SDW correlation function K_s decreases progressively with increasing V (i.e., when moving deeper into the CDW regime). This behavior illustrates alternatively the smoothness of the CDW-SDW transition in finite systems. The fact that K_s does not vanish exactly (as is with the case within a mean-field approach) is a result of quantum fluctuations. Besides, we also compare the absolute error in the ground state obtained variationally, $\delta E = \langle\Psi_A|H|\Psi_A\rangle - \langle\Psi_0|H|\Psi_0\rangle$, to the total correlation energy, $E_{corr} = E_{HF} - \langle\Psi_0|H|\Psi_0\rangle$ (E_{HF} is the total Hartree-Fock ground state energy); see the curve for $\delta = \delta E/E_{corr}$ in Fig. 2(c). The trial state that possesses the correct symmetry $|\Psi_A\rangle$ represents a better approximation—both qualitatively and quantitatively—for the exact ground state $|\Psi_0\rangle$ than that with broken symmetry ($|\varphi_{1,2}\rangle$). Notice also that δ vanishes exponentially in the strong coupling limit. In this limit, the function $|\Psi_A\rangle$ provides accurate estimates of the exact ground state properties.

Summarizing the comparison reveals that unlike the states with broken symmetry $|\varphi_{1,2}\rangle$, the symmetry-adapted BCS-trial wave functions $|\Psi_{A,B}\rangle$, provide a satisfactory framework for describing finite rings. The reason is that, although approximate, the expressions (6) of the functions $|\Psi_{A,B}\rangle$ account for the collective tunneling of electrons. As expected from intuitive physical reasons (Sec. II), this effect should play an important role at mesoscopic sizes.

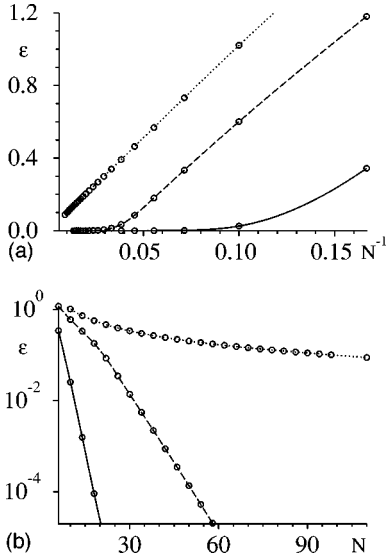

FIG. 3. For closed-shell systems, the lowest excitation energy ε behaves as a HOMO-LUMO gap ($\varepsilon \sim 1/N$) for small sizes (N) and as a tunneling splitting ($\ln \varepsilon \sim -N$)) for large N, indicating a crossover from weak to strong correlations. The parameter values are $t=1$ and, increasing downwards, $U=V=0.5;1;2$. Lines are guides to the eye.

V. WEAK VERSUS STRONG CORRELATIONS IN MESOSCOPIC RINGS

Two limits are encountered in the study of interacting systems. In the limit of weak correlations, a system can be described in terms of (almost) independent quasiparticles. Such a description does not hold any more in the opposite limit of strong correlations. Usually, one moves from the former case to the latter by starting with a collection of free particles and switching on interaction(s) between them. From this standpoint, mesoscopic systems are more interesting than infinite systems, because there exists another route between the two limits: not only by increasing interaction strengths (like U and/or V) but also by increasing the size N of the system.

In this section, we shall demonstrate this explicitly for the chosen model (1). This is possible within the variational approach based on the symmetry-adapted trial functions (6), because this method can be applied to rings of mesoscopic sizes, much larger than those for which numerical exact diagonalization can be carried out. Calculations clearly indicate the crossover from a weak-correlation regime to a strong-correlation regime with increasing size. To illustrate this, we present in Fig. 3 the N dependence of the lowest-excitation energy $\varepsilon \equiv \langle\Psi_B|H|\Psi_B\rangle - \langle\Psi_A|H|\Psi_A\rangle$.

