Quantum coherence and decoherence of correlated electron states in the one-dimensional charge-density-wave–spin-density-wave phase transition

Norikazu Tomita*
Institute of Materials Structure Science, 1-1 Oho, Tsukuba, Ibaraki, 305-0801, Japan
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The charge-density-wave (CDW)–spin-density-wave (SDW) phase transition of the one-dimensional extended Hubbard model is investigated in the strong correlation regime, from the viewpoint of the quantum coherence or decoherence of the two correlated states. In the finite-size system, the CDW wave function, near the phase boundary, has the significant quantum fluctuations due to the SDW domains. The superposition of these SDW domains leads to the quantum coherence between the CDW and SDW wave functions. However, the scaling analysis shows that the density of the SDW fluctuations becomes asymptotically zero in the infinite-size limit, which indicates the decoherence of the two states in the bulk phase transition.

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I. INTRODUCTION

The quantum phase transition, quantum fluctuation, and quantum nucleation have been attracting much interest in fundamental physics for a long time.[1] Now, the clarifying of these quantum phenomena is believed also to help us understand the quantum effects in the unconventional phases, such as the high-temperature superconductivity[2] and quantum paraelectrics.[3] Furthermore, in addition to the historical ^{3}He-^{4}He liquid mixtures,[4,5] the quantum phase transition has also been reported for the organic charge-transfer complexes.[6] Thus, the research on the fluctuations and nucleation in the quantum phase transition has been becoming quite important.

A one-dimensional (1D) electron system is a good target to study the quantum phase transition, since no thermal phase transition occurs in it due to the large quantum fluctuations. A charge-density-wave (CDW)–spin-density-wave (SDW) phase transition of the 1D extended Hubbard model is a simple but interesting example, which has rich information on the quantum effects in the phase transition. Its Hamiltonian is given by

$$H = -t\sum_{l,\sigma}^{N}(a_{l,\sigma}^{\dagger}a_{l+1,\sigma} + a_{l+1,\sigma}^{\dagger}a_{l,\sigma}) + U\sum_{l}^{N} n_{l,\uparrow}n_{l,\downarrow} + V\sum_{l}^{N} n_l n_{l+1}, \tag{1}$$

where $n_l = n_{l,\uparrow} + n_{l,\downarrow}$ and N represents the system size. The half-filled case, where the number of electrons is equal to N, is considered. In Eq. (1), t, U, and V denote the transfer energy between the neighboring sites, on-site and nearest-neighbor-site Coulomb repulsions, respectively. In the following calculations, all the energies are scaled by t, and the periodic boundary condition is imposed.

So far, the CDW–SDW phase transition has widely been studied by many methods,[7–25] and, for example, it has been clarified that the phase boundary deviates slightly from the Hartree-Fock (HF) result $U=2V$ to the CDW side ($U<2V$), due to the electron correlation effects. The recent theories have further pointed out the bond order wave (BOW) ground state near the CDW–SDW phase boundary[17–19,22–25] or just on the phase boundary[20] in the weak and intermediate correlation regimes. Although the precise phase diagram is not determined yet, the CDW–SDW phase transition is now believed to be mediated by the BOW ground state, such as CDW–BOW–SDW, in the weak and intermediate correlation regimes. On the other hand, the direct CDW–SDW phase transition of the first order is realized in the strong correlation regime.

Although the ground state behaviors have thus extensively been studied, we do not have sufficient information on the quantum fluctuations in this system yet, which is also important to understand the nature of the transition.

In this paper, the direct CDW–SDW phase transition in the strong correlation regime is studied by the resonating Hartree-Fock (Res-HF) method, from the viewpoint of the quantum coherence and decoherence of the two correlated states. Here, the quantum coherence of the two states, denoted by A and B phases, for example, is accomplished by the coherent superposition of the B phase domains in the wave function for the A phase, and vice versa. These counter-phase domains work as the quantum fluctuations in the quantum phase transition. In the second order phase transition, this quantum coherence is realized and the electron state changes continuously from one state to another by changing the weight of the counter-phase domains. In the first order phase transition, on the other hand, this quantum coherence is cut off, and the two different phases cannot be continuously connected by the quantum fluctuations. In the previous paper, we have tried to clarify the quantum fluctuation effects on the CDW–SDW phase transition.[26] We have shown that the SDW (CDW) domains appear in the CDW (SDW) wave function near the phase boundary. However, the system size was restricted up to $N=22$, and we could not elucidate how the phase transition is characterized from the quantum fluctuations. In this paper, it will be shown that the density of the SDW domains in the CDW wave function becomes asymptotically zero in the infinite-size limit, though the small SDW domains persist near the phase boundary. Thus, the quantum coherence between the CDW and SDW states is cut off, and the phase transition becomes of the first order in the infinite-size system.

