Coexistence of spiral spin-density waves and superconductivity: Ground-state properties

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The interplay between phonon mediated and bare intrasite Coulomb electron-electron interactions is considered in the formation of superconducting and spin-density-wave ground states. A model Hamiltonian is solved in the mean-field approximation and the symmetry of its ground state analyzed in detail. The considered broken symmetries tend to destroy each other in general, but, in some cases, there is coexistence of superconductivity and spiral-spin-density-wave order in the ground state.

The existence of ground states with more than one coexisting broken symmetry is an old and very appealing problem.[1-4] Among the many different possible situations, the coexistence of superconductivity and magnetic order is one of the more studied ground states with more than one broken symmetry.[5-7] The magnetic moments tend to break the Cooper pairs destroying the superconducting order, and making the coexistence of superconductivity and magnetism very unlikely. In this work, however, we show that, in some cases, spiral-spin-density-wave (SSDW) ordering of itinerant electrons can coexist with superconductivity in the ground state of the system. This ground state has already been discussed in the literature[8,9] and it has been suggested as being present in some heavy fermion systems.[8] Also, the interplay between superconductivity and magnetic order has been recently discussed in the case of the new high-T_c superconductors.[10,11]

The model Hamiltonian we will handle in this work for a quasi-one-dimensional system has the following form:

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_U+\mathcal{H}_{e\text{-ph}}\,, \tag{1}$$

$$\mathcal{H}_0=\sum_{k,\sigma}\varepsilon_k n_{k\sigma}\,, \tag{2}$$

where ε_k stands for the band dispersion. We take here a simple one-dimensional free-electron parabola. The energy units are chosen so as the Fermi energy is 4. The occupation number for electrons of momentum k and spin σ is indicated by $n_{k\sigma}$. The other two terms of (1) are

$$\mathcal{H}_U=\frac{U}{2}\sum_{i,\sigma}n_{i\sigma}n_{i\bar{\sigma}}\,, \tag{3}$$

σ being the spin index ($\sigma\neq\bar{\sigma}$), and

$$\mathcal{H}_{e\text{-ph}}=\frac{1}{2}\sum_{\substack{k,k',q\\ \sigma,\sigma'}}[V(k,q)+V(k',q)]\,c^{\dagger}_{k+q,\sigma}c_{k',\sigma}c^{\dagger}_{k'-q,\sigma'}c_{k,\sigma'}\,. \tag{4}$$

The operator c ($c^{\dagger}$) stands for the destruction (creation) electron operator. The effective electron-electron interaction function $V(k,q)$ takes the standard form

$$V(k,q)=\begin{cases}-(V_0/N) & \text{if } |\varepsilon_k-\varepsilon_f|<\hbar\omega_d \text{ and } |\varepsilon_{k+q}-\varepsilon_f|<\hbar\omega_d,\\ 0 & \text{otherwise,}\end{cases} \tag{5}$$

$\hbar\omega_d$ being the Debye energy.

In the Hamiltonian we have two distinct electron-electron interactions. The bare Coulomb repulsive interaction is represented by the on-site term U. The interaction V_0 represents an attractive interaction due to intermediated phonons. We have therefore two competing interactions as well as two different ground-state orderings. The interplay between them is the main purpose of this work.

We have solved the Hamiltonian in the mean-field approximation. It should be noticed that special care has to be taken when solving the above problem in the mean-field approximation. The decoupling of the different terms of $\mathcal{H}$ has to be done carefully to obtain consistent results. The procedure to solve the above Hamiltonian follows the work of Balseiro and Falicov to study the coexistence of superconductivity and charge-density waves.[6]

In order to understand first the effect of the interactions in the superconducting and spin-density-wave ground states we have solved the above Hamiltonian in both cases independently. We consider first the spin-density-wave ground state.

We study the mean-field solution of the Hamiltonian (1) considering only the possibility of SSDW ordering in the ground state.[12] The formation of the SSDW is originated by electron-hole coupling at k_f and $-k_f$ giving rise to a new periodicity (commensurate or not with the original one) governed by the vector $Q=2k_f$. The mean-field Hamiltonian of the total Hamiltonian (1) is in this case,

$$\mathcal{H}_{\rm DW}=\sum_{k,\sigma}\xi_k n_{k\sigma}+\sum_k g(k-Q/2)(c^{\dagger}_{k-Q/2,\sigma}c_{k+Q/2,\bar{\sigma}}+\text{H.c.})+\frac{g_0^2}{U}-\frac{g_1g_2}{V_0}\,, \tag{6}$$

where ξ_k stands for the energy bands referred to the Fermi level. The order parameter has the following form:

