Higher grade hybrid model of layered superconductors

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Summary A hybrid discrete-continuous model of layered superconductors with interlayer Josephson couplings of arbitrary range is constructed. The conditions required by gauge invariance and thermodynamical stability of the model are determined. Some important special cases, in particular transition to the classic Lawrence-Doniach model, are discussed. The conditions for presence of alternating solutions and the possibilities to describe such states of a superconductor by the continuum or bi-continuum models are examined. The enhancement of superconductivity caused by the presence of higher order Josephson couplings is shown.

1 Introduction

Most of the high-temperature superconductors like e.g. YBCO or BSCCO have a layered structure. Such a strongly anisotropic situation results in the fact that the material properties and behaviour of the fields in direction (say z axis) orthogonal to the layers is totally different from the behaviour in directions parallel to layers. [4, 1, 8]. The idea originally proposed by Lawrence and Doniach (LD) [7] is to consider the Ginzburg-Landau order parameter $\psi$ as a function of two continuous variables (say $x$ and $y$) and one discrete variable $n$ - the index of the layer. The form of the free-energy

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functional proposed in [7] and, after a modification, presented e.g. in [5] takes into account the Josephson coupling between the nearest neighbour layers. The exact solutions for this case are given in [6]. The higher grade hybrid model, proposed in this paper, admits also couplings between more distant neighbours - up to a (given, but arbitrary) range $K$.

Let us look at the layered superconductor as a one-dimensional chain of atomic planes with Josephson’s bonds between them. Such bonds will be called J-links. The interplanar distance will be denoted by $s$. We assume the following convention for indexing the planes and links. If we locate the point $z = 0$ at an atomic plane, then the $z$-coordinate of any plane, equal $ns$, may be represented by the integer $n$, while the $z$-coordinate of the center of any interplanar gap, equal $ls$, by the half-integer $l$. Choosing the point $z = 0$ at the center of an interplanar gap - we index the planes by half-integers and the gaps by integers.

2 The hybrid model of grade K

Let us consider the free-energy functional $\mathcal{F}$ for a layered superconductor. We shall denote by $\psi_n$ the order parameter associated to the layer indexed by the number $n$. Its complex conjugate (c.c.) will be denoted by $\bar{\psi}_n$. The symbol $m_{ab}$ and $m_c$ will denote the in-plane and tunneling effective mass of superconducting current carriers, respectively. We start from the free energy functional of the following form

$$\mathcal{F} = \mathcal{F}_0 + \mathcal{F}_s + \frac{1}{8\pi} \int B^2 d^3 x.$$  \hspace{1cm} (1)

The term $\mathcal{F}_0$ describes the normal state, while $\mathcal{F}_s$ the superconducting one. The superconducting term is composed of two parts:

$$\mathcal{F}_s = \mathcal{F}_p + \mathcal{F}_J,$$  \hspace{1cm} (2)

where the part

$$\mathcal{F}_p = \sum_n F_n$$  \hspace{1cm} (3)

describes the contribution of atomic planes, while $\mathcal{F}_J$ corresponds to interplanar Josephson’s bonds. For any plane indexed by $n$ the free energy $F_n$
has the 2D Ginzburg-Landau form (in general, the parameters can depend on $n$)

$$F_n = s \int dxdy \left\{ \frac{\hbar^2}{2m_{ab}} |(D\psi)_n|^2 + \alpha_0 |\psi_n|^2 + \frac{1}{2} \beta |\psi_n|^4 \right\},$$  

(4)

where we have introduced the 2-dimensional continuous operator $D$ (covariant derivative)

$$D_\rho = \partial_\rho - \frac{ie^*}{\hbar c} A_\rho, \quad \rho = x, y. \tag{5}$$

The form (4) of the functional $F_p$ already ensures its invariance with respect to the gauge transformation

$$A \to A' = A + \nabla \Lambda, \quad \psi_n \to \psi'_n = \psi_ne^{i\frac{e}{\hbar c} \Lambda}, \quad \bar{\psi}_n \to \bar{\psi}'_n = \bar{\psi}_ne^{-i\frac{e}{\hbar c} \Lambda},$$  

(6)

(2-dimensional $A$ and $\nabla$ for this case). The standard variational treatment of the functional $F_s$ with respect to $A_\rho$, $\rho = x, y$, gives the standard in-plane components of the superconducting current

$$j_\rho = -\frac{ie^*}{2m_{ab}} (\bar{\psi}_n \partial_\rho \psi_n - \psi_n \partial_\rho \bar{\psi}_n) - \frac{e^*2}{m_{ab}c} A_\rho |\psi_n|^2, \quad \rho = x, y. \tag{7}$$

