BAND STRUCTURE OF LOCAL PAIRS.
MATHEMATICAL TOOLS.

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Abstract
A system of strongly interacting fermions in a solid state is discussed. As an example, a structure of singlet and triplet coupled 2-particle states and their excitation spectra are investigated. It is shown that an account of intersite fermion interaction leads to new boson modes. Their number depends on dimensionality of a system. It is shown also that a reasonable choice of Hamiltonian parameters leads to a small effective mass of local pairs. A problem of interaction of coupled states with external fields are discussed. The calculations are carried out for intermediate and strong fermion–fermion coupling. The same analysis can be performed for another sorts of pairings like d-wave.

1 Introduction

The discovery of high-temperature superconductors (HTSC) that differ drastically from conventional superconductors leads to a great number of theoretical models. A small coherence length in HTSC–materials indicates that a size of fermion pairs, which is crucial for the superconducting properties, should be of the order of lattice parameter.

In this paper the formalism of tightly binding fermions in solids is developed. The main tool is extended Hubbard model with a fermion-fermion intersite attraction. The origin of the attraction could be ‘phononic’, ‘excitonic’ [1], ‘plasmonic’ [2] or ‘magnonic’ [3].

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Last years indicate the power of the bipolaron theory \cite{4}, \cite{5} and one could identify the local pairs and bipolarons – local pairs with phonon mechanism of 2-fermion attraction. The presence of the attraction changes the band structure significantly. Fermions being placed on different sites are coupled into pairs. The continuum of electron-hole pairs is situated above the local pair bands and does not overlap with them both in the normal and superconducting phases – see discussion in \cite{6}. It is the main difference of BCS-like theories and local pair ones.

The pair size seems to be of the same order of the distance between pairs that appears to be rather difficult for theoretical analysis. Nevertheless there are some papers \cite{6}, \cite{7} that are devoted to this complex intermediate region of crossover from Cooper pair regime to local pair one.

A presence of a superconducting state indicates an existence of boson type excitations, that are able to form a condensate at low temperatures. But there are fermions (electrons) in solids as the only charge carriers from the beginning that interact with phonons and other quasiparticles in crystal. This interaction in HTSC – materials is very complicated both for experimental and theoretical investigations. As a result, a large variety of superconductivity models has been developed. Most of papers deal with a ground state and excitation spectra on the basis of an attractive or repulsive Hubbard model (see review \cite{8}). Although a generalization to a more realistic and complicated situation is not obvious, several interesting papers have been recently appeared \cite{6}, \cite{9}, \cite{10}. In \cite{6} the authors considered in detail a ground state of such a system with rather general form of interaction in site representation. In \cite{9} the Green function method was applied to the boson spectra excitations. But the latter work was motivated by Auger experiments in noble metals and only fermion – fermion repulsion was taken into account.

This work is devoted to the investigation of the boson excitations - their band structure, interaction with each other and with external fields.

We start with rather general form of fermion – fermion interaction to be able to describe a large variety of interaction forms in different HTSC – materials. To be more definite, we postulate the effective Hamiltonian for fermi excitations in site representation in the form:

\[
H = -\mu \sum_{M} c_{M}^\dagger c_{M} + \sum_{M,N} t(m - n) c_{M}^\dagger c_{N} + \frac{1}{4} \sum_{M,N,M',N'} U_{M,N,M',N'} c_{M}^\dagger c_{N}^\dagger c_{M'} c_{N'} + \sum_{M,N} B_{M,N} c_{M}^\dagger c_{N}. \tag{1}
\]

Here \(\mu\) is the chemical potential, and for example \(M = (m, s)\), where \(m\) represents the site index, \(s\) is the spin projection of the fermion, \(c_{M}^\dagger, c_{M}\) are the operators for fermion creation and annihilation on the site \(m\) with the spin projection \(s = \pm \frac{1}{2}\), \(U_{M,N,M',N'}\) - is the matrix element of fermion interaction. This matrix is antisymmetric in its first and second pairs of indices separately.
\[ U_{MN,M'N'} = -U_{NM,M'N'} = -U_{MN,N'M'} \]

A hopping integral \( t(m-n) \) characterizes the fermion motion and describes a kinetic energy in a momentum representation. \( B_{MN} \) represents an arbitrary external field.

It must be stressed here that only fermi statistics of primordial quasiparticles is important. One can keep in mind polarons, holes, magnons and so on. The question is if the interaction is strong enough to form the local pairs or we have Cooper pairs in high-\( T_c \) superconductors as in the ordinary ones. A mathematical method in the latter case has been developed quite accurately.

The method, developed in this paper for the description of the local pairs is based on a functional integral technique \([11]\), that was widely used in different theoretical investigations (see, for example, \([12]\), \([19]\), \([13]\)). It was applied to a single-polaron problem \([14]\) and is used here for the local pair description of strongly interacting fermions. Calculations appear to be rather simple in the case of short-distance interaction. Furthermore mathematical difficulties increase slightly with a number of accounted sites.

Below the general formalism is presented for an arbitrary form of fermion-fermion interaction. Detailed calculations of spectra excitations and a structure of the pairs are discussed. Several applications of the developed method were considered in papers \([15]\), devoted to tunneling and \([16]\), where it was shown that experimental data on neutron scattering and infrared absorption spectra are in good agreement with predictions of local pair model.