By inspecting the curves for $U=V=1$ of Figs. 3(a) and 3(b), one can see that the linear dependence of $\varepsilon(N)$ on $1/N$

for small sizes ($N<N_c$) changes to an exponential dependence, $\ln \varepsilon(N) \sim -N$, beyond a certain size ($N>N_c$). The crossover value N_c is very sensitive to changes of interaction strengths. The stronger the coupling, the higher is the value of N_c. The crossover value is larger than all the sizes employed in Fig. 3 for $U=V=0.5$, while it is smaller for $U=V=2$. This is why, in the *whole N* range shown in Fig. 3, the $\varepsilon(N)$ curve is practically linear in Fig. 3(a) for $U=V=0.5$, and in Fig. 3(b) for $U=V=2$. This behavior of $\varepsilon=\varepsilon(N)$ has a clear physical interpretation. For $N<N_c$ (weak correlation or single-particle regime), the main interaction effect is to renormalize the single-particle gap. There, $\varepsilon(N)$ plays the role of a (renormalized) HOMO-LUMO gap ($\varepsilon \sim t/N$ for $U=V=0$). In the opposite case, $N>N_c$ (strong correlation or collective regime), $\varepsilon(N)$ is the result of the tunneling of electrons through an energy barrier. Semiclassically, the tunnel-splitting energy should be proportional to the transmission coefficient τ over a distance of the order of the lattice constant a through a barrier of height $E_B \approx E_{corr}$ (see below) of an object of mass $M \approx Nm$ [$m \approx \hbar^2/(2ta^2)$ being the electron mass]. This yields $\log \tau \sim -a\sqrt{2E_BM}/\hbar \sim -\sqrt{E_{corr}N/t} \propto N$. The proportionality to N is the result of the fact that for larger sizes $E_{corr} \propto N$. The size-dependence $\ln \varepsilon \sim -N$, similar to that of $\ln \tau$, is a clear indication of the *collective* nature (i.e., $M \propto N$) of this effect, in accord with the qualitative analysis of Secs. I and II. The above considerations also allow us to unravel the physical meaning of the critical size N_c. The crossover between weak and strong correlation regimes (alternatively, between single particle and collective excitations) occurs when the exponent entering the expression of τ is of the order of unity, i.e., $E_{corr} \sim t/N$. This relation has a clear physical interpretation: at $N \sim N_c$, the system can rapidly tunnel between the two classically equivalent configurations, because the energy of single electron-hole excitations ($\sim t/N$) is comparable to the energy barrier ($\sim E_{corr}$). This is analogous to the crossover between normal (undimerized) and dimerized regimes encountered in mesoscopic Peierls rings.[5] In that case, the critical size corresponds to an energy barrier $V(Q=0) - V(Q_{MF})$ as determined by the symmetric adiabatic double well potential $V(Q)=V(-Q)$ [Q is the dimerization coordinate and $V_{\min}=\min_Q V(Q)$] which is comparable to the phonon frequency Ω; see Ref. 5 for details. The correspondence between the case of Ref. 5 and the present one is the following: $V(Q=0) \rightleftharpoons E_{HF}$, $V_{min} \rightleftharpoons \langle \Psi_A|H|\Psi_A\rangle$, and $t/N \rightleftharpoons \Omega$. Unfortunately, unlike V_{min}, the (almost) exact energy $\langle \Psi_A|H|\Psi_A\rangle$ cannot be evaluated analytically, so that a straightforward estimation of E_{corr}, and hence, of the present quantity N_c is impossible.

It is also interesting to examine the size dependence of relevant average properties, like the CDW and SDW correlation functions $K_{c,s}$. To understand the results collected in Figs. 4(a) and 4(b), one should first remember that, for the values used there ($U=V$), an infinite system would be in the CDW regime ($U<2V$). The twofold degenerate mean-field ground state would be a CDW condensate characterized by an extensive CDW correlation function ($K_c \propto N$) and vanishing SDW correlations ($K_s=0$). As illustrated in Fig. 4, differences exist between the properties of the states $|\Psi_A\rangle$ and $|\Psi_B\rangle$ for sufficiently small sizes. The weaker the coupling, the broader is the N range where the properties are significantly size dependent and the larger are the differences between the states $|\Psi_A\rangle$ and $|\Psi_B\rangle$: compare the curves for $U=V=0.5$, 1, and 2 in Fig. 4.