Let us now construct the term $F_J$ in the free-energy. In general it is a functional which can depend on all $\psi_n, \bar{\psi}_n$ and on the vector potential $A$. Consider first the global gauge transformation, i.e. $\Lambda = \text{const}$ in (6). The invariance condition for $F_J$ implies that its density $F_J$ fulfills the relation

$$\frac{\partial F_J}{\partial \psi_n} \psi_n - \frac{\partial F_J}{\partial \bar{\psi}_n} \bar{\psi}_n = 0 \tag{8}$$

for each $n$ separately. That means that the functional $F_J$ depends on the fields $\psi$ only through the combinations $\bar{\psi}_n \psi_k$.

Now we shall consider the local gauge transformation with $\Lambda$ depending only on the variable $z$, but first let us introduce the following new variables

$$\hat{\psi}_n = \psi_ne^{ip_{1n}} \tag{9}$$

(and the appropriate complex conjugate), with

$$p_{1n} = \frac{e^*}{\hbar c} \int_{n\hbar}^{(n+1)\hbar} A_z \, dz. \tag{10}$$
The vanishing of the variation of $\mathcal{F}_J$ with respect to $\Lambda$ gives the condition
\[
\sum_n \frac{\delta \mathcal{F}_J}{\delta \hat{\psi}_n} \frac{\partial \hat{\psi}_n}{\partial \hat{\psi}_n} + c.c. + \frac{\partial \mathcal{F}_J}{\partial A_z} \frac{\partial A_z}{\partial \Lambda} = 0, \tag{11}
\]
which, together with the condition of global gauge invariance, implies explicit independence of $\mathcal{F}_J$ of $A_z$.

The simplest gauge invariant expression for the energy of J-link between $n$-th and $(n + q)$-th planes will have the following form
\[
\epsilon_{qn} = \frac{1}{2} \{ \zeta_{qn}\bar{\psi}_n\psi_n + \eta_{qn}\bar{\psi}_{n+q}\psi_{n+q} - (\gamma_{qn}\bar{\psi}_n\psi_{n+q}e^{-ip_{qn}} + c.c.) \}, \tag{12}
\]
where the exponent $p_{qn}$ is defined by the formula
\[
p_{qn} = \frac{e^*}{\hbar c} \int_{nq}^{(n+q)s} A_z dz. \tag{13}
\]

Let us note that for the model invariant with respect to the time reversal we have $\gamma_{qn} = \bar{\gamma}_{qn}$. In general, the coupling parameters $\zeta$, $\eta$, $\gamma$ as well as in-plane parameters $\alpha_0$ and $\beta$ can be different for different planes (which is the case for superconductors composed of various atomic planes). However, in this paper we shall consider the array of identical planes, hence the parameters will not depend on index $n$. That implies that $\eta_q = \bar{\zeta}_q$. Hence instead of (12) we shall use
\[
\epsilon_{qn} = \frac{1}{2} \{ \zeta_q (|\psi_n|^2 + |\psi_{n+q}|^2) - \gamma_q (\bar{\psi}_n\psi_{n+q}e^{-ip_{qn}} + c.c.) \}. \tag{14}
\]

Let $P$ denote the (finite or infinite, but ordered) set of all indices of planes, and let $Q = \{1, 2, ..., K\}$. The planes connected with the $n$-plane by Josephson coupling select the following subset of $Q$
\[
P_n = \{ q \in Q : (n + q)eP \}. \tag{15}
\]
Thus, the gauge invariant functional $\mathcal{F}_J$ for the hybrid model of grade $K$ has the density of the following form
\[
\mathcal{F}_J = \sum_{n \in P} \sum_{q \in P_n} \epsilon_{qn}, \tag{16}
\]
with $\epsilon_{qn}$ given by (14). The coupling parameters $\zeta_q$ and $\gamma_q$ vanish for $q > K$. Every J-link is represented in (16) by exactly one term.
3 Comparison with anisotropic GL model

To compare our hybrid model (HM) with the continuum GL model, we shall consider the infinite medium. In that case the summation index may be shifted by the integer $q$. Moreover $P_n = Q$. This implies that

$$F_J = \frac{1}{2} \sum_n \sum_q \left\{ 2(\zeta_q - \gamma_q)|\psi_n|^2 + \gamma_q|\psi_n + qe^{-ip\gamma_q} - \psi_n|^2 \right\}$$  \hspace{2cm} (17)

For very weak field $A_z$ and very small dependence of $\psi_n$ on $n$ we have the correspondence rules which allows us to pass from the hybride to the continuum models.

