Fundamental excitations in layered superconductors with long-range Josephson couplings

by

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February 2, 2008

Abstract

The present paper develops the ideas introduced in cond-mat/0312673. The construction of a hybrid discrete-continuous model of layered superconductors is briefly presented. The model bases on the classic Lawrence-Doniach scenario with admitting, however, long-range interactions between atomic planes. Moreover, apart from Josephson couplings they involve the proximity effects. The range of interactions, K, can, in principle, be arbitrary large. The solutions corresponding to the range K=2 are exposed. The fundamental excitations are understood as deviations from stable ground states. The formulae for energy of those excitations are constructed. The possible shapes of dispersion curves are analysed. For each type of shape the corresponding values of physically measurable quantities like effective mass and bandwidth are expressed by coupling parameters.

1 Introduction

The layered structure of superconductor implies a very strong structural anisotropy which may be characterised by relation between $\xi_c$ – the coherence length in the direction perpendicular to layers – and the interlayer distance $s$. In the limiting case $\xi_c >> s$ the 3D anisotropic Ginzburg–Landau model

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is well applicable [1, 2, 3, 8]. On the other side, in the case $\xi_c \leq s$, a much better description is given by Lawrence–Doniach model: a stack of 2D GL planes with Josephson links between adjacent planes [4, 9]. Similar model has been used in [5, 7, 6, 10]. However, there exist superconducting materials like $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ or $\text{Tl}_2\text{Ba}_2\text{CaCu}_2\text{O}_8$, which have $\xi_c/s$ between 1.5 and 2, i.e. too small for GL and too high for LD.

The higher grade hybrid model (HM) [11, 12, 13, 14], presented here, patches the gap between those extreme cases, admitting Josephson-type couplings (we shall call them J-links) between distant planes. The range $K$ of J-links is a global parameter of the model. $K=0$ denotes the stack of non-interacting GL planes, $K=1$ – J-links between nearest planes only, $K=2$ – J-links between nearest and next nearest planes, and so on.

Like in LD model we consider two continuous independent variables understood as in-plane coordinates $x, y$. The third independent variable is discrete: it denotes the ordinal number of the plane $n$.

We shall use the following notation:

$\begin{cases} 
\psi_n - \text{the order parameter associated to the layer indexed by } n \\
\bar{\psi}_n - \text{its complex conjugate (c.c.)}, \\
m_{ab} - \text{in-plane effective mass of superconducting current carriers}, \\
m_c - \text{out-of-plane}
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2 Free energy functional

Contribution to the superconducting component of the free energy contains 2 parts: from GL planes and from J-links.

$$
\mathcal{F}_s = s \sum_n \int dx dy \left\{ \frac{\hbar^2}{2m_{ab}} |(D\psi)_n|^2 + \alpha_0 |\psi_n|^2 + \frac{1}{2} \beta |\psi_n|^4 \right\} + \frac{s}{2} \sum_{n \in P} \sum_{q \in P_n} \int dx dy \left\{ \xi_q (|\psi_n|^2 + |\psi_{n+q}|^2) - \gamma_q (\bar{\psi}_n \psi_{n+q} e^{-ip_{qn}} + \text{c.c.}) \right\},
$$

where $P$ denotes the set of indices of all planes, $P_n$ refers to planes which are J-linked to the plane $n$. Every J-link is represented by exactly one term.
The symbol $D$ denotes the 2-dimensional operator of covariant derivative

$$D_{\rho} = \partial_{\rho} - ie^* \frac{\bar{A}_{\rho}}{\hbar c}, \quad \rho = x, y. \quad (2)$$

The third component of the vector potential $A_z$ appears in the exponent

$$p_{qn} = \frac{e^*}{\hbar c} \int_{ns} \overline{(n+q)s} A_z dz. \quad (3)$$

3 Comparison with the anisotropic GL model

To compare our hybrid model (HM) with the continuum GL model, we shall consider the infinite medium. In that case the component of free energy connected with J-links has the form

$$F_J = \frac{1}{2} \sum_{n} \sum_{q} \left\{ 2(\zeta_q - \gamma_q)|\psi_n|^2 + \gamma_q|\psi_{n+q}e^{-ip_{qn}} - \psi_n|^2 \right\}. \quad (4)$$

For very weak fields $A_z$ and very slow dependence of $\psi_n$ on $n$ we have the correspondence rules which, in the long wave limit, allow us to pass from the hybrid to the 3D continuum. Applying the rules formulated in [14] one obtains

$$\mathcal{F}_s \rightarrow \int d^3x \left\{ \frac{\hbar^2}{2m_{ab}} |D\psi|^2 + \frac{1}{2} q^2 s^2 \gamma_q |D_3\psi|^2 + \alpha_0 |\psi|^2 + \sum_{q} [ (\zeta_q - \gamma_q)|\psi|^2 + \frac{1}{2} \beta |\psi|^4] \right\}. \quad (5)$$