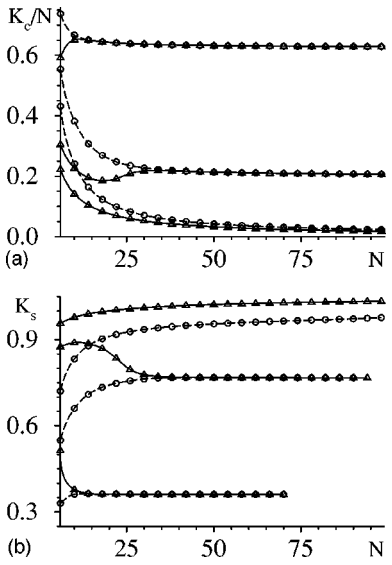

FIG. 4. The size dependence of the normalized CDW correlation function K_c/N (a) and absolute SDW correlation function K_s (b) for closed-shell systems in the lowest energy states $|\Psi_A\rangle$ and $|\Psi_B\rangle$ (triangles and circles, respectively). Lines are guides to the eye. The parameter values $U/t=V/t=0.5;1;2$ increase upwards in (a) and downwards in (b) for $N \geqslant 50$.

In Fig. 4(a), we show the N dependence of the normalized CDW correlation function K_c/N. K_c/N saturates for $N \rightarrow \infty$, indicating the presence of a well-defined CDW condensate in infinite systems. The semiclassic (mean-field) picture becomes qualitatively correct in the thermodynamic limit. At large enough sizes, the tunneling splitting ε becomes vanishingly small. The states $|\Psi_A\rangle$ and $|\Psi_B\rangle$ become almost degenerate and are characterized by almost equal CDW correlations, in agreement with the qualitative discussion of Sec. I.

It is also useful to compare the different behaviors exhibited by the curves of Figs. 4(a) and 4(b). Notice that the former refers to the *normalized* CDW correlation function K_c/N, whereas the latter refers to the *absolute* SDW correlation function K_s. Both quantities saturate in the thermodynamic limit. The CDW condensate becomes more pronounced with increasing N, while the SDW is not condensed; unlike in the mean-field description, weak SDW correlations exist ($K_s \neq 0$) but are practically determined solely by size-independent quantum fluctuations. This behavior resembles that of the mean-square lattice displacement $\langle Q^2 \rangle = \langle (a + a^\dagger)^2 \rangle$ (a and $a^\dagger$ are phonon operators). For a condensed-phonon field (static lattice distortion), $\langle Q^2 \rangle$ is proportional to N, whereas for normal (noncondensed phonons) it tends to a N-independent value determined by quantum-phonon fluctuations ($\langle Q^2 \rangle = 1$ for free phonons); see, e.g., Ref. 5. The picture emerging from this analysis is consistent to that of a

smooth CDW-SDW transition discussed in Sec. II and indicates two alternative routes towards a well-defined CDW state: by increasing the size (for $V>U/2$) or the coupling strength (e.g., V at fixed U).

VI. OPEN SHELL CASE

So far, we have shown that the symmetry-adapted trial functions (6) are suitable to describe periodic (PBC) rings with $N=4n+2$ sites in the CDW regime. This is also the case of antiperiodic (ABC) rings with $N=4n$ sites. There are only several minor differences between the cases $N=4n+2$ with PBC and $N=4n$ with ABC. In the latter case, the ground state also has, in the whole $(U/t,V/t)$-plane, the same symmetries: they are those of the states $|CDW_+\rangle$ and $|SDW_-\rangle$ (*not* $|SDW_+\rangle$, cf. Table I). The functions $|\Psi_A\rangle$ and $|\Psi_B\rangle$ have the same symmetries as the states $|CDW_+\rangle$ and $|CDW_-\rangle$, respectively. The different spin-flip symmetry (F^- for $N=4n+2$ with PBC, but F^+ for $N=4n$ with ABC) is the consequence of the fact that the transformation $\hat{F}$ interchanges an odd (even) number of parentheses in Eq. (6) in the former (latter) case, since κ is (half-) integer. The physical properties for $N=4n+2$ with PBC and $N=4n$ and ABC are quite similar, because both correspond to closed shells: the ground state of the noninteracting systems is nondegenerate (the HOMO-LUMO gap does not vanish). Analogous to the situation encountered in Peierls mesoscopic rings,[5] the points on the curves displaying the N dependence of relevant physical properties for the case $N=4n+2$ and PBC smoothly interpolates between those for the case $N=4n$ and ABC.

