SPIN DENSITY WAVES AND SUPERCONDUCTIVITY IN STRONGLY CORRELATED ELECTRON SYSTEMS

D.F. Digor[a], L.A. Dohotaru[b], P. Entel[c], V.A. Moskalenko[a,d] and M.I. Vladimir[b]

[a]*Institute of Applied Physics, Academy of Sciences of Republic of Moldova, MD-2028, Republic of Moldova.*
[b]*Technical University, Chisinau, MD-2064, Republic of Moldova.*
[c]*Institute of Physics, University of Duisburg-Essen, Duisburg Campus, 47048 Duisburg, Germany.*
[d]*BLTP, Joint Institute for Nuclear Research, 141980 Dubna, Russia*

A special diagram technique recently proposed for strongly correlated electron systems is used to study the peculiarities of a spin-density-wave (SDW) in competition with superconductivity. This method allows to formulate the Dyson equations for the renormalized electron propagators of the coexisting phases of SDW antiferromagnetism and superconductivity. We find the surprising result that triplet supercondctivity appears provided that we have coexistence of singlet superconductivity and SDW antiferromagnetism.

In many investigations of the conditions, in which the superconducting state at the high temperatures arises, the exclusive role is given to the strong Coulomb interactions of the electrons in the system. The Coulomb interactions can also be the cause of the appearance of the spin-density-wave (SDW) state. The aim of the present paper is to investigate the influence of this interaction on the competition of the above mentioned states.

In the case of strongly correlated electrons considered here, the strong on-site electron repulsion is (together with the number of electrons per site) the dominant parameter of the theory. As an elemental model, which takes this into account, we use the Hubbard Hamiltonian [1] and the method of broken symmetry [2] in order to discuss the coexistence of a SDW with spiral polarization and superconductivity.

The Hubbard Hamiltonian has the form:

$$H^0 = -\mu \sum_{i\sigma} c^+_{i\sigma} c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad H^1 = \sum_{ij\sigma} t(j-i) c^+{}_{j\sigma} c_{i\sigma}.$$

Here c_i and c_i^+ are the destruction and creation operators of the electrons at site i, respectively; μ is the chemical potential of the system, $t(j-i)$ is the transfer matrix element and U is on-site Coulomb repulsion.

In order to take into account from the beginning the static SDW, we use the following unitary transformation,

$$\widehat{H} = \Omega H \Omega^{-1}$$

with the unitary operator Ω defined by

$$\Omega = \prod_i \exp\left(i\theta_i S_i^z\right), \ \theta_i = (\mathbf{Q}\cdot\mathbf{R}_i),$$

where S_i^z is the z -component of the electron spin operator at site i. After such a transformation the electron operators $c_{i\sigma}$ and $c_{i\sigma}^{?}$ take the form ($\sigma = \pm 1$):

$$\tilde{c}_{i,\sigma} = \Omega c_{i,\sigma} \Omega^{-1} = c_{i,\sigma} \exp\left(-i \frac{1}{2} \sigma (\mathbf{Q} \cdot \mathbf{R}_i) \right), \quad \tilde{c}_{i\sigma}^{+} = \Omega c_{i\sigma}^{+} \Omega^{-1} = c_{i,\sigma}^{+} \exp\left(i \frac{1}{2} \sigma (\mathbf{Q} \cdot \mathbf{R}_i) \right),$$

This new ground state is characterized by the wave vector $\mathbf{Q}$. The new tunneling matrix element,

$$t_{\sigma}(\mathbf{R}_j - \mathbf{R}_i) = t(\mathbf{R}_j - \mathbf{R}_i) \cdot \exp\left(i \frac{1}{2} \sigma \left[\mathbf{Q} \cdot (\mathbf{R}_j - \mathbf{R}_i) \right] \right),$$

depends now on the wave vector and on the spin of the tunneling electrons. The Fourier transform of this new matrix element is equal to