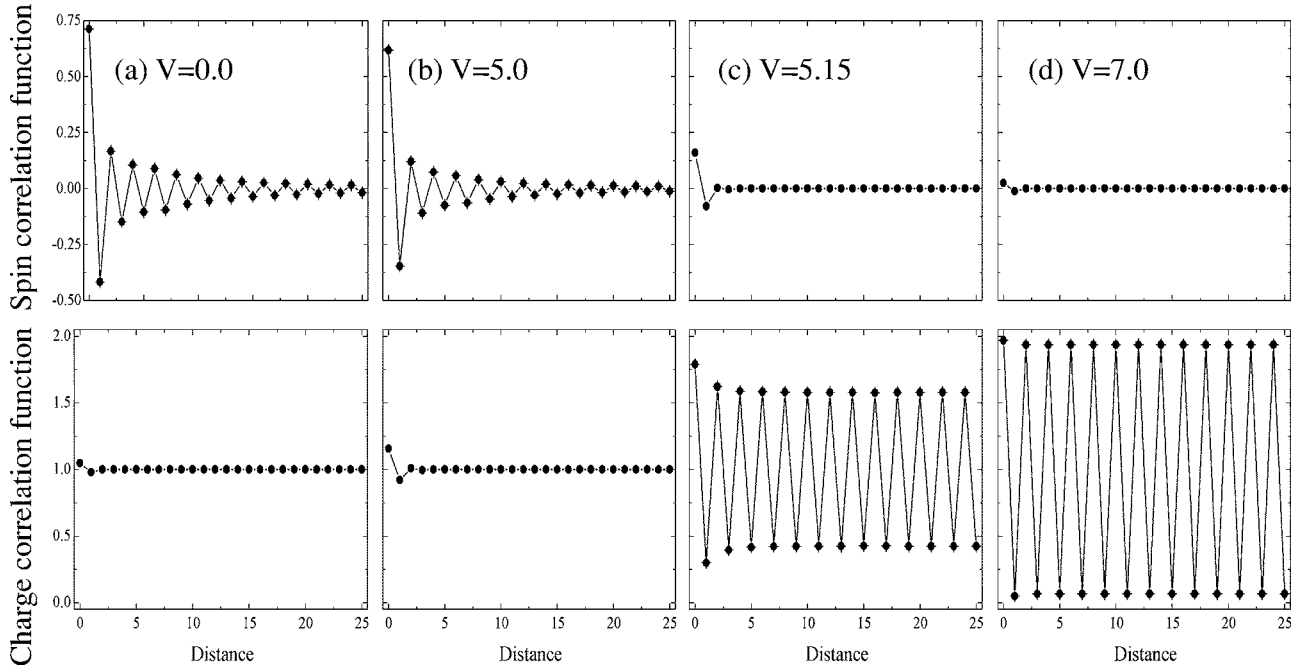

FIG. 1. V-dependence of the overall structures of the spin and charge correlation functions for $N=50$ at $U=10$. The Res-HF results with $N_S=30$ S-dets (black circles) are compared with those with $N_S=20$ S-dets (crosses) for the spin correlation functions in the SDW region and charge correlation functions in the CDW region.

This viewpoint is important also for the preliminary understanding of the quantum nucleation. In general, the first order phase transition starts with creation of islands or domains of the true ground state in the quasistable state. Then, these domains trigger the complete phase transition to the true ground state. In the low temperature limit, where the system cannot thermally go beyond the potential barrier, the domains are created by the quantum tunneling effect. This creation of the domains of the true ground state, in the first step of the quantum phase transition, is called the quantum nucleation. In this research, the quantum fluctuations due to the survived SDW domains in the CDW wave function are suggested to evolve into the quantum nucleation, which triggers the CDW–SDW phase transition, when the system goes to the SDW region. The subject of the present research is, thus, to clarify the nature of the first order quantum phase transition through the quantum fluctuations, and not to determine the phase diagram precisely. We are also interested in the quantum nucleation, which is characteristic of the first order phase transition. Since the CDW–BOW or BOW–SDW phase transition is suggested to be continuous,[17–19,22–25] the BOW-mediated phase transition is not suitable for the research on the quantum nucleation, and it will be studied elsewhere.

This paper is organized as follows. In Sec. II, the Res-HF method is briefly reviewed. In Sec. III, this method is applied to the CDW–SDW phase transition in the 1D extended Hubbard model. The correlation structures and quantum fluctuations are clarified in this section. Finally, a summary is given in Sec. IV.

II. METHOD

The Res-HF method constructs a many-body wave function by superposition of nonorthogonal Slater determinants (S-dets),[27] such as

$$|\Psi\rangle = \sum_{n=1}^{N_S} C_n \sum_G P^G |\phi_n\rangle. \tag{2}$$

Here, the broken symmetry S-dets are employed to generate the Res-HF wave function, and N_S represents the number of the S-dets. This is a natural extension of the unrestricted Hartree-Fock (UHF) approximation, in which the electron correlations are partially described by a single broken symmetry S-det, to the multi-S-det approach for the strongly correlated electron systems. To recover the original symmetry, we apply the Peierls-Yoccoz[28] and spin[29] projections to the constituting S-dets $|\phi_n\rangle$. The projections are symbolically denoted by P^G in Eq. (2). The 1D N-electron periodic system has the D_N symmetry, and both the CDW and SDW ground states belong to the same singlet A_1^+ irreducible representation, where the indices 1 and + represent the even parity of the reflection and electron-hole symmetries, respectively. The wave function is now explicitly given by

$$|\Psi\rangle = \sum_{n=1}^{N_S} C_n \sum_{m=0}^{N-1} T^m (1+R)(1+R^{e\text{-}h}) P^S |\phi_n\rangle, \tag{3}$$

where T makes the translation of the S-det by one site, while P^S, R, and R^{e-h} represent the spin projection, C_2 rotation in the D_N symmetry, and the electron-hole conversion, respectively. A similar method has been developed independently

