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Stripes and superconductivity in one-dimensional self-consistent model

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We show that many observable properties of high temperature superconductors can be obtained in the frameworks of one-dimensional self-consistent model with included superconducting correlations. Analytical solutions for spin, charge and superconductivity order parameters are found. The ground state of the model at low hole doping is a spin-charge solitonic superstructure. Increasing of doping leads to the phase transition to superconducting phase. There is a region of doping where superconductivity, spin density wave and charged stripe structure coexist. The charge density modulation presents in the vicinity of vortices (kinks in the 1D model) in the superconducting state.

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Recently discovered stripe phases in doped antiferromagnets (cuprates and nickelates) [1] have attracted attention to the problem of coupled spin and charge order parameters in the electron systems. Theoretical [2 – 5] and experimental [6 – 10] evidence indicate the possibility that their ground state exhibits spin and charge density waves (SDW and CDW), either competing, or coexisting with superconductivity. Numerical mean-field calculations [2 – 4] suggest a universality of the spin-charge multi-mode coupling phenomenon in repulsive electronic systems of different dimensionalities. Families of the cuprate high-transition-temperature superconductors show antiferromagnetism and superconductivity. For the $La_{2-x}Sr_xCuO_4$ family there is another ordering tendency – unidirectional charge-spin density wave, i.e. "stripes". Recent neutron scattering experiment of Lake et al. shows that moderate magnetic field makes fluctuating stripes quasi static [6]. An important development in the theory of the cuprate superconductors is the prediction that in addition to antiferromagnetism and superconductivity there is a tendency toward stripe ordering [2 – 4]. This prediction is corroborated by experiments [1, 11]. A recent neutron scattering experiment shows that a moderate magnetic field can turn a fluctuating stripe order into a quasi static one in the optimum doped cuprates [7]. The vortex state can be regarded as an inhomogeneous mixture of a superconducting spin fluid and a material containing a nearly ordered antiferromagnet.

In this paper we present the one-dimensional effective model describing stripe phase at low hole doping and superconductivity state at higher doping. An exact analytical solution of the Hartree-Fock problem at and away from half-filling is found. Our theory predicts an amazing duality between the spin density wave and superconducting order, and implies the presence of stripes near a superconducting vortex, and superconductivity near a stripe dislocation.

The Hamiltonian $H = H_0 + H_s$ consists of two parts: the Hubbard Hamiltonian with on-site repulsion $U > 0$:

$$H_0 = -t \sum_{\langle i,j\rangle \sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} - \mu \sum_{i.\sigma} \hat{n}_{i,\sigma}, \quad (1)$$

and the interaction part including superconducting correlations

$$H_s = \sum_i \Delta_s(i) c^\dagger_{i,\uparrow} c^\dagger_{i,\downarrow} + \text{h.c.}, \quad (2)$$

where Δ_s is the superconducting order parameter, μ is the chemical potential. The case of the Hubbard model (1) was considered in details earlier [12]. The self-consistent analytical solution for the charge-spin solitonic superstructure was found as a function of a hole doping. It was shown that effects of commensurability led to a pinning of stripe structure at rational filling points $|\rho - 1| = m/n$.

In the continual self-consistent approximation the effective Hamiltonian can be derived similar [12]. We obtain

$$\begin{aligned} H = \int dx \{ &\Psi^\dagger_\sigma \left(-i\frac{\partial}{\partial x}\right) \hat{\sigma}_z \Psi_\sigma + \Delta(x)\Psi^\dagger_\sigma \hat{\sigma}_+ \Psi_\sigma + \\ &+ \Delta^*(x)\Psi^\dagger_\sigma \hat{\sigma}_- \Psi_\sigma + \alpha\rho(x)\Psi^\dagger_\sigma \Psi_\sigma + \\ &+ \Delta_s(-\Psi^\dagger_{+,\uparrow}\Psi^\dagger_{-,\downarrow} + \Psi^\dagger_{-,\uparrow}\Psi^\dagger_{+,\downarrow}) + \\ &+ \Delta^*_s(-\Psi_{-,\downarrow}\Psi_{+,\uparrow} + \Psi_{+,\downarrow}\Psi_{-,\uparrow}) + \\ &+ \frac{|\Delta|^2}{\pi\lambda} + \frac{|\Delta|^2_s}{\pi\lambda_s} - \frac{\alpha}{2}\rho^2 \}, \end{aligned} \quad (3)$$