$$\left\{ \begin{array}{l}
\sum_n \rightarrow \frac{1}{s} \int dz,
\frac{1}{qs}(\psi_{n+q} - \psi_n) \rightarrow \psi_n'(z),
e^{-ip\gamma_q} \rightarrow 1 - \frac{i}{\hbar}\epsilon^s q s A_z.
\end{array} \right. \hspace{2cm} (18)$$

Applying the rules to the functional (2) with (4) and (17) one obtains

$$F_s \rightarrow \int d^3x \left\{ \frac{\hbar^2}{2m_{ab}} |D\psi|^2 + \alpha_0|\psi|^2 + \frac{1}{2} \beta|\psi|^4 + \sum_q \left[ (\zeta_q - \gamma_q)|\psi|^2 + \frac{1}{2} q^2 s^2 \gamma_q |D_3\psi|^2 \right] \right\}.$$  \hspace{2cm} (19)

Hence, we have the following relation between $m_c$ – the effective mass in $z$–direction (in anisotropic GL model) and the coupling parameters $\gamma_q$:

$$\frac{1}{m_c} = \frac{s^2}{\hbar^2} \sum_q q^2 \gamma_q.$$  \hspace{2cm} (20)

The presence of J-links modifies also the parameter $\alpha_0$ to the form:

$$\alpha = \alpha_0 + \sum_q (\zeta_q - \gamma_q).$$  \hspace{2cm} (21)

4 Field equations

By computing the variation of the functional $F$ with respect to $A_z$ one obtains the Maxwell equation for the $z$–components of current density and curl $H$

$$\frac{1}{c} J(z) = \frac{1}{4\pi} \left( \text{curl} \ H \right)_z,$$  \hspace{2cm} (22)
where
\[ J(z) = i\frac{Se^*}{2\hbar c} \sum_{n \in P} \sum_{q \in P_n} \left\{ \gamma_q \bar{\psi}_n \psi_{n+q} e^{-ip_{qn}} - \text{c.c.} \right\} \chi_{qn}(z), \] (23)

\( P_n \) is given by (25), and the quantity \( p_{qn} \) by (13). The symbol \( \chi_{qn}(z) \) denotes the characteristic function of the interval \([ns, (n + q)s]\). Let us note that for any layer \( ns < z < (n + 1)s \) the expression \( J(z) \) does not depend on the value \( z \); only the ends of the interval are important. To better see the structure, let us first extend the set \( Q \) on the negative values
\[ \bar{Q} = \{-K, ..., -2, -1, 1, 2, ..., K\}, \] (24)
and introduce the symbols
\[ \sigma_{qn} = \begin{cases} 1 & \text{if } (n + q) \in P, \\ 0 & \text{otherwise}. \end{cases} \] (25)

Then the expression for Josephson current \( J_l \) describing tunneling across the interplanar gap indexed by \( l \) (half integer if \( P \) contains integers) will have the form
\[ J_l = i\frac{Se^*}{2\hbar c} \sum_{q \in \bar{Q}} \sum_{n \in P_l} \left\{ \gamma_q \sigma_{qn} \bar{\psi}_n \psi_{n+q} e^{-ip_{qn}} - \text{c.c.} \right\}, \] (26)

where
\[ P_l = \{ n \in P : n < l < n + q \}. \] (27)

By computing the variation of the functional \( F_s \) with respect to \( \bar{\psi}_n \), one obtains the equations
\[ -\frac{\hbar^2}{2m_{ab}} D^2 \psi_n + \bar{\alpha} \psi_n + \beta|\psi_n|^2 \psi_n + \] (28)
\[ -\frac{1}{2} \sum_{q \in \bar{Q}} \gamma_q (\sigma_{qn} \psi_{n+q} e^{-ip_{qn}} + \sigma_{-qn} \psi_{n-q} e^{ip_{n-q}}) = 0, \]
where instead of \( \alpha_0 \) we have introduced
\[ \bar{\alpha} = \alpha_0 + \sum_q \sigma_{qn} \zeta_q \] (29)
depending of \( n \), for finite \( P \).
The ground states

Let us now consider the plane-uniform states of HM in the absence of magnetic field. The order parameter is then independent of the in-plane variables and the net supercurrents vanish. In detailed calculations we shall focus our attention on the grade $K = 2$, which seems to be sufficiently illustrative to grasp the idea on what is going on. The generalization to grades $K > 2$, although more complicated algebraically, is straightforward. In the region far from the boundary all the coefficients $\sigma_{qn} = 1$. For $K = 2$ the condition of vanishing Josephson current is equivalent to

$$\gamma_1(\bar{\psi}_n \psi_{n+1} - \text{c.c.}) + \gamma_2(\bar{\psi}_n \psi_{n+2} + \bar{\psi}_{n-1} \psi_{n+1} - \text{c.c.}) = 0.$$  