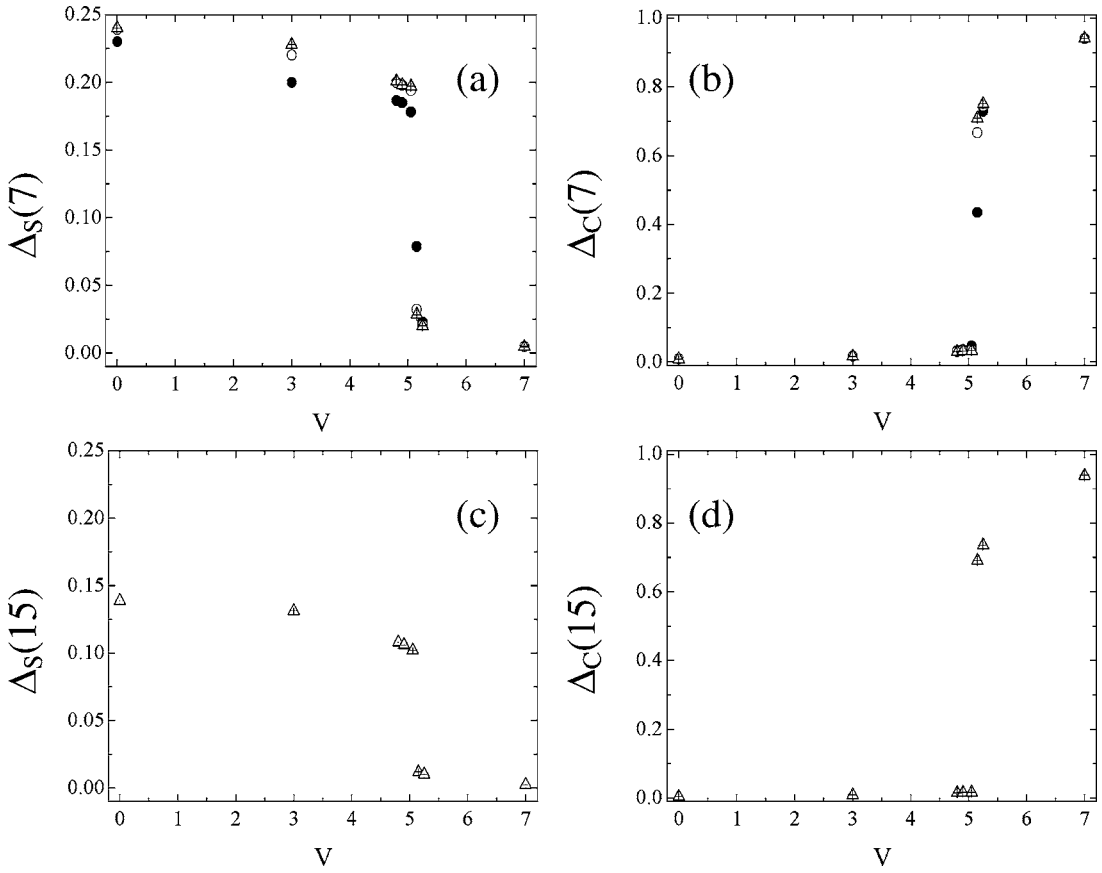

FIG. 2. V-dependence of the order parameters at $U=10$. (a) and (b) show Δ_S and Δ_C at $m=7$, while (c) and (d) show those at $m=15$. Black and white circles in (a) and (b) represent the Res-HF results for $N=14$ and 22, while white triangles and crosses in (a)–(d) denote the results for $N=30$ and 50.

by another group.[30] One of the most important points in the Res-HF method is that the orbitals in every S-det are newly determined by the direct optimization method[31] to minimize the many-body state energy. This orbital optimization improves the Res-HF wave function quite significantly. The author showed in the previous paper[32] that the Res-HF method can describe the electron correlation effects very efficiently for the 1D Hubbard model at any filling, where we have the exact Lieb-Wu solution.[33,34] In addition, by looking at the structures of the constituting S-dets, we can directly obtain information on the quantum fluctuations.

Now, we mention how to prepare the initial S-dets for the Res-HF wave functions. Since the orbital optimization is a time-consuming process,[31] the choosing of the proper initial S-dets is important to save the computational time. In the previous papers,[31,32] it was shown that the dominant quantum fluctuations in the half-filled Hubbard model are described by the translational and vibrational motions of the SDW neutral solitons. Here, the soliton is a topological defect which converts the phase of the SDW. A neutral soliton has spin of 1/2 and no charge, while a charged soliton has charge of e and no spin. In the present study, we start the Res-HF wave function for the SDW state with the superposition of the UHF S-dets representing the neutral soliton pairs with different distances. In the CDW region, we also prepare the S-dets representing the charged solitons as well as the neutral ones for the initial Res-HF wave function. As shown in the following sections, however, some of these solitons disappear after the orbital optimization, and the SDW (CDW) domains appear in the Res-HF CDW (SDW) wave functions, especially near the phase boundary. This shows the importance of the orbital optimization. In fact, the CDW solitons no longer work as the dominant quantum fluctuations in the CDW system, unlike the SDW soliton in the SDW system. In the following calculations, the Res-HF wave functions are constructed by $N_S=30$ S-dets for $N=50$, and $N_S=20$ S-dets for the smaller systems. It should be noted that the following Res-HF results are not significantly modified even if the numbers of S-dets are further increased.