It implies the modification of GL parameter $\alpha_0$ to the form

$$\alpha = \alpha_0 + \sum_{q} (\zeta_q - \gamma_q) \quad (6)$$

and gives the following relation between the GL effective mass in $z-$direction and the coupling parameters.

$$m_c = \left( \frac{s^2}{\hbar^2} \sum_{q} q^2 \gamma_q \right)^{-1}, \quad (7)$$
4 Field equations

By computing the variation of the functional \( F_s \) with respect to \( \bar{\psi}_n \), one obtains the equations

\[-\frac{\hbar^2}{2m_{ab}} D^2 \psi_n + \bar{\alpha} \psi_n + \beta |\psi_n|^2 \psi_n - \frac{1}{2} \sum_{q \in \bar{Q}} \gamma_q \sigma_{qn} \psi_{n+q} e^{-i p_{qn}} = 0 \]  

(8)

where

\[\bar{\alpha} = \alpha_0 + \frac{1}{2} \sum_{q \in \bar{Q}} \sigma_{qn} \zeta_q\]  

(9)

depends of \( n \) for finite \( P \). The quantities

\[\bar{Q} = \{-K, ..., -2, -1, 1, 2, ..., K\}, \quad \sigma_{qn} = \begin{cases} 1 & \text{if } (n + q) \nu P \\ 0 & \text{otherwise} \end{cases}\]  

(10)

have been introduced to describe the finite range of J-links.

The expression for Josephson current \( J_l \) describing tunnelling across the interplanar gap indexed by \( l \) (half integer if planes are indexed by integers) will have the form

\[J_l = \frac{se^*}{2i \hbar} \sum_{q \in \bar{Q}} \sum_{n \in P_{lq}} \{\gamma_q \sigma_{qn} \bar{\psi}_n \psi_{n+q} e^{-i p_{qn}} - \text{c.c.}\},\]  

(11)

where

\[P_{lq} = \{n \in P : n < l < n + q\}.\]  

(12)

5 The ground states

Consider now the plane-uniform states of HM in the absence of magnetic field. Let us concentrate on the case \( K = 2 \). The condition of vanishing Josephson current is equivalent to

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

(13)

and the equations (8) take the form

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

(14)
Solutions with constant amplitude and difference of phase between adjacent atomic planes, obtained by the ansatz $\psi_n = C e^{i n \theta}$ form 3 classes of states with $C^2 = -\alpha^*/\beta$:

- **uniform**: $\psi_n = C$, $\alpha^* = \alpha_0 + \zeta_1 + \zeta_2 - \gamma_1 - \gamma_2$,
- **alternating**: $\psi_n = (-1)^n C$, $\alpha^* = \alpha_0 + \zeta_1 + \zeta_2 + \gamma_1 - \gamma_2$,
- **phase modulated**: $\psi_n = C e^{\pm i n \theta}$, $\theta = \arccos(-\frac{\gamma_1}{4 \gamma_2})$.

(15)

The phase modulated solutions exist if the parameters $\gamma_1$ and $\gamma_2$ fulfill the relation $|\gamma_1| \leq 4|\gamma_2|$. Then $\alpha^*$ is connected with the coupling constants by the formula

$$\alpha^* = \alpha_0 + \zeta_1 + \zeta_2 + \gamma_2 (1 + \frac{\gamma_1^2}{8 \gamma_2^2}).$$

(16)

The straight lines $\gamma_1 + 4 \gamma_2 = 0$, $\gamma_1 - 4 \gamma_2 = 0$, and $\gamma_1 = 0$ divide the plane $(\gamma_1, \gamma_2)$ into 3 regions (shown in Fig. 1 of [14]). Both the uniform and the alternating solutions always exist. However, in the region $\ominus$: $\gamma_1 > 0$, $\gamma_1 + 4 \gamma_2 > 0$, only the uniform solution is stable, while in the region $\oplus$: $\gamma_1 < 0$, $\gamma_1 - 4 \gamma_2 < 0$, only the alternating solution is stable. The region $\otimes$: $\gamma_2 < 0$, $4 \gamma_2 < \gamma_1 < -4 \gamma_2$, excludes the stability of both the uniform and the alternating solutions but, in contrast to that, ensures the existence and stability of the phase modulated solutions. In the sector (N): $\gamma_2 > 0$, $|\gamma_1| < 4 \gamma_2$, the phase modulated solutions exist but are unstable.

Note that, irrespectively of the values and signs of $\gamma_1$, $\gamma_2$, a stable ground state solution always exists.