(30)

and the equations (28) take the form

$$\bar{\alpha} \psi_n + \beta |\psi_n|^2 \psi_n - \frac{1}{2} \left[ \gamma_1 (\psi_{n+1} + \psi_{n-1}) + \gamma_2 (\psi_{n+2} + \psi_{n-2}) \right] = 0.$$  

(31)

We shall look for solutions with constant amplitude and difference of phase between neighbouring atomic planes, so we use the ansatz

$$\psi_n = C e^{in\theta}.$$  

(32)

The result is the equation

$$\bar{\alpha} + \beta C^2 - \gamma_1 \cos \theta - \gamma_2 \cos 2\theta = 0,$$  

(33)

with the condition

$$\gamma_1 \sin \theta + 2\gamma_2 \sin 2\theta = 0.$$  

(34)

Solving (34) with respect to $\theta$, we obtain 3 variants: (a1) $\theta = 0$, (a2) $\theta = \pi$, and (a3) $\cos \theta = -(\gamma_1 / 4\gamma_2)$. The solution $C$ to (33) has the form $C^2 = -\alpha^*/\beta$, where $\alpha^*$ depends on the variant. The variant (a1) implies the uniform solution to (31):

$$\psi_n = C,$$  

(35)

with

$$\alpha^* = \alpha_0 + \zeta_1 + \zeta_2 - \gamma_1 - \gamma_2,$$  

(36)

what is the case of equation (21) for grade $K=2$. In the variant (a2) the solution to (31) has the alternating form

$$\psi_n = \pm C,$$  

(37)
with
\[ \alpha^* = \alpha_0 + \zeta_1 + \zeta_2 + \gamma_1 - \gamma_2. \] (38)

Finally, in the variant (a3), the solution exists if the parameters \( \gamma_1 \) and \( \gamma_2 \) fulfill the relation
\[ |\gamma_1| \leq 4|\gamma_2|. \] (39)

Then the parameter \( \alpha^* \) is connected with the coupling constants by the formula:
\[ \alpha^* = \alpha_0 + \zeta_1 + \zeta_2 + \gamma_2(1 + \frac{\gamma_1^2}{8\gamma_2^2}). \] (40)

There are two independent solutions
\[ \psi_n = Ce^{\pm \theta}, \quad \theta = \arccos(-\frac{\gamma_1}{\gamma_2}). \] (41)

They will be referred to as the phase modulated states. The solutions degenerate at the extremities \( |\gamma_1| = 4|\gamma_2| \).

So far we confined our discussion to the existence of solutions which could serve as candidates for the ground state. The question of stability of the solutions will be addressed in the next section.

Let us note that the condition \( \sin \theta = 0 \) admits the solutions (35) and (37) for hybrid model of any grade K. Contrary to that, the analogues of the conditions (a3) and (39) can deliver, depending on the grade and the coupling parameters, any number from 0 to \( 2(K-1) \) modulated solutions.

### 6 Stability

To examine the stability of the solutions presented in the previous section, we shall analyze the Hessian matrix of the free energy \( F_s \) describing small deviations from the ground state. The problem reduces to examining the function
\[ \mathcal{E}(C, \theta) = \tilde{\alpha}C^2 + \frac{1}{2}\beta C^4 - C^2(\gamma_1 \cos \theta + \gamma_2 \cos 2\theta). \] (42)

The solutions found in the previous section are stationary points of \( \mathcal{E} \). If \( \gamma_2 = 0 \), then the stability of the solutions depends on the sign of \( \gamma_1 \). If \( \gamma_2 \neq 0 \) then the sign of the respective eigenvalue depends on the values of the
parameters $\gamma_1$ and $\gamma_2$. For $\theta$ different from 0 and $\pi$ the dependence has form according to the function

$$f(\gamma_1, \gamma_2) = \gamma_2(\gamma_1 + 4\gamma_2)(\gamma_1 - 4\gamma_2).$$

(43)

The straight lines $\gamma_1 + 4\gamma_2 = 0$ and $\gamma_1 - 4\gamma_2 = 0$ divide the plane $\gamma_1, \gamma_2$ into 4 regions (see Figure 1).

As explained above, both the uniform and the alternating solutions always exist. However, in the region

$$(A): \gamma_1 > 0, -\gamma_1 < 4\gamma_2 < \gamma_1,$$

(44)

only the uniform solution (35) is stable.