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where $\lambda = 2\alpha/\pi$ is a dimensionless spin coupling constant, λ_s is a dimensionless superconductor coupling constant, $\hat{\sigma}_{z,x}$ are the Pauli matrices, $2\hat{\sigma}_{\pm} = \hat{\sigma}_x \pm \hat{\sigma}_y$, $\alpha = U/4t$; the Plank constant is taken as unity, and the length is measured in the units of the lattice (chain) period a. In these units momentum and wavevector are dimensionless, and velocity and energy posses one and the same dimensionality. The vector ${\Psi_\sigma}^T \equiv (\Psi_{\sigma+}, \Psi_{\sigma-})$ is defined in terms of the right- left-moving $\Psi_{\sigma\pm}$, which constitute the wave function:

$$\Psi_\sigma(x) = \Psi_{+,\sigma} e^{ik_F x} + \sigma \Psi_{-,\sigma} e^{-ik_F x} \tag{4}$$

where $\sigma = \pm 1$ for a spin $\uparrow$ and $\downarrow$ respectively. The Fermi-momentum is $k_F = \pi\bar{\rho}/2$, where in the case of half-filling the average number of electrons per site equals $\bar{\rho} = 1$, i.e. $k_F = \pi/2$. The slowly varying real functions $\Delta(x)$ and $\rho(x)$ are defined as $\langle \hat{n}(x) \rangle = \rho(x)$, $\langle \hat{S}^z(x) \rangle = -\Delta(x)\cos(\pi x)/\alpha$. The continual approximation requires that $\alpha, \lambda, \lambda_s \ll 1$ (weak coupling limit). Note that the constraint $\lambda = 2\alpha/\pi$ for the Hubbard model is not necessary in a general case, our results remain valid for independent $\alpha, \lambda, \lambda_s \ll 1$.

Introduce $\bar{\rho}$ and $\tilde{\rho}$ as $\rho(x) = \bar{\rho} + \tilde{\rho}(x)$, $\int \tilde{\rho}(x) dx = 0$. Then the term $\alpha\bar{\rho}\Psi^\dagger\Psi$ in Eq. (3) is the shift of the chemical potential or the energy, and the term $\alpha\tilde{\rho}\Psi^\dagger\Psi$ can be excluded by the unitary transformation (see [12, 13])

$$\Psi_\pm(x) \longrightarrow \exp(\mp i\alpha \int^x \tilde{\rho}\, dx')\Psi_\pm(x).$$

Under this transformation the spin order parameter modifies as $\Delta(x) \longrightarrow \exp(2i\alpha \int^x \tilde{\rho}\, dx')\Delta(x)$.

We can diagonalize the total Hamiltonian $H = H_0 + H_s$ by performing a unitary Bogolubov transformations

$$\Psi_\sigma(x) = \sum_n \gamma_{n,\sigma} u_{n,\sigma}(x) - \sigma \gamma^+_{n,-\sigma} v^*_{n,-\sigma}(x) \tag{5}$$

which have the form

$$\Psi_{\pm,\sigma} = \sum_n \gamma_{n,\sigma} u_\pm \pm \gamma^+_{n,-\sigma} v^*_\mp \tag{6}$$

in terms of right and left components $u_\pm$, $v_\pm$ defined as

$$f_\sigma(x) = f_{+,\sigma} e^{ik_F x} + \sigma f_{-,\sigma} e^{-ik_F x}, \quad f = u, v. \tag{7}$$

New operators γ, γ^+ satisfy the fermionic commutative relations $\{\gamma_{n,\sigma}, \gamma^+_{m,\sigma'}\} = \delta_{m,n}\delta_{\sigma,\sigma'}$. The transformations (5) must diagonalize the Hamiltonian H:

$$H = E_g + \sum_{\epsilon_n > 0} \epsilon_n \gamma^+_{n,\sigma}\gamma_{n,\sigma}, \tag{8}$$

$$E_g = \sum_{\epsilon_n < 0} \epsilon_n + \int dx \left(\frac{|\Delta|^2}{\pi\lambda} + \frac{|\Delta|_s^2}{\pi\lambda_s} - \frac{\alpha}{2}\rho^2 \right),$$

where E_g is the ground state energy and $\epsilon_n > 0$ is the energy of excitation n.