III. RESULTS AND DISCUSSION

First, we show, in Fig. 1, the V-dependence of the overall structures of the spin and charge correlation functions for $N=50$ at $U=10$. These correlation functions are defined by

$$F_{\mathrm{Spin}}(l) = \frac{\langle \Psi | \mathbf{S}_l \cdot \mathbf{S}_0 | \Psi \rangle}{\langle \Psi | \Psi \rangle}, \tag{4}$$

$$F_{\mathrm{Charge}}(l) = \frac{\langle \Psi | n_l \cdot n_0 | \Psi \rangle}{\langle \Psi | \Psi \rangle}, \tag{5}$$

where

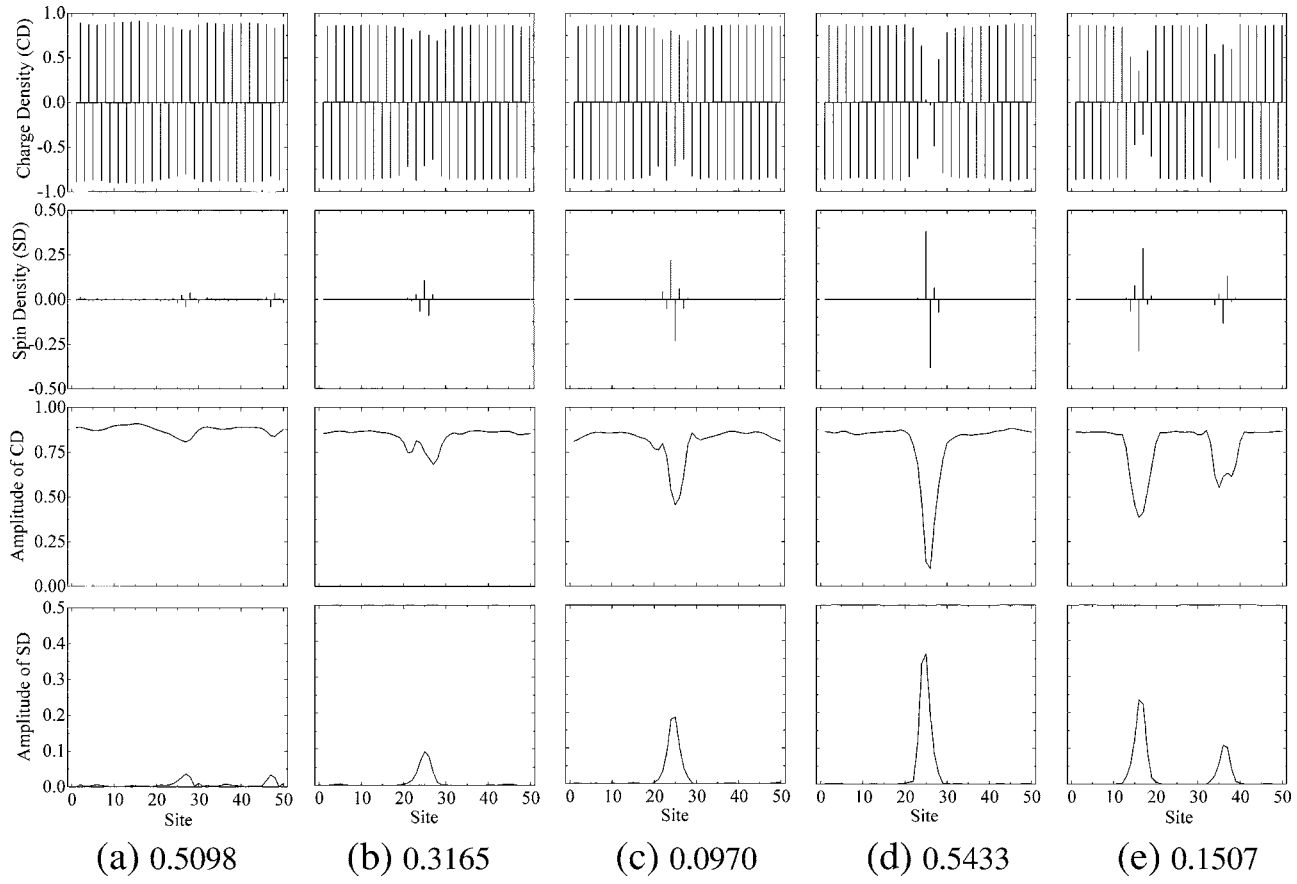

FIG. 3. Electronic structures of five typical S-dets generating the Res-HF wave function at $(U,V)=(10,5.15)$ for $N=50$. Charge density is measured from the half-filling. The numeral in each S-det denotes the probability to find that S-det in the Res-HF wave function.