$$e_{\sigma}(\mathbf{k}) = e(\mathbf{k} + \sigma \frac{1}{2} \mathbf{Q}),$$

where $e(\mathbf{k})$ is the Fourier transform of the initial matrix element. This unitary transformation rotates the transversal components of the electron spin operator:

$$\Omega S_i^x \Omega^{-1} = \cos(\mathbf{Q} \cdot \mathbf{R}_i) \cdot S_i^x - \sin(\mathbf{Q} \cdot \mathbf{R}_i) \cdot S_i^y,$$

$$\Omega S_i^y \Omega^{-1} = \cos(\mathbf{Q} \cdot \mathbf{R}_i) \cdot S_i^x + \sin(\mathbf{Q} \cdot \mathbf{R}_i) \cdot S_i^x.$$

In this paper we discuss the properties of a SDW having one of the two spiral polarizations. Therefore, in order to obtain non zero values of thermodynamical averages of the transverse components of the spin operator, it is necessary to break the spin conservation law of the initial Hamiltonian. This is realized by adding to the Hamiltonian a source term for the formation of the SDW. In our case this term corresponds to one of the transversal components of the full spin operator of the system. This allows for the formation of anomalous expectation values. After the renormalization of these quantities the source is removed restoring the initial Hamiltonian. This procedure allows to introduce from the beginning the static spin wave corresponding broken symmetry of the ground state. Let us emphasize that this method does not correspond to the concept of mean field approximation used in work [3]. Instead we investigate the properties of the renormalized one-particle Matsubara Green's functions for the case of coexisting superconductivity and SDW phases:

$$G_{\sigma\sigma'}(x - x') = -\langle T c_{\mathbf{x}\sigma}(\tau) \bar{c}_{\mathbf{x}'\sigma'}(\tau') U(\beta) \rangle_0^c, \quad F_{\sigma\sigma'}(x - x') = -\langle T c_{\mathbf{x}\sigma}(\tau) c_{\mathbf{x}'\sigma'}(\tau') U(\beta) \rangle_0^c,$$

$$\bar{F}_{\sigma\sigma'}(x - x') = -\langle T \bar{c}_{\mathbf{x}\sigma}(\tau) \bar{c}_{\mathbf{x}'\sigma'}(\tau') U(\beta) \rangle_0^c.$$

Here $U(\beta)$ is the evolution operator, $x = (\mathbf{x},\ \tau)$ and $c_{\mathbf{x},\sigma}(\tau)$ is the electron operator in the interaction representation.

We use a new diagrammatic method, recently elaborated by us for strongly correlated systems, based on a generalized Wick theorem and a new conception of irreducible Green's functions [4,5]. The irreducible Green's functions describe all spin, charge and pairing fluctuations which are possible in the system. Thus, an approximate knowledge of these quantities will allow a serious discussion of the occurrence of multiple phase transitions and competition between different phases. The infinite sum of these new elements leads to new correlation functions, $Z_{\sigma\sigma'}$, $Y_{\sigma\sigma'}$ and $\bar{Y}_{\sigma\sigma'}$, which are the most essential elements of the theory describing spin, charge and pairing tendencies. The Dyson equations for the delocalized Green's functions, $G_{\sigma\sigma'}$, $F_{\sigma\sigma'}$ and $\bar{F}_{\sigma\sigma'}$, contain these correlation functions together with the electronic energy, $e_\sigma(\mathbf{k}) = e(\mathbf{k} + \sigma\,\frac{1}{2}\mathbf{Q})$, for different values of spin σ and SDW wave vector $\mathbf{Q}$. The simplest form of these equations can be obtained by using the matrix notation for the full Green's functions $\hat{G}(k)$ ($k = \mathbf{k},\ i\omega$),