Following [14] we obtain the eigenvalue equations

$$\hat{H}\chi = \epsilon\chi, \tag{9}$$

where

$$\hat{H} =$$

$$= \begin{pmatrix} -i\frac{\partial}{\partial x} + \alpha\rho & \Delta & \Delta_s & 0 \\ \Delta^* & i\frac{\partial}{\partial x} + \alpha\rho & 0 & \Delta_s \\ \Delta_s^* & 0 & i\frac{\partial}{\partial x} - \alpha\rho & \Delta \\ 0 & \Delta_s^* & \Delta^* & -i\frac{\partial}{\partial x} - \alpha\rho \end{pmatrix},$$

$\chi^T = (u_+, u_-, v_+, v_-)$, and self-consistent conditions

$$\rho(x) = 2\sum [(u_+^* u_+ + u_-^* u_-) f + (v_+^* v_+ + v_-^* v_-)(1-f)], \tag{10}$$

$$\Delta(x) = -4\lambda[\sum u_-^* u_+ f - \sum v_-^* v_+ (1-f)], \tag{11}$$

$$\Delta_s = 2\lambda_s \sum (1-2f)[v_+^* u_+ + v_-^* u_-], \tag{12}$$

where $f = 1/(\exp[\epsilon/T] + 1)$. We omitted spin indices since in our representation for wave functions all equations are diagonal over spin.

At first, consider homogeneous state with constant $\Delta = |\Delta|\exp[i\varphi]$, $\Delta_s = |\Delta_s|\exp[i\varphi_s]$ and $\rho(x) = \bar{\rho} \equiv \equiv N/L$. The average spin density has the form $< S_z > \propto \propto \mathrm{Re}(\Delta\exp(2ik_F x)$. Neglecting trivial dependence on $\bar{\rho}$ we obtain two branch spectrum $\epsilon_\pm^2 = k^2 + (|\Delta| \pm |\Delta_s|^2)^2$, with wave functions $u, v \propto \exp[ikx]$ satisfying the symmetry relations

$$v_+ = \pm u_- \exp i[\varphi - \varphi_s],\ v_- = \pm u_+ \exp -i[\varphi + \varphi_s]. \tag{13}$$

The self-consistent equations read

$$|\Delta| = \frac{\lambda}{L}[F_+ + F_-], \quad |\Delta_s| = \frac{\lambda_s}{L}[F_+ - F_-], \tag{14}$$

where $F_\pm = \sum_\epsilon [(|\Delta| \pm |\Delta_s|)/\epsilon_\pm] \tanh[\epsilon_\pm/T]$. At zero temperature we obtain

$$\frac{2}{\lambda} = \log\frac{4\epsilon_F^2}{||\Delta|^2 - |\Delta_s|^2|} + \frac{|\Delta_s|}{|\Delta|}\log\left|\frac{|\Delta| - |\Delta_s|}{|\Delta| + |\Delta_s|}\right|. \tag{15}$$

The second equations is derived from the first one by substitution $\lambda \to \lambda_s$, $\Delta \leftrightarrow \Delta_s$. The minimum of the ground state energy E_g is achieved at the state $\Delta = 2\epsilon_F \exp[-1/\lambda]$, $\Delta_s = 0$ for the case $\lambda > \lambda_s$, and $\Delta_s = 2\epsilon_F \exp[-1/\lambda_s]$, $\Delta = 0$ for the case $\lambda < \lambda_s$.

In general case parameters λ, λ_s depend on the doping concentration $h = |\rho - 1|$. It is well known that the coupling constant λ monotonically decreases with doping from λ_0 at $\rho = 1$ to the value $\lambda_0/2$ in the limit $|\rho - 1| \gg \Delta/v_F$ (due to the absence of umklapp scattering at $\rho \neq 1$) [15]. If we suppose that superconducting part H_s comes from next neighboring site repulsion (as considered for 2D CuO plane model) $H_s \sim \sim V\rho_n\rho_{n\pm1}$, then the self-consistent equation becomes $\Delta_s \sim V\langle\Psi_{n,\downarrow}\Psi_{n\pm1,\uparrow}\rangle \to 2V\cos k_F a\langle\Psi_\downarrow(x)\Psi_\uparrow(x)\rangle$ in the continual approximation. The coupling constant $\lambda_s \sim \sim (2/\pi)V\cos(\pi\rho/2)$ increases with hole doping $h = 1 - \rho$. If the ground state of undoped system is antiferromagnet state ($\lambda > \lambda_s$), phase transition to superconducting state will take place at some doping h_c where $\lambda = \lambda_s$. Two phases (SDW and SC) with $\Delta = \Delta_s \neq 0$ can coexist at this point. For detailed investigation of the phase transition more rigorous consideration of quantum fluctuations is necessary.