$$\mathbf{S}_l = \frac{1}{2} \sum_{\gamma,\delta=\uparrow\downarrow} a^{\dagger}_{l,\gamma}(\sigma)_{\gamma\delta} a_{l,\delta}, \tag{6}$$

$$n_l = n_{l,\uparrow} + n_{l,\downarrow}. \tag{7}$$

$\mathbf{S}_l$ is the spin density at the lth site with the Pauli spin matrices $\sigma=(\sigma_1,\sigma_2,\sigma_3)$, and n_l is the electron charge density at the lth site. In Fig. 1, for comparison, the Res-HF results with $N_S=20$ S-dets are also shown by the crosses for the spin (charge) correlation functions in the SDW (CDW) regime. As mentioned in the preceding section, we cannot find any significant difference between the results with $N_S=20$ and $N_S=30$ S-dets. From Figs. 1(a) and 1(b), we can see that the spin correlation function does not have a real long-range order even in the SDW region. Thus, as is already established in the Hubbard system, we can safely say that the SDW state is a Mott insulator with a quasi-long-range order. In the CDW region, on the other hand, we can see, from Figs. 1(c) and 1(d), that the charge correlation function has a long-range order. This long-range order will cause the spontaneous translational symmetry breaking in the infinite-size system.

Then, let us see the CDW–SDW phase transition through the order parameters. In this research, the following quantities $\Delta_S(m)$ and $\Delta_C(m)$ are taken as the order parameters, which reflect the spin and charge correlation structures up to the mth neighboring site, respectively,

$$\Delta_S(m) = \frac{\sum_{l=0}^{l=m} (-1)^l F_{\mathrm{Spin}}(l)}{m+1}, \tag{8}$$

$$\Delta_C(m) = \frac{\sum_{l=0}^{l=m} (-1)^l F_{\mathrm{Charge}}(l)}{m+1}. \tag{9}$$

As shown in Fig. 1, the CDW system has a long-range ordering. In this case, the order parameter does not depend on m so largely. On the other hand, the 1D SDW system does not have a real long-range order, and the sum of the SDW correlation function divided by the system size goes to zero when the system size becomes infinite $(m\to\infty)$. Therefore, we had better cut m at a finite value to focus on the relevant correlation structures. In this research, $m=7$ and $m=15$ are employed to reflect both the spin and charge correlation structures appropriately into the order parameters, and also to see the m-dependence of the order parameters.

Figures 2(a) and 2(b) show the V-dependences of $\Delta_S(7)$ and $\Delta_C(7)$, respectively, at $U=10$. Black and white circles represent the results for $N=14$ and 22, respectively, while the triangles and crosses denote those for $N=30$ and 50, respectively. Both order parameters change discontinuously at the