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. The presence of coupling constants $\zeta_q$ allows to take into account the proximity effect between atomic planes. According to the formula (16) one can obtain a negative $\alpha^*$ starting from a positive $\alpha_0$. It means that under appropriate coupling one can obtain superconductivity by stacking planes which originally are in normal state.
The HM with K=1 has in general two coupling parameters, \( \zeta \) and \( \gamma \). In particular cases it is related to known models:

\( \zeta = \gamma > 0 \Rightarrow \) LD model, uniform solution, no enhancement.
\( \zeta = \gamma < 0 \Rightarrow \) Theodorakis model, alternating solution, proximity effect, enhancement.

6 The excited states

The physical interpretation of the model requires adequate understanding of the excited states. In the present section we shall consider the excited states as deviations from the ground states determined in the previous section. The results presented here for K=2 may be directly generalized to the case of arbitrary K [13].

For two reasons the problem will be treated in the linear context:
(a) The nonlinearity is present in the equations through the term \( |\psi|^2 \) only, hence the excitations which do not change the modulus \( |\psi| \) (we shall call them phase excitations) may be treated in the framework of linear equations exactly.
(b) For the excitations changing the modulus of the order parameter, one can solve the problem in linear approximation, valid for weakly excited states. From the microscopic point of view one speaks here on the collective excitations of the Cooper pair condensate.

Let us first consider the phase excitations. We substitute the function

\[
\psi_n = f e^{i\theta_n}, \text{ where } f = \text{const.} \tag{17}
\]

into the equation

\[
(\tilde{\alpha} + \beta |\psi|^2)\psi_n - \frac{1}{2} [\gamma_1(\psi_{n+1} + \psi_{n-1})\psi_n + \gamma_2(\psi_{n+1} + \psi_{n-1})\psi_n] = \epsilon\psi_n. \tag{18}
\]

Then we obtain

\[
\tilde{\alpha} + \beta |\psi|^2 - \frac{1}{2} [\gamma_1(e^{i(\theta_{n+1} - \theta_n)} + e^{i(\theta_{n-1} - \theta_n)}) + \gamma_2(e^{i(\theta_{n+2} - \theta_n)} + e^{i(\theta_{n-2} - \theta_n)})] = \epsilon(\theta), \tag{19}
\]

which should be independent of \( n \). In consequence, \( \theta_n = n(\theta_0 + \theta) + \text{const} \) and

\[
\epsilon(\theta) = \tilde{\alpha} + \beta f^2 - [\gamma_1 \cos (\theta_0 + \theta) + \gamma_2 \cos 2(\theta_0 + \theta)], \tag{20}
\]
where $\theta_0$ corresponds to the ground state determined in the Section 5. The particular values $\theta_0 = 0$ and $\theta_0 = \pi$ represent the uniform and alternating ground states, respectively. The remaining values of $\theta_0$ represent the phase modulated ground states.

The expression for the energy of a phase excitation has the form:

$$\epsilon(\theta) - \epsilon(0) = \gamma_1(\cos \theta_0 - \cos (\theta_0 + \theta)) + \gamma_2(\cos 2\theta_0 - \cos 2(\theta_0 + \theta)), \quad (21)$$

where $\epsilon(0)$ denotes the energy of ground state

$$\epsilon(0) = \hat{\alpha}(\theta_0) + \beta f^2. \quad (22)$$

Now we shall examine the modular excitations. Let us consider once more the equation (18) but this time we shall take into account that $\psi_n \rightarrow f + \delta \psi_n$, where $f$ denotes a uniform ground state. After linearization one obtains equation of the same shape, with $f^2$ in place of $|\psi|^2$ and $\delta \psi$ in place of $\psi$. Taking excitation $\delta \psi_n = ae^{ink}$ with arbitrary constant amplitude $a$ and wave vector $k$ (it is sufficient to consider excitations with $k_x = 0 = k_y$), after some calculations like in the case of phase modulated excitations, one obtains the excitation energy corresponding to wave vector $k$ (with respect to the ground state $k = 0$

$$\epsilon_1 = \epsilon_k - \epsilon_0 = \gamma_1(1 - \cos ks) + \gamma_2(1 - \cos 2ks) \quad (23)$$

valid in the region of stability of uniform ground state: $\gamma_1 > 0, \gamma_1 + 4\gamma_2 > 0$. Similar procedure performed for the alternating ground state delivers the formula

$$\epsilon_2 = -\gamma_1(1 - \cos ks) + \gamma_2(1 - \cos 2ks) \quad (24)$$

in the region of stability of alternating ground state: $\gamma_1 < 0, -\gamma_1 + 4\gamma_2 > 0$.