So far we considered uniform state with Δ, $\Delta_s = = \text{const}$. Since symmetry relations between wave function components (13) are independent of absolute values ($|\Delta|$, $|\Delta_s|$), we assume that these relations are valid also in a general case of nonuniform order parameters. Substituting (13) to (9) we obtain in the case of constant phases φ, φ_s equations

$$[-i\sigma_z\frac{d}{dx} + \tilde{\Delta}\sigma_+ + \tilde{\Delta}^*\sigma_-]\mathbf{u} = \epsilon\mathbf{u}, \qquad (16)$$

where $\mathbf{u}^T = \{u_+, u_-\}$, $\tilde{\Delta} = (\Delta \pm \Delta_s)\exp[i\varphi]$. These equations are eigenvalue equations for the Peierls model, were studied in [15, 16]. The dependance on ρ in (1) was excluded by means of wave function transformation $u_\pm, v_\pm \to \exp\{\mp i\alpha\int\rho dx\}u_\pm, v_\pm$. The term $\alpha\int dx\rho^2/2$ in the total energy E_g is responsible for commensurate effects and pinning of the system at rational doping ($h = m/n$) points [12].

Consider the system with $\lambda > \lambda_s$. At $\bar{\rho} = 1$ the ground state is antiferromagnet with constant $\Delta = \Delta_0$, $\rho = \bar{\rho}$ and $\Delta_s = 0$. As a result of doping kink states are formed with local level $\epsilon = 0$ at the center of the gap 2Δ. The single kink solution of (1) is $\tilde{\Delta}_1 = \Delta + \Delta_s = \Delta_0\tanh(\Delta_0 x + a/2)$, $\tilde{\Delta}_2 = \Delta - \Delta_s = = \Delta_0\tanh(\Delta_0 x - a/2)$ with arbitrary shift a. The wave functions and the excitation spectrum read

$$u_\pm \propto (\pm\epsilon + k + i\Delta_0\tanh\xi)e^{ikx}e^{\pm i\pi/4}, \quad \epsilon^2 = k^2 + \Delta_0^2, \qquad (17)$$

$$u_{0,\pm} \propto \frac{\exp[\pm i\pi/4]}{\cosh^2\xi}, \quad \epsilon = 0, \qquad (18)$$

where $\xi = \Delta_0 x \pm a/2$. The order parameters Δ, Δ_s take form

$$\Delta_s = \frac{\Delta_0\sinh a}{2(\cosh^2\Delta_0 x + \sinh^2 a/2)}, \quad \Delta = \frac{\Delta_0\tanh\Delta_0 x}{1 + \frac{\sinh^2 a/2}{\cosh^2\Delta_0 x}}.$$

For the case $a = 0$ we obtain $\Delta_s \equiv 0$, $\Delta = \Delta_0\tanh\Delta_0 x$, $\rho \propto 1/\cosh^2\Delta_0 x$. It is a one stripe solution found in [12]. The shift $0 < a \ll 1$ leads to the appearance of the region around the stripe with $\Delta_s \neq 0$, so that $\rho \propto 1/\cosh^2\Delta_0 x$, $\Delta_s \propto a/\cosh^2\Delta_0 x$. The quasiparticle spectrum is independent of a, therefore the equilibrium position a is defined by minimization of the potential energy

$$\delta W(a) = \frac{\Delta_0}{\pi}\left|\frac{1}{\lambda_s} - \frac{1}{\lambda}\right|\frac{a}{\tanh a} + \frac{\Delta_0\alpha}{4}\frac{\frac{a}{\tanh a} - 1}{\sinh^2 a}. \qquad (19)$$

The minimum of the energy (19) is reached at $a = 0$ for $\gamma \equiv \alpha\pi\lambda\lambda_s/4|\lambda - \lambda_s| - 2.5 < 0$. For small a the inequality $\gamma < 0$ is possible if λ and λ_s are not very close to each other ($|\lambda - \lambda_s| \gtrsim \alpha\lambda\lambda_s$). The nontrivial minimum $a \neq 0$ exist only in the small region $|\lambda - \lambda_s| \lesssim \alpha\lambda\lambda_s$ around the transition point $\lambda = \lambda_s$, where $\gamma > 0$. Stripe and superconductivity phases coexist in this region: $\Delta_s, \Delta, \rho(x) \neq 0$. The equilibrium shift a is small $a \propto \sqrt{\gamma}$ if $\gamma \ll 1$, but it l logarithmically diverges $a \propto \log\gamma$ in the limit $\lambda_s \to \lambda$.