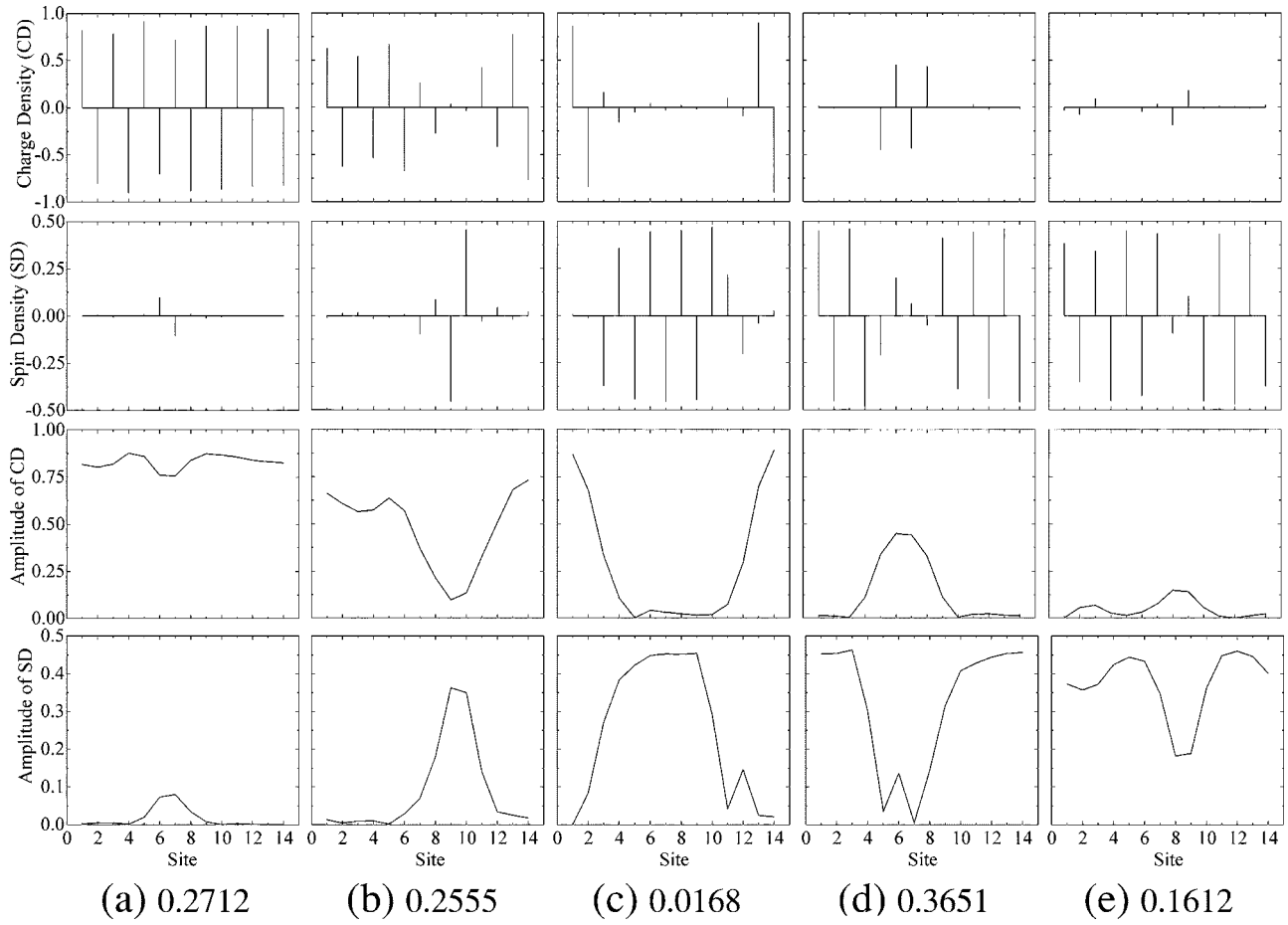

FIG. 4. Electronic structures of five typical S-dets at $(U,V)=(10,5.15)$ for $N=14$.

phase boundary ($V\approx 5.1$). In the case of $N=14$, however, jumps of $\Delta_S(7)$ and $\Delta_C(7)$ at the phase boundary are much smaller than those of $N=22$, 30, and 50. This finite-size effect is discussed in the following paragraphs from the viewpoint of the quantum coherence or the avoided crossing. Figures 2(c) and 2(d) show the V-dependences of $\Delta_S(15)$ and $\Delta_C(15)$, respectively, where the triangles and crosses denote the results for $N=30$ and 50 as in Figs. 2(a) and 2(b). By comparing Figs. 2(a) and 2(c), we can see that the amplitude of Δ_S becomes smaller as m is increased. This is because the SDW system does not have a real long-range order. If we took $m\to\infty$, the amplitude of Δ_S would be zero. Thus, to see the relevant spin correlation structure, as mentioned above, we had better cut m at a finite value. The present results indicate that both $\Delta_S(7)$ and $\Delta_S(15)$ show the relevant change in the SDW correlation structure appropriately. On the other hand, as seen from Figs. 2(b) and 2(e), Δ_C hardly depends on m, since the CDW system has a real long-range order. The discrete changes in both the spin and charge order parameters in the strong correlation regime agree with the previous results,[8–10,12,13,15–17,19,20,24,25] and they indicate the first order phase transition in this correlation regime.

Now, let us investigate this phase transition through the quantum fluctuations. Figures 3 and 4 show the structures of five typical S-dets, generating the Res-HF wave functions for $N=50$ and $N=14$, respectively. In both figures, (U,V) is set at $(10,5.15)$, which is in the CDW region very close to the phase boundary. In these figures, the spin density (SD) represents the z component of $\mathbf{S}_l$, while the charge density (CD) is measured from the half-filling, such as

$$\mathrm{SD}(l)=\tfrac{1}{2}(n_{l,\uparrow}-n_{l,\downarrow}), \tag{10}$$

$$\mathrm{CD}(l)=n_{l,\uparrow}+n_{l,\downarrow}-1. \tag{11}$$

The numeral in each S-det denotes the probability to find a symmetry projected S-det in the Res-HF wave function. Since the Res-HF wave function $|\Psi\rangle$ is constituted of nonorthogonal S-dets $|\phi_n\rangle$, this probability p_n is explicitly given by

$$p_n=\left|\langle\Psi|\sum_{m=0}^{N-1}T^m(1+R)(1+R^{e\text{-}h})P^S|\phi_n\rangle\right|^2. \tag{12}$$

We should note that because of nonorthogonality of the S-dets, the sum of their probabilities is not equal to 1, though only the typical S-dets are depicted here. The Res-HF wave functions, shown in Figs. 3 and 4 indicate that the SDW domains appear in the CDW ground state near the phase boundary, and the CDW amplitudes are reduced where the SDW domains arise. In the Res-HF calculations, as mentioned in Sec. II, the broken-symmetry S-dets, shown in Figs. 3 and 4, are projected onto the subspace of the singlet A_1^+ irreducible representation with the group integration intro-