As already noted in Sec. II, our results obtained by means of the exact numerical diagonalization for small sizes indicated that notable differences between closed ($N=4n+2$ with PBC and $N=4n$ with ABC) and open ($N=4n$ with PBC and $N=4n+2$ with ABC) shells, known from previous investigations on weakly correlated systems,[10,4,5] also exist in the case of strong correlations. To exemplify, one can refer to the CDW-SDW transition. According to the qualitative analysis of Sec. II, one can conclude that a CDW-SDW transition should necessarily occur by changing the model parameters from $1\ll U/t<2V/t$ to $U/t>2V/t\gg 1$. The inspection of Table I shows that a transition $|CDW_\mu\rangle \rightleftharpoons |SDW_\nu\rangle$ in open-shell rings must be accompanied by a change in the ground state symmetry ($\mu,\nu=\pm$). This indicates a *sharp* CDW-SDW transition in these cases, as explicitly shown in Ref. 13, contrasting to the smooth one found in Sec. II.

Trial functions possessing the symmetries of the states $|CDW_\pm\rangle$ can also be constructed for open shells. However, their form is more complicated than those of Sec. III, just because of the ground state degeneracy of the free electron gas. To illustrate the difficulty, one should note that to construct two singlet states with the symmetries of $|CDW_+\rangle$ and $|CDW_-\rangle$ in the absence of interaction, one should superpose each time two distinct states out of the six degenerate ground states. In view of the above considerations, instead of $|\varphi_{1,2}\rangle$ and $|\psi_{1,2}\rangle$, one can try to use the functions

$$|\xi_{1,2}\rangle=[\pm Ar_\downarrow^\dagger r_\uparrow^\dagger \pm Bl_\downarrow^\dagger l_\uparrow^\dagger + C(r_\downarrow^\dagger l_\uparrow^\dagger - r_\uparrow^\dagger l_\downarrow^\dagger)] \times \prod_{\sigma,k} (a_{k,\sigma}^\dagger \cos\theta_k \pm b_{k,\sigma}^\dagger \sin\theta_k)|0\rangle,$$

$$|\eta_{1,2}\rangle=[\pm Br_\downarrow^\dagger r_\uparrow^\dagger \pm Al_\downarrow^\dagger l_\uparrow^\dagger + C(r_\downarrow^\dagger l_\uparrow^\dagger - r_\uparrow^\dagger l_\downarrow^\dagger)] \times \prod_{\sigma,k} (a_{k,\sigma}^\dagger \cos\theta_{-k} \pm b_{k,\sigma}^\dagger \sin\theta_{-k})|0\rangle,$$

where k increases by unity from $-N/4+1/2$ to $N/4-1/2$, $r_\sigma=b_{-N/4-1/2,\sigma}$, $l_\sigma=a_{-N/4-1/2,\sigma}$, $A=\sin\alpha\cos\beta$, $B=\sin\alpha\sin\beta$ and $C=2^{-1/2}\cos\alpha$ $(A^2+B^2+2C^2=1)$. These functions are of broken symmetry, but they can be used to define the trial functions with correct symmetries:

$$|\Phi_{A,B}\rangle \propto |\xi_1\rangle + |\eta_1\rangle \pm |\xi_2\rangle \pm |\eta_2\rangle. \tag{8}$$

Straightforward analysis shows that the functions $|\Phi_A\rangle$ and $|\Phi_B\rangle$ represent singlet states with the symmetries of $|CDW_+\rangle$ and $|CDW_-\rangle$, respectively. We have used the functions $|\Phi_{A,B}\rangle$ to minimize the total energy by adjusting the variational parameters $\{\theta_p\}$, α and β. For small systems, we have compared the results of exact numerical diagonalization[13] with those deduced variationally by using the functions $|\Phi_{A,B}\rangle$. Although not as accurate as in the closed-shell case, the proposed variational approach can still reproduce exact ground state properties of open-shell systems within a few percent; see Fig. 5(a) for illustration.