On the other hand, in the region

$$(B): \gamma_2 > 0, -4\gamma_2 < \gamma_1 < 4\gamma_2,$$

(45)

both the solutions (35) and (37) are stable (the uniform one in the right and the alternating one in the left part of the region), while in the region

$$(C): \gamma_1 < 0, -\gamma_1 < 4\gamma_2 < \gamma_1,$$

(46)
only the alternating solution (37) is stable. The region

\[(D): \gamma_2 < 0, \ 4\gamma_2 < \gamma_1 < -4\gamma_2,\]  \hspace{1cm} (47)

excludes the stability of both the uniform and the alternating solutions but, in contrast to that, ensures the existence and stability of the modulated solutions (41). In the region (45) the modulated solutions exist but are unstable.

Let us note that in the regions (45) and (46) of stability of the alternating solution (37) one can apply the construction of bi-continuum solution presented in [9].

7 Enhancement of the superconductivity

The association of the formulae (36), (38) and (40) with the regions of stability of the ground state shows that, for suitable relations between the coupling constants \(\gamma_1\) and \(\gamma_2\), one can make the parameter \(\alpha^*\) more negative than \(\alpha_0\). In consequence, the 3D superconductivity can turn out enhanced with respect to the 2D superconductivity in the atomic planes. Such a possibility has been indicated in literature [2]. In further discussion we shall count the enhancement with respect to the origin located at \(\tilde{\alpha}\) given by (29). It is convenient to introduce the polar coordinates \(\gamma\) and \(\varphi\) in the plane \(\gamma_1, \gamma_2\):

\[\gamma_1 = \gamma \cos \varphi, \ \gamma_2 = \gamma \sin \varphi,\]  \hspace{1cm} (48)

and the notation

\[\varphi_0 = \arctan \left(\frac{1}{4}\right).\]  \hspace{1cm} (49)
Fig. 2. Enhancement of superconductivity by Josephson currents: $\Delta \alpha$ vs. $\varphi$

The quantity $\Delta \alpha = \alpha^* - \tilde{\alpha}$ as a function of the coupling angle $\varphi$ is plotted in Figure 2 (the numerical values are computed for $\gamma = 1$).

In the uniform state (36) we have

$$\Delta \alpha = \sqrt{2} \gamma \sin(\varphi - \frac{3}{4} \pi), \quad -\varphi_0 \leq \varphi \leq \pi - \varphi_0.$$  \hspace{1cm} (50)

The minimum $\Delta \alpha$ (hence the maximum enhancement) is reached at $\varphi = \frac{\pi}{4}$ and equals $-\sqrt{2} \gamma$.

In the alternating state (38), in turn, one obtains

$$\Delta \alpha = \sqrt{2} \gamma \sin(\varphi + \frac{3}{4} \pi), \quad +\varphi_0 \leq \varphi \leq \pi + \varphi_0$$  \hspace{1cm} (51)

with the minimum value $-\sqrt{2} \gamma$ reached at $\varphi = \frac{3}{4} \pi$.

The enhancement for the phase modulated state (40) is represented by

$$\Delta \alpha = \gamma \sin \varphi (1 + \frac{1}{8} \text{ctg}^2 \varphi), \quad -\pi + \varphi_0 \leq \varphi \leq -\varphi_0.$$  \hspace{1cm} (52)

In this case the minimum equals $-\gamma$ and is reached at $\varphi = -\frac{\pi}{2}$. Hence, the maximum enhancement in this case is smaller than in the uniform and alternating states.

8 Special cases

The hybrid model of grade 0 (HM with $K=0$) reduces formally to uncoupled (2 dimensional) Ginzburg-Landau model for each atomic plane. The HM
with K=1 has in general two coupling parameters ζ and γ. If they are equal to one another, one obtains the Lawrence-Doniach model with parameter α = α₀, and the effective mass in z–direction given by the formula

\[ \frac{1}{m_c} = \frac{s^2}{\hbar^2} \gamma. \]  

Due to \( \gamma > 0 \) the LD model has only one stable ground state solution, namely the uniform one. The interplanar coupling gives neither enhancement nor suppression of the critical temperature. Although the Josephson current coupling places the model on the enhancement side, the effect is precisely annulled by ζ = γ.

Let us note that, in the enhancement mechanism discussed above, the 2D superconductivity of the planes is not a prerequisite for the 3D superconductivity of the array of the planes. In fact, one can obtain the negative \( \alpha^* \) starting from positive \( \alpha_0 \). This is in concordance with ideas expressed in Anderson’s discussion of his Dogma V in [3].

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