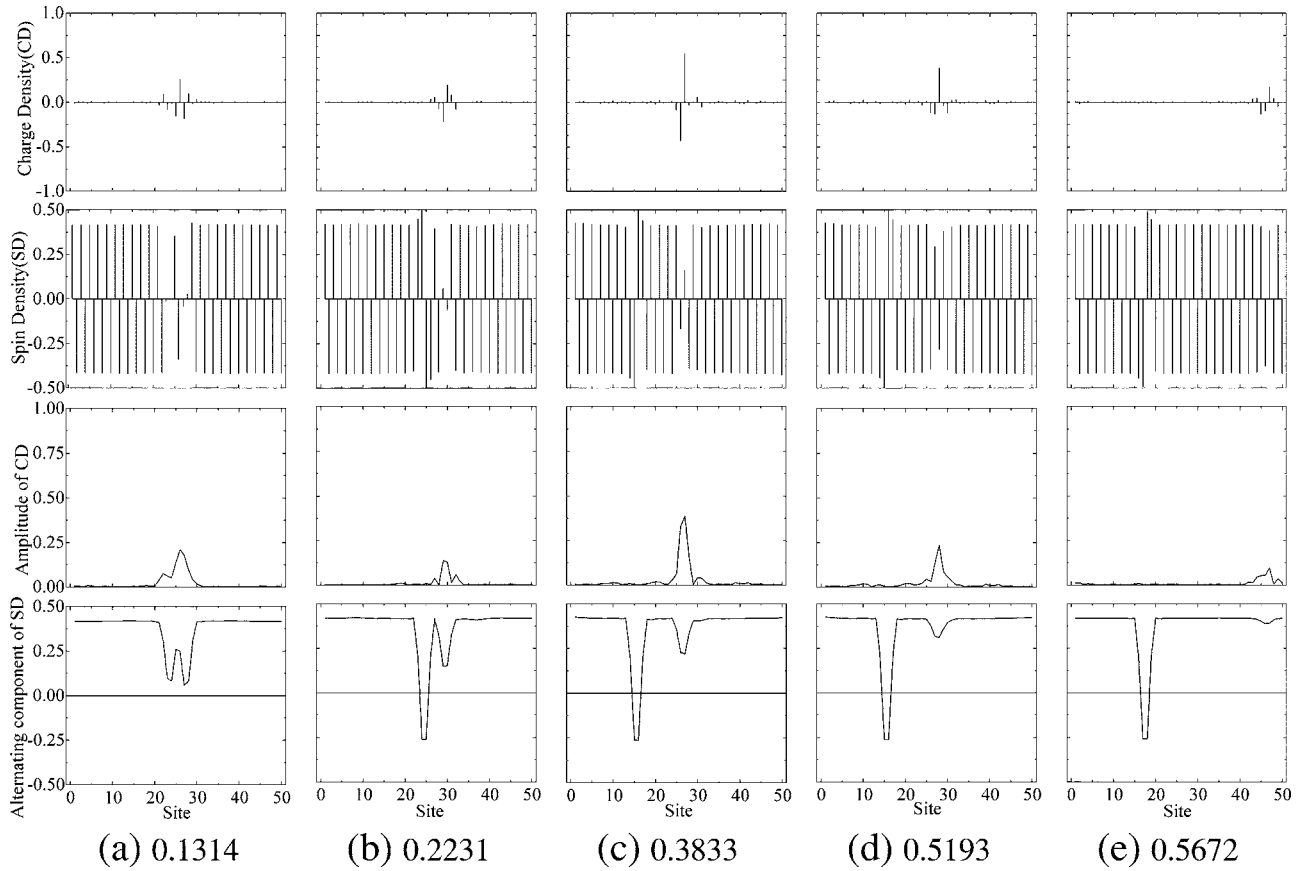

FIG. 5. Electronic structures of five typical S-dets generating the Res-HF wave function for $N=50$ at $(U,V)=(10,5)$, which lies in the SDW region near the phase boundary. The alternating component of the SD at the bottom of each figure represents both the phase and amplitude of the SDW.

duced by Peierls and Yoccoz. Then, in Fig. 3(a)–3(d) represent the quantum fluctuations due to the expanding and contracting motions of the SDW domains, while the S-dets, shown in Fig. 3(e), include two SDW domains. The rest of the S-dets severally include a single SDW domain whose size is in between (a) and (d). On the other hand, as shown in Fig. 4, the Res-HF wave function for $N=14$ has much larger SDW domains near the phase boundary. In fact, as shown in Figs. 4(d) and 4(e), some S-dets include the larger SDW domains than the CDW ones, though the most S-dets consist of the dominant CDW components with the smaller SDW domains, like Figs. 4(a) and 4(b). This large SDW contribution in the Res-HF CDW wave function for $N=14$ is consistent with the continuous changes in the order parameters shown in Figs. 2(a) and 2(b).

For comparison, in Fig. 5, we show five typical S-dets generating the Res-HF wave function for $N=50$ at $(U,V)=(10,5)$, which lies in the SDW region close to the phase boundary. In Figs. 5(a)–5(e), the alternating component of the spin density shown at the bottom of each figure represents both the amplitude and phase of the SDW. Here, the defect, which converts the SDW phase + to − across the horizontal zero line, denotes the SDW neutral soliton. While the S-det shown in Fig. 5(a) contains two confined CDW domains, the S-dets shown in Figs. 5(b)–5(e) include the SDW neutral soliton pair on the left-hand side as well as the CDW domain on the right-hand side. Thus, in contrast to the CDW case, the Res-HF SDW wave function still has the quantum fluctuations due to the SDW solitons even near the phase boundary. However, as seen from Fig. 5, these SDW neutral solitons do not affect the CDW component, and therefore, we can safely say that they work for the stabilization of the SDW state, as clarified in the Hubbard model.[31,32]

Thus, from Figs. 3–5 we can see that the relevant fluctuations in the CDW-SDW phase transition are the SDW domains in the CDW wave function and the CDW domains in the SDW wave function.