So we obtain that an increasing of doping for the system with $\lambda > \lambda_s$, $\gamma < 0$ at $\rho = 1$ leads to the forming of the periodic structure of charged kinks $\Delta = = \Delta_0\tanh\Delta_0 x$, which acquires the form at $h = |\rho - 1| \gg \gg v_F/\Delta_0$ [12]

$$\Delta \sim \Delta_0\sqrt{k}\,\mathrm{sn}[\Delta_0 x/\sqrt{k}, k], \; \rho(x) - \bar{\rho} \propto \Delta^2 - \bar{\Delta}^2,$$

where $K(k)$ is the Elliptic Integral of the first kind, sn(.,k) is the Jacobi elliptic function, $|\bar{\rho} - 1| = = \Delta_0/2K(k)\sqrt{k}$.

The superconducting order parameter order $\Delta_s \neq 0$ appears in the considered case at some higher doping level where γ becomes positive. In a small region $|\lambda - \lambda_s| \lesssim \alpha\lambda\lambda_s$ around the transition point $\lambda = \lambda_s$, where $\gamma > 0$, superconductivity and spin/charge orders coexist: $\Delta_s, \Delta, \rho(x) \neq 0$. In the particular case of the model with $\alpha = 0$ this region is reduced to the point $h = h_c$. A more complicated analysis beyond the scope of the used mean field approximation is required at this point to take into account strong quantum fluctuations, including the zero mode due to the degeneration of the ground state with respect to the shift a of two sublattices.

The opposite region $\lambda < \lambda_s$ can be studied using the duality properties of the model. It is easy to see that eigenvalues ϵ_n of equations (9) are invariant under transformation $\Delta \longleftrightarrow \Delta_s$. Indeed, if we simultaneously exchange $\Delta \longleftrightarrow \Delta_s$ and $u_-(x) \longleftrightarrow v_+(x)$ in Eq. (9) the Hamiltonian (9) is not changed (without unimportant terms with $\rho(x)$) . Therefore the ground state energy E_g in (8) is invariant under the transformations $\Delta \longleftrightarrow \Delta_s$, $\lambda \longleftrightarrow \lambda_s$. Therefore we can apply obtained above solutions for the superconductivity phase. We find that in the region $\gamma > 0$ the ground state is superconductor with $\Delta_s = \text{const}$, $\Delta = 0$. The one-dimensional analogue of the vortex in two- or three-dimensional systems is the kink: $\Delta_s = \Delta_0 \tanh \Delta_0 x$.

Due to the duality symmetry the charge density $\rho(x)$ has the same expression as for the kink in spin density wave. Therefore we obtain that the charge density is not zero in the vicinity of the kink

$$\rho(x) \sim \frac{1}{\cosh^2 \Delta_0 x} \cos(2\pi|\rho - 1|). \qquad (20)$$

Similar to the previous case ($\lambda > \lambda_s$) we find that near the transition point ($\lambda \sim \lambda_s$, $\gamma > 0$) a stripe structure can arise. In the limit $0 < \gamma \ll 1$, $|\bar{\rho} - 1| \gg \Delta_0/v_F$ we obtain

$$\Delta(x) \propto \sin \pi|\bar{\rho} - 1|x, \quad \tilde{\rho}(x) \propto \cos 2\pi|\bar{\rho} - 1|x, \quad a \propto \sqrt{\gamma}.$$

To conclude, we have found the self-consistent mean-field analytical solution for the ground state structure of the quasi-one-dimensional electronic system with spin, charge and superconducting correlations. We have found that for an appropriate choice of parameters the ground state is striped charge/spin density wave structure at low hole doping. The stripe configuration is pinned at rational points $|\rho - 1| = m/n$ with the pinning energy $\propto \exp(-Cn)$ substantial for small n, which can lead to the stability of the stripe picture. The phase transition to the superconductivity state takes place at some doping level. Both superconductivity and spin/charge density wave order parameters can coexist in a some small region near this point.

The model is self-dual: The eigenfunction equations are invariant with respect to transformations $\lambda \leftrightarrow \lambda_s$, $\Delta \leftrightarrow \Delta_s$. Therefore properties of superconducting state can be derived from the low doping consideration. In particular, we obtained that charge stripes can exist as in low doping spin density wave state as in superconducting state in the vicinity of spatially nonuniform configurations of Δ_s, for example, vertices (kinks in one dimension).

Though this one-dimensional model can be applied rather to quasi-one-dimensional systems than to high-temperature quasi-two-dimensional anisotropic superconductors, it shows some properties peculiar to high-temperature superconductors (one-dimensional stripe structure at low doping and superconductivity at a higher doping, etc.). Therefore our results can be useful for understanding of high-temperature phenomenon. For describing anisotropic properties of real systems a two-dimensional model consideration is required to take into account an important contribution from nodal quasiparticles.

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