The case of phase-modulated ground state is more complicated due to the lack of invariance with respect to the time reversal. The result in this case reads

$$\epsilon_3 = \gamma_1(\cos \theta_0 - \cos (\theta_0 + ks)) + \gamma_2(\cos 2\theta_0 - \cos 2(\theta_0 + ks)) \quad (25)$$

and is valid in the third region of stability of ground states:

$$\gamma_2 < 0, \quad |\gamma_1| < 4|\gamma_2| \quad (26)$$

The quantity $\theta_0$ in (25) equals the value of the variable $\theta$ determined by (15).
The calculation of the first and second derivatives of functions $\epsilon_1$, $\epsilon_2$ and $\epsilon_3$ describing excitation energy allows us to discuss shapes of dispersion curves in several sectors of the plane $(\gamma_1, \gamma_2)$ and to obtain the expressions for bandwidth $W$ and effective mass $m_c$. It is sufficient to plot the curves on the interval $[0, \pi]$. The Fig. 1 contains examples of all 6 possible shapes of dispersion curves.

The first and second derivatives of excitation energy are expressed by the same formulae for both the east and nord-east sectors (the region of stability of the uniform state):

$$
\epsilon_1' = s(\gamma_1 + 4\gamma_2 \cos ks) \sin ks, \quad \epsilon_1'' = s^2 \gamma_1 \cos ks + 4\gamma_2(2\cos^2 ks - 1). \quad (27)
$$

The effective mass, expressed by $\epsilon_1'(k = 0)$, is then for both E and NE sectors given by the same formula:

$$
m_c = \frac{\hbar^2}{s^2}(\gamma_1 + 4\gamma_2)^{-1}. \quad (28)
$$

However, the expressions for bandwidth are different. In the E sector $\epsilon_1' \geq 0$, the dispersion curve is monotonic, and the bandwidth $W$ is expressed by the difference of values of $\epsilon_1$ at the ends of interval $[0, \pi]$:

$$
W = 2\gamma_1. \quad (29)
$$

In the NE sector the dispersion curve reaches maximum at the point $ks = \theta$, where $\theta$ is determined by (15), ($\theta < \pi/2$ for NW sector and $\theta > \pi/2$ for NE one). The expression for bandwidth calculated as $\epsilon_1(\theta) - \epsilon_1(0)$ has the form

$$
W = \gamma_1 + 2\gamma_2 + \frac{\gamma_1^2}{8\gamma_2}. \quad (30)
$$

In the region of stability of the alternate state, i.e. in the nord-western and western sectors, the formulae for the first and second derivatives of excitation energy $\epsilon_2$ have the form (27) with $\gamma_1$ replaced by $-\gamma_1$. Hence the substitution of $|\gamma_1|$ instead of $\gamma_1$ into (29) gives bandwidth for western sector; the same substitution into (30) leads to the bandwidth for nord-western sector. The
expression for effective mass for both NW and W sectors may be obtained from (28) by the same substitution again and has the form

$$m_c = \frac{\hbar^2 s^2}{2 (|\gamma_1| + 4\gamma_2)^{-1}}.$$  \hfill (31)

For the region of stability of the phase-modulated foundamental states, i.e. for both southern sectors, we have

$$\epsilon_3' = s[\gamma_1 + 4\gamma_2 \cos(\theta + ks)] \sin(\theta + ks)$$  \hfill (32)

and

$$\epsilon_3'' = s^2[\gamma_1 \cos(\theta + ks) + 4\gamma_2 (2 \cos^2(\theta + ks) - 1)]$$  \hfill (33)

with $\theta$ expressed by (15). In the interval $[0, \pi]$ $\epsilon_3' = 0$ if $\theta + ks = 0$ or $\theta + ks = \pi$, or else $\cos(\theta + ks) = \cos(\theta)$. That implies that $\epsilon_3$ has minimum at $ks = \theta$ ($\theta > \pi/2$ for SW sector and $\theta < \pi/2$ for SE one).

The expression for bandwidth in SW sector is equal to the difference $\epsilon_3(\theta) - \epsilon_3(0)$ and in SE sector $\epsilon_3(\pi) - \epsilon_3(\theta)$. The common formula for the bandwidth has the form

$$W = |\gamma_1| + 2|\gamma_2| + \frac{\gamma_1^2}{8|\gamma_2|}.$$  \hfill (34)

while the effective mass in both southern sectors is given by

$$m_c = \frac{\hbar^2}{s^2} \frac{4|\gamma_2|}{16\gamma_2^2 - \gamma_1^2}.$$  \hfill (35)

This completes the discussion of bandwidths and effective masses for all the types of ground states.

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Fig. 1. Classification of dispersion curves, grade K=2