In the presence of an Aharonov-Bohm (AB) magnetic flux ϕ (flux unit hc/e) threading a ring, the first term in parenthesis of Eq. (1) should be replaced by $c_{j,\sigma}^\dagger c_{j+1,\sigma}\exp(2\pi i\phi/N)+c_{j+1,\sigma}^\dagger c_{j,\sigma}\exp(-2\pi i\phi/N)$.[14] This yields a flux-dependent ground state varying periodically with the flux $E_G(\phi)=E_G(\phi+1)$ and a persistent electric current $j\propto -\partial E_G/\partial\phi$ oscillating with ϕ. The average over a half-period of the latter $j_{av}\propto E_G(1/2)-E_G(0)$ can be taken as a measure of the amplitude of j oscillations. The above ϕ-dependent phase factor can be accounted for by twisting the boundaries; the difference $E_G(1/2)-E_G(0)$ represents the difference between the ground state energies computed with periodic and antiperiodic boundary conditions at zero flux; see, e.g., the second part of Ref. 5 and references cited therein. Figure 5(b) illustrates that the j_{av} curve obtained variationally reasonably reproduces the exact one in the CDW region relatively close to the CDW-SDW transition $(2V/U\gtrsim 1)$. For such a case, we also present in Fig. 5(c) the size dependence of j_{av} obtained by using the trial functions (6) and (8). Figures 5(b) and 5(c) also show a fact important for observability: for moderate couplings, the persistent current is not very much diminished with respect to the values for free electrons.

However, some important properties of open-shell rings cannot be correctly described by means of the functions $|\Phi_{A,B}\rangle$. A spectacular finding we reported recently for open-shell clusters described by model (1) is the occurrence of quantum-phase transitions driven by tunneling.[13] As a result of quantum tunneling, by varying the parameters U/t and V/t, the ground state can change, e.g., from a state with the

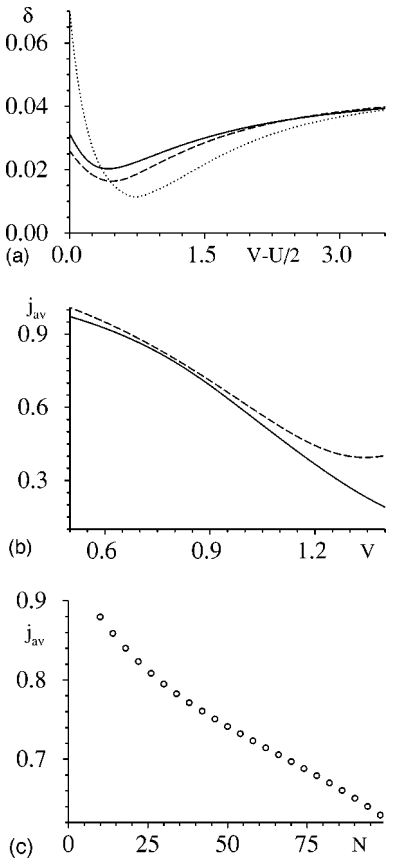

FIG. 5. (a) Absolute error in the ground state energy divided by the exact correlation energy for antiperiodic ten site clusters. $\delta \equiv (\langle \Psi_A|H|\Psi_A\rangle - \langle \Psi_0|H|\Psi_0\rangle)/(E_{HF} - \langle \Psi_0|H|\Psi_0\rangle)$ for $U=5;2.5;1$ (solid, dashed, and dotted lines, respectively). The comparison with Fig. 2 illustrates that the variational results for open shells are much less accurate than for closed shells. (b),(c) Persistent current averaged over an AB half-period normalized to its value for free electrons at $t=U=1$: (b) exact versus variational results for $N=10$ (solid and dashed lines, respectively); (c) N dependence of the variational results for $V=0.7$.

symmetry of $|CDW_+\rangle$ to a state with the $|CDW_-\rangle$ symmetry. This result has been obtained for small clusters for which the numerical exact diagonalization can be carried out, and it would be desirable to investigate such unusual phenomena at larger sizes as well. To this purpose, a physically transparent and reliable approach of the type proposed here would be very useful. Unfortunately, such CDW-to-CDW quantum-phase transitions cannot be described by means of Eq. (8). We found that the state $|\Phi_A\rangle$ is *always* energetically lower than state $|\Phi_B\rangle$. As such, one should expect variational results significantly deviating from exact ones in the region where the ground state has the symmetry of $|\Phi_B\rangle$. Therefore, the disagreement between the two j_{av}-curves of Fig. 5(b) for V values beyond the point $V=0.75$ of the CDW-to-CDW transition is not surprising.