$$\hat{G}(k) = \begin{pmatrix} G_{\uparrow\uparrow}(k) & G_{\uparrow\downarrow}(k) & F_{\uparrow\downarrow}(k) & F_{\uparrow\uparrow}(k) \\ G_{\downarrow\uparrow}(k) & G_{\downarrow\downarrow}(k) & F_{\downarrow\downarrow}(k) & F_{\downarrow\uparrow}(k) \\ \bar{F}_{\downarrow\uparrow}(k) & \bar{F}_{\downarrow\downarrow}(k) & -G_{\downarrow\downarrow}(-k) & -G_{\uparrow\downarrow}(-k) \\ \bar{F}_{\uparrow\uparrow}(k) & \bar{F}_{\uparrow\downarrow}(k) & -G_{\downarrow\uparrow}(-k) & -G_{\uparrow\uparrow}(-k) \end{pmatrix}$$

with mass operator $\hat{e}(k)$:

$$\hat{e}(\mathbf{k}) = \begin{pmatrix} e_\uparrow(\mathbf{k}) & o & 0 & 0 \\ 0 & e_\downarrow(\mathbf{k}) & o & o \\ 0 & 0 & -e_\downarrow(-\mathbf{k}) & 0 \\ 0 & 0 & 0 & -e_\uparrow(-\mathbf{k}) \end{pmatrix}$$

and correlation matrix $\hat{Z}(k)$:

$$\hat{Z}(k) = \begin{pmatrix} Z_{\uparrow\uparrow}(k) & Z_{\uparrow\downarrow}(k) & Y_{\uparrow\downarrow}(k) & Y_{\uparrow\uparrow}(k) \\ Z_{\downarrow\uparrow}(k) & Z_{\downarrow\downarrow}(k) & Y_{\downarrow\downarrow}(k) & Y_{\downarrow\uparrow}(k) \\ \bar{Y}_{\downarrow\uparrow}(k) & \bar{Y}_{\downarrow\downarrow}(k) & -Z_{\downarrow\downarrow}(-k) & -Z_{\uparrow\downarrow}(-k) \\ \bar{Y}_{\uparrow\uparrow}(k) & \bar{Y}_{\uparrow\downarrow}(k) & -Z_{\downarrow\uparrow}(-k) & -Z_{\uparrow\uparrow}(-k) \end{pmatrix}$$

leading to the following matrix equation for $\hat{G}(k)$:

$$\hat{G}(k) = \hat{\Lambda}(k)\left[1 + \hat{e}(k)\cdot\hat{G}(k)\right], \quad \hat{\Lambda}(k) = \hat{G}^{(0)} + \hat{Z}(k),$$

Here $\hat{G}^{(0)}$ is the matrix of the local Green's function [4,5]. As remarked before, the system of Dyson equations allows the additional appearance of triplet superconductivity in the presence of singlet superconductivity and a spiral SDW state (or the appearance of a SDW if singlet and triplet superconductivity coexist).

In order to close the equations of motion for the full Green's functions it is necessary to add to them the corresponding equations for the correlation functions. Since the Dyson equations for these functions do not exist we must use appropriate approximations, which are based on the procedure of summing the most important diagrams. Here we use the local in coordinate space approximation for these quantities which is obtained by summing one class of diagrams containing the simplest two-particle irreducible Green's functions $G_2^{(0)irr}$ [4,5]. These diagrams give the main contribution to this theory.

$$Z_{\sigma\sigma}(i\omega) = -\frac{1}{\beta N}\sum_{\mathbf{k}}\sum_{\omega_1}\tilde{G}_2^{(0)irr}[\sigma, i\omega; \sigma, i\omega_1 \mid \sigma, i\omega_1; \sigma, i\omega]\, e_\sigma^2(\mathbf{k})\, G_{\sigma\sigma}(\mathbf{k} \mid i\omega_1)$$
$$+ \tilde{G}_2^{(0)irr}[\sigma, i\omega; \bar{\sigma}, i\omega_1 \mid \bar{\sigma}, i\omega_1; \sigma, i\omega]\, e_{\bar{\sigma}}^2(\mathbf{k})\, G_{\bar{\sigma}\bar{\sigma}}(\mathbf{k} \mid i\omega_1),$$
$$Z_{\sigma\bar{\sigma}}(i\omega) = -\frac{1}{\beta N}\sum_{\mathbf{k}}\sum_{\omega_1}\tilde{G}_2^{(0)irr}[\sigma, i\omega; \bar{\sigma}, i\omega_1 \mid \sigma, i\omega_1; \bar{\sigma}, i\omega]\, e_\sigma(\mathbf{k})\, e_{\bar{\sigma}}(\mathbf{k})\, G_{\sigma\bar{\sigma}}(\mathbf{k} \mid i\omega_1),$$