$$g(k-Q/2)=\begin{cases}-g_0+g_1+g_2 & \text{if } |\varepsilon_{k-Q/2}-\varepsilon_f|<\hbar\omega_d \text{ and } |\varepsilon_{k+Q/2}-\varepsilon_f|<\hbar\omega_d,\\ -g_0+g_1 & \text{otherwise,}\end{cases} \quad (7)$$

where

$$g_0=\frac{U}{N}\sum_k\langle c^\dagger_{k+q,\sigma}c_{k,\bar\sigma}\rangle\,, \quad (8a)$$

$$g_1=\frac{V_0}{2N}\sum_k{}''\langle c^\dagger_{k+q,\sigma}c_{k,\bar\sigma}\rangle\,, \quad (8b)$$

$$g_2=\frac{V_0}{2N}\sum_k\langle c^\dagger_{k+q,\sigma}c_{k,\bar\sigma}\rangle\,. \quad (8c)$$

The double prime of (8b) indicates that only states such that $|\varepsilon_{k-Q/2}-\varepsilon_f|<\hbar\omega_d$ and $|\varepsilon_{k+Q/2}-\varepsilon_f|<\hbar\omega_d$ have to be considered.

The new one-electron bands have the form given in Fig. 1 and are given by the following equation:

$$\omega_{1,2k}=\tfrac{1}{2}(\xi_{k-Q/2}+\xi_{k+Q/2}) \pm[(\xi_{k-Q/2}-\xi_{k+Q/2})^2+4g^2(k-Q/2)]^{1/2}\,. \quad (9)$$

The self-consistent equations for the order parameters take the following form:

$$g_0=\frac{U}{N}\sum_k\frac{g(k-Q/2)}{\omega_{1,k}-\omega_{2,k}}\Theta(\varepsilon_f-\omega_{2,k})\,, \quad (10a)$$

$$g_1=\frac{V_0}{2N}\sum_k{}''\frac{-g_0+g_1+g_2}{\omega_{1,k}-\omega_{2,k}}\Theta(\varepsilon_f-\omega_{2,k})\,, \quad (10b)$$

$$g_2=\frac{V_0}{2N}\sum_k\frac{-g_0+g_1+g_2}{\omega_{1,k}-\omega_{2,k}}\Theta(\varepsilon_f-\omega_{2,k})\,. \quad (10c)$$

The self-consistent solution of Eqs. (10a)-(10c) gives the order parameters of the pure SSDW ground state. Results of the calculation for g_0 are shown in Fig. 2(a) for $U=10.5$ and $\hbar\omega_d=0.5$ in the same units in which the Fermi energy is 4. Similar results are obtained for the other g's and for other variables of the intrasite Coulomb repulsion parameter U. We observe the existence of a stable SSDW ground state for values of V_0 larger than U.

In the case of a pure superconducting ground state without magnetic order, the reduced Hamiltonian has the following form:

$$\mathcal{H}_{\rm red}=\sum_{k,\sigma}\xi_{k\sigma}n_{k\sigma}-\tfrac{1}{2}\sum_{k,\sigma}\Delta(k)(c^\dagger_{k\sigma}c^\dagger_{-k\sigma}+\text{H.c.}) -\frac{\Delta_1^2}{U}+\frac{\Delta_2^2}{V_0}\,. \quad (11)$$

ξ_k stands for the noninteracting elementary excitations energies and $\Delta(k)$ is given by

$$\Delta(k)=\begin{cases}-\Delta_1+\Delta_2 & \text{if } |\varepsilon_k-\varepsilon_f|<\hbar\omega_d,\\ \Delta_1 & \text{otherwise,}\end{cases} \quad (12)$$

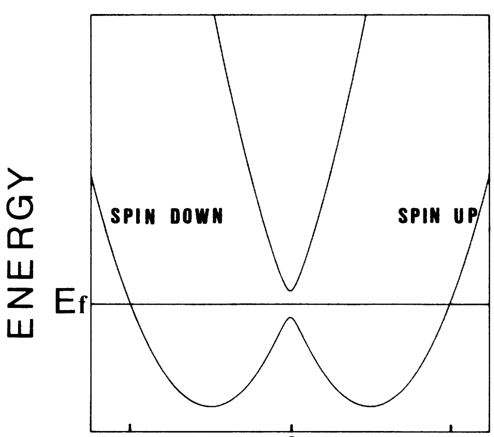

FIG. 1. One-electron bands in the pure SSDW ground state. The width of the gap at $k=0$ is of the order of magnitude of the order parameter g [see Eq. (9)]. The Fermi level is indicated.