VII. SUMMARY AND OUTLOOK

In this paper, we have developed an approach based on symmetry-adapted trial functions of BCS-type that is reasonably accurate, and applied it to mesoscopic rings described by an extended-Hubbard model at half-filling. To demonstrate its usefulness, we have applied this method to point out and investigate a phenomenon occurring in the systems under consideration that was ignored by previous investigators: the collective tunneling of electrons between two CDW configurations that are classically equivalent. Recently, a quantum tunneling of electrons has been inferred from experiments on double layers in gallium arsenide quantum wells.[15] There, the two lowest energy states can also be expressed approximately as the symmetric and antisymmetric superpositions of two wave functions, analogous to the present case. Similar situations are encountered, e.g., in NH_3 molecules[16] and dimerized systems,[5] where the symmetry, broken within semiclassical (mean-field) approximations, is restored by quantum tunneling. What makes the difference between those cases and ours is the origin of the tunneling (phononic and not electronic).

We have shown that the symmetry-adapted trial functions of BCS-type proposed here can be used to describe reliably mesoscopic systems with closed shells. Most of the interest in mesoscopic rings stems from the Aharonov-Bohm effect and the related persistent currents. Therefore, it would be useful to develop a reliable and physically transparent approach able to provide the flux dependence of relevant quantities. As discussed in Sec. VI, a quantitative treatment of the flux dependence would require, first, a reliable description of the open-shell case and, second, trial functions changing continuously between the closed- and open-shell cases. In view of the limitations of the approach based on Eq. (8), further investigations on a suitable choice of symmetry-adapted trial wave functions to describe open-shell systems with mesoscopic sizes represent a necessary first step.

The different symmetries of the two states $\Psi_{A,B}$ of lowest energy can be exploited in optical studies for a correct classification of the excited states. For low temperatures $T(<\varepsilon)$, only optical transitions from the state Ψ_A are possible, while for $T\sim\varepsilon$ the transitions from the state Ψ_B also contribute to the spectrum. The optical absorption in the state Ψ_B could be extracted by comparing the two spectra. In weakly correlated systems, the tunneling also yield pairs $\Psi_{\mu,\nu}$ of *excited* states that are nearly degenerate ($|E_\mu - E_\nu| \sim \varepsilon$) and of different symmetries. Out of them, a single transition can contribute to either spectrum (say $\Psi_A \rightarrow \Psi_\mu$ and $\Psi_B \rightarrow \Psi_\nu$). Strong correlations may yield excitations that do not necessarily consist of pairs of almost degenerate states; hence, one can expect a more significant difference between the two aforementioned spectra. Of course, this is possible only for sizes corresponding to sufficiently large values of the tunneling splitting. According to the present evaluations (cf. Fig. 3), $\varepsilon \sim 1$ meV ($\varepsilon \sim 10$ K) for $N\sim 50$ at moderate couplings ($t,U,V \sim 1$ eV). The strong dependence of ε on the interaction strengths [cf. Fig. 1(b)] could be exploited once it is possible to fabricate ordered nanostructures of rings consisting of quantum dots. Controlled modifications of the model parameters (t,U,V) could be achieved by controlled modifications in size and spacing of such quantum-dot systems.

The present theoretical study shows interesting effects

due to quantum tunneling in commensurate systems of strongly correlated electrons. We hope that this will also stimulate the experimental interest in investigations on such systems. A direct experimental study of such phenomena becomes imaginable in view of the recent achievements of nanometer-scale site-control techniques for the growths of individual quantum dots on semiconductor surfaces.[17]

ACKNOWLEDGMENTS

I.B. thanks Professor E. Dormann and Professor H. von Löhneysen for valuable discussions. The work at Karlsruhe has been financially supported by the Sonderforschungsbereich 195.

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[12] The full spatial symmetry of the Hamiltonian (1) can be described by the point group C_{Nv} (or D_N). The trial functions $|\Psi_A\rangle$ and $|\Psi_B\rangle$ transforms according to the one-dimensional irreducible representations A_1 and B_1, respectively.

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