$$\bar{Y}_{\bar{\sigma}\sigma}(i\omega) = -\frac{1}{\beta N}\sum_{\mathbf{k}}\sum_{\omega_1}\tilde{G}_2^{(0)\,irr}[\sigma, i\omega_1; \bar{\sigma}, -i\omega_1 \mid \sigma, i\omega; \bar{\sigma}, -i\omega]\, e_\sigma(\mathbf{k}) e_{\bar{\sigma}}(-\mathbf{k})\, \bar{F}_{\bar{\sigma}\sigma}(\mathbf{k} \mid i\omega_1),$$

$$\bar{Y}_{\sigma\sigma}(i\omega) = -\frac{1}{2\beta N}\sum_{\mathbf{k}}\sum_{\omega_1}\tilde{G}_2^{(0)\,irr}[\sigma, i\omega_1; \sigma, -i\omega_1 \mid \sigma, i\omega; \sigma, -i\omega]\, e_\sigma(\mathbf{k}) e_{\sigma}(-\mathbf{k})\, \bar{F}_{\sigma\sigma}(\mathbf{k} \mid i\omega_1).$$

The kernels $\tilde{G}_2^{(0)\,irr}$ of these equations are the simplest irreducible two-particle Green's functions, which obey spin and frequency conservation [4,5]. These equations for the correlation functions together with the Dyson equations lead to a closed system of equations.

Summary

The main equations for the renormalized one-particle Green's and correlation functions of strongly correlated electron systems have been derived for the mixed phases of coexisting SDW with spiral polarization and superconductivity. As model Hamiltonian we have used the single-band Hubbard model; in the corresponding diagrammatic expansion recently proposed for the description of strongly correlated electron systems the electron transfer term is used as the perturbative term. The new elements of the theory correlation functions appear, which contain the most important spin, charge and pairing fluctuations. The correlation functions together with the full Green's functions are the main elements of the new diagrammatic approach. We have then established the exact Dyson equations for the delocalized Green's functions; with respect to the equations for the correlation functions we have used simple, but in the sense of retaining the most important contribution approximations. The influence of a spiral polarized SDW on the appearance of triplet superconductivity and vice versa has been shown.

Acknowledgements

P. Entel and V.A. Moskalenko would like to thank the Steering Committee of the Heisenberg-Landau Program for the Grant, which supports this work. P. Entel would like to thank the Bogoliubov Laboratory of Theoretical Physics of JINR (Dubna) for its hospitality. V.A. Moskalenko thanks the theory group of the Institute of Physics of the University of Duisburg-Essen for its hospitality and the SFB 445 for financial support. V.A. Moskalenko and V.I.Vladimir thank the High Department of Science and Technology of the Moldova Republic Government for a Grant.

References

[1] J. Hubbard, Proc. Roy. Soc. A 276, 233 (1963).
[2] Н.Н. Боголюбов, Ротапринт ОИЯИ, Д-781, Дубна, 1961 г.; Physikalische Abhandlungen aus der S.U. 6, 1, 113, 229 (1962).
[3] K. Machida, Solid State Commun., 41, 217, (1982).
[4] M.I. Vladimir and V.A. Moskalenko, Teor. Mat. Fiz. 82, 428, (1990) [Theor. Math. Phys. 82, 301, (1990)].
[5] S.I. Vacaru, M.I. Vladimir, and V.A. Moskalenko, Teor. Mat. Fiz. 85, 248, (1990) [Theor. Math. Phys. 85, 1185 (1990)].