Here, the following scenario is given for this quantum phase transition. Since both the CDW and SDW wave functions belong to the same singlet A_1^+ irreducible representation, the electron state should change continuously from the CDW to the SDW and vice versa in the finite-size system. The origin of such a continuous change is the finite off-diagonal resonance between the two wave functions, having the same symmetry. The finite off-diagonal resonance causes the mixing of the two states, and as a result, the SDW (CDW) domains appear in the CDW (SDW) wave function. The coherent superposition of these SDW (CDW) domains brings about the quantum coherence between the CDW and SDW states in the finite-size system. Thus, the continuous change in the order parameters for $N=14$ shown in Figs. 2(a) and 2(b), and the large quantum fluctuations due to the SDW domains in the Res-HF CDW wave function shown in Fig. 4

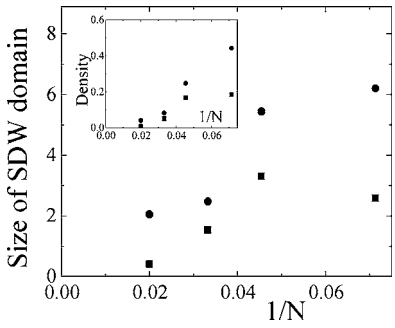

FIG. 6. N-dependence of the size of the SDW domain at $(U,V)=(10,5.15)$ (black circles), and (10, 10) (black squares). The inset shows the density of the SDW domains to the system size.

are explained by this quantum coherence. The quantum coherence is a natural extension of the well-known avoided crossing for the diatomic molecule, in which the two potential curves for the two independent wave functions having the same symmetry cannot cross due to the finite off-diagonal resonance between the two wave functions.

However, the above discussion is for the finite-size systems. To understand the bulk phase transition correctly, we must remove the finite-size effects. In fact, as shown in Fig. 2, the changes in the order parameters become much more discrete as the system size is increased. To elucidate the role of the quantum fluctuations in the bulk phase transition, we show in Fig. 6 the expectation value of the size of the SDW domains in the CDW ground state, as a function of the system size. This expectation value W_{SDW} is given by

$$W_{\mathrm{SDW}} = \frac{\sum_{n=1}^{N_S} p_n W_{\mathrm{SDW}}(n)}{\sum_{n=1}^{N_S} p_n}, \tag{13}$$

where $W_{\mathrm{SDW}}(n)$ represents the size of the SDW domain in the nth S-det $|\phi_n\rangle$, and the p_n is the probability of $|\phi_n\rangle$ defined by Eq. (12). Black squares and circles represent the results for $(U,V)=(10,10)$ and (10, 5.15), which lie in the deep CDW region and near the phase boundary, respectively. Although the size of $N=50$ might be small for the accurate extrapolation, we can see that near the phase boundary, the size of the SDW domains stays finite in the infinite-size limit, while it goes to zero in the deep CDW region. On the other hand, as shown in the inset of Fig. 6, the density of the SDW domains is extrapolated to zero even near the phase boundary, as well as in the deep CDW regions, in the infinite-size limit. This result means that the mixing ratio of the SDW domain in the CDW wave function becomes zero in the infinite-size system, even near the CDW–SDW phase transition, which indicates the decoherence of the CDW and SDW states. Eventually, the CDW wave function becomes asymptotically orthogonal to the SDW wave function at the phase boundary, and the transition becomes of the first order in the infinite-size system.

Finally, we mention the possible relationship of the quantum fluctuations and quantum nucleation. Figure 6 shows that the size of the SDW domains increases as the system moves from the deep CDW region to the phase boundary. Though the CDW–SDW phase transition is of the first order due to the decoherence of the two states, the SDW domains stay finite at $(U,V)=(10,5.15)$ even in the infinite-size limit. Therefore, it is suggested that when the CDW system crosses the transition point to the SDW region, the quantum fluctuations due to the SDW domains can naturally evolve into the quantum nucleation, which triggers the CDW–SDW phase transition. Thus, we can regard these SDW domains as the precursor of the quantum nucleation in the first order quantum phase transition. The precise mechanism of this quantum nucleation will be studied elsewhere.

IV. SUMMARY

The Res-HF calculations have shown that the quantum fluctuations due to the SDW (CDW) domains, induced by the off-diagonal resonance, lead to the quantum coherence of the CDW and SDW states, and the electronic state changes continuously in the finite-size system. However, the scaling analysis has indicated the decoherence of the two correlated states in the bulk phase transition, since the density of the counter-phase domains becomes asymptotically zero. These results agree with the discontinuous behaviors of the order parameters at the phase boundary when the system size is increased. Finally, it has been suggested that the finite counter-phase domain in the infinite-size system would be the precursor of the quantum nucleation.

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*Present address: Department of Physics, Graduate School of Science and Technology, Yamagata University, Kojirakawa-machi 1-4-12, Yamagata, 990-8560, Japan

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