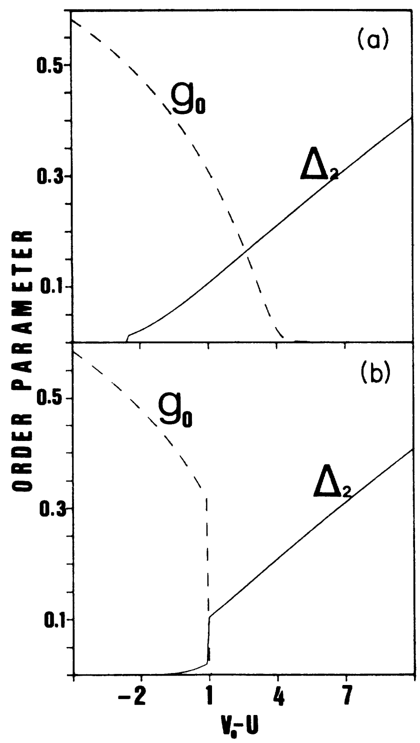

FIG. 2. Order parameters of the SSDW (g_0) and superconductivity (Δ_2) vs V_0-U for $U=10.5$. (a) The two electronic orderings are assumed to be independent. (b) The complete mean-field Hamiltonian is considered [Eq. (16)]. The parameters Δ_2 and g_0 are indicated by solid and dashed lines, respectively.

and the order parameters are

$$\Delta_1 = \frac{U}{N}\sum_k \langle c_{k\sigma}^{\dagger} c_{-k\bar{\sigma}}^{\dagger}\rangle , \qquad (13a)$$

$$\Delta_2 = \frac{V_0}{N}\sum_k{}' \langle c_{k\sigma}^{\dagger} c_{-k\bar{\sigma}}^{\dagger}\rangle , \qquad (13b)$$

where the prime in the last summation indicates that only states within $\hbar\omega_d$ from the Fermi level are considered.

The self-consistent equations for the order parameters (13) are

$$\Delta_1 = \frac{U}{N}\sum_k \frac{\Delta(k)}{2\omega_k} , \qquad (14a)$$

$$\Delta_2 = \frac{V_0}{N}\sum_k{}' \frac{-\Delta_1+\Delta_2}{2\omega_k} , \qquad (14b)$$

where ω_k is the dispersion relation obtained after diagonalization of $\mathcal{H}_{\text{red}}$,

$$\omega_k = [\xi_k^2 + \Delta^2(k)]^{1/2} . \qquad (15)$$

The variation of the order parameter Δ_2 vs $V_0 - U$ (for $U = 10.5$ and $\hbar\omega_d = 0.5$) is shown in Fig. 2(a). Similar results are obtained for Δ_1 and for other values of U. The most interesting aspect of this result is the fact that the superconducting ground state is stable for values of the Coulomb interaction parameter U much larger than the attractive interaction parameter V_0. This clearly indicates, as in the pure SSDW case, that the effective electron-electron interaction cannot be represented by a single parameter as it is usually done.

Looking at Fig. 2(a) we observe that, if the SSDW and the superconductivity are considered independently, there is a large region of values of $U - V_0$ such that both broken symmetries exist simultaneously.

To study the competition between both the electron-electron interactions and the electronic ordering we have considered the Hamiltonian (1) in the mean-field approximation in the following form:

$$\mathcal{H}_{\text{MF}} = \mathcal{H}_{\text{DW}} + \mathcal{H}_{\text{red}} . \qquad (16)$$

The diagonalization of this Hamiltonian can be performed by a Bogoliubov transformation.[5] After the diagonalization the different order parameters can be calculated self-consistently as in the single broken symmetry case. The numerical solution has some subtleties, but the stable ones can be finally obtained. Results of the calculations for Δ_2 and g_0 for the same values of the parameters as before are shown in Fig. 2(b). Similar results are obtained for other sets of parameters.

From the results of our calculations we can conclude the following.

(i) The interplay between SSDW and superconductivity is such that they tend to destroy each other, as is apparent comparing Figs. 2(a) and 2(b). This is partially in contradiction with the results of Machida and co-worker,[8,9] who suggest an enhancement of the superconductivity due to the presence of spin-density waves. This discrepancy is due to the fact that these authors consider only competition between interactions and neglect the competition between the different symmetries involved as it is done in this work, and also to the fact that their result holds for non-*s*-wave superconductors. In addition, the decoupling of the Hamiltonian is different from ours.

(ii) In spite of the overall weakening of the SSDW and the superconductivity there is a region of coexistence of both orderings. This is essentially due to the fact that electrons with momentum $Q/2$ and $-Q/2$ are weakly affected by the SSDW, as can be seen in Fig. 1, and since they have opposite spin, can couple to form Cooper pairs. The reduction of the superconducting order parameter in Fig. 2(b) with respect to Fig. 2(a) corresponds essentially to an $\exp(-2)$ factor since only half of the electrons participate in the superconductivity. The electrons at $k=0$ produce the SSDW and are not affected by the superconductivity.

(iii) The parameters U and V_0 play a very rich role in the formation of SSDW and superconducting ground states. Their effect cannot be simulated by a single electron-electron interaction parameter if proper handling of the Hamiltonian (1) is made.

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