## 2 General formalism

### 2.1 Main equations

The Hamiltonian \( H \) in the form (1) is quite general and its origin is not discussed here. The external field \( B \) is written in a general form too. This form includes the interaction with electromagnetic field and neutrons, for example. Let's start with partition function of the system in a functional integral form \([12]\):

\[
Z = \text{Spe}^{-\beta H} = \int Dc^* Dc \exp S[c^*, c],
\]

\[
S[c^*, c] = \int_0^\beta d\tau \left[ \sum_A c^*_A \dot{c}_A - H(c^*, c) \right]
\]

\[
= \int_0^\beta d\tau \left[ \sum_A c^*_A \dot{c}_A + \sum_{AB} r_{AB} c^*_A \dot{c}_B - \sum_{ABA'B'} \frac{1}{4} U_{ABA'B'} c^*_A \dot{c}_B c^*_A \dot{c}_B c^*_A \dot{c}_A \right],
\]

\[
r_{AB} = (\mu - \omega_{pA}) \delta_{AB}.
\]
Expression (2) is written in momentum representation where complex index $A = (p_A, s_A)$ includes quasimomentum and spin projection of a fermion; $\omega_{p_A}$ is the fermion spectrum determined as a Fourier transform of the hopping integral; $c_A^\dagger(\tau), c_A(\tau)$ are independent grassman variables; $\beta = 1/T$ is the inverse temperature. The external field $B$ is omitted in this section. To get rid of the four grassman variables product in the exponent and introduce the bosonic variables $\psi_{AB}(\tau), \psi_{AB}(\tau)^*$ one can use the Hubbard – Stratonovich transformation [17], [7] which is usually applied to consideration of bosonic fields of one argument that describes boson motion as a whole. In this latter case all the information about the internal structure of the bound state is lost, though the results of conventional BCS – theory of superconductivity are reproduced [12], [18]. But as far as we intend to study the internal pair structure and the interaction of the pairs with external fields we should use more complex bosonic fields $\psi_{AB}(\tau), \psi_{AB}(\tau)^*$. In this case expression (2) is transformed into:

$$Z = \int Dc^\dagger Dc D\psi^\dagger D\psi e^{S_e},$$

$$S_e = \int_0^\beta d\tau \left[ \sum_A c_A^\dagger c_A + \sum_{AB} \left[ r_{AB} c_A^\dagger c_B + \frac{1}{2} \psi_{AB}^* c_A c_B + \frac{1}{2} \psi_{AB} c_A^\dagger c_B^\dagger \right] \right] + \sum_{ABA'B'} \psi_{AB}^* U_{ABA'B'}^{-1} \psi_{A'B'},$$

(3)

Our central problem is to obtain equations for the wave functions of the coupled states and to find their solutions for the chosen form of interaction term. An imaginary “time” Fourier – transformation gives:

$$S_e = \sum_{\varepsilon AB} (r_{AB} + i\varepsilon\delta_{AB}) c_A^\dagger(\varepsilon) c_B(\varepsilon) + \frac{1}{2} \sum_{\varepsilon' AB} \psi_{AB}^*(\varepsilon + \varepsilon') c_A(\varepsilon)c_B(\varepsilon')$$

$$+ \frac{1}{2} \sum_{\varepsilon' AB} \psi_{AB}(\varepsilon + \varepsilon') c_A^\dagger(\varepsilon)c_B^\dagger(\varepsilon') + \sum_{EABA'B'} \psi_{AB}^*(E) U_{ABA'B'}^{-1} \psi_{A'B'},$$

where Matsubara frequencies $\varepsilon = (2n + 1)\pi/\beta, \varepsilon' = (2n' + 1)\pi/\beta$ due to antiperiodic boundary conditions for fermionic variables and $E = 2\pi n/\beta$ due to periodic boundary conditions for boson dynamic variables. Now one can integrate out the grassman variables [12]:

$$Z = \int D\psi^* D\psi e^{S_b},$$

$$S_b = \sum_{ABA'B'E} \psi_{AB}^*(E) U_{ABA'B'}^{-1} \psi_{A'B'}(E) + Tr(\ln Y),$$

(4)
\[ Y_{AB}(\varepsilon, \varepsilon') = \begin{pmatrix} (r_{AB} + i\varepsilon \delta_{AB})\delta_{\varepsilon, \varepsilon'} & \psi_{AB}(\varepsilon + \varepsilon') - (r_{AB} + i\varepsilon \delta_{AB})\delta_{\varepsilon, \varepsilon'} \\ \psi_{AB}^*(\varepsilon + \varepsilon') & -(r_{AB} + i\varepsilon \delta_{AB})\delta_{\varepsilon, \varepsilon'} \end{pmatrix}. \]

Boson dynamic variables \( \psi_{AB}^*, \psi_{AB} \) having been introduced, the expression (4) remains not very suitable for the further analysis. Next step is to expand the action \( S_b \) around a classical action \( S_b[\psi_{cl}] \). (\( \delta S_b/\delta \psi_{cl} = 0 \) by definition). The simplest case \( \psi_{cl} = 0 \), takes place: a) in a normal phase (by definition), b) near critical temperature, where a condensate density is small, and c) in a low fermion density limit. Calculations for \( \psi_{cl} \neq 0 \) were discussed in [19]. Here we will be interested in the normal phase of the system.

Let’s expand the effective action \( S_b \) (4) in Taylor series up to the second order in fields \( \psi_{AB}^*, \psi_{AB} \) around trivial classical trajectory \( \psi_{cl} = 0 \). A fourth order in the fluctuation describes interaction of pairs and was discussed in [20]. As it was shown in ref. [21], this term is small in a low-density region and/or for a weak fermion interaction. Here we neglect the pair interaction and limit ourselves to the study of boson excitation spectra and their interaction with external fields. Simple, but tedious calculations lead to quadratic part of the effective boson action:

\[ S_b^{(2)} = \sum_{ABA'B'E} \psi_{AB}^*(E) \tilde{D}_{ABA'B'}(E) \psi_{A'B'}(E), \]

\[ \tilde{D}_{ABA'B'}(E) = \frac{1}{4} \cdot \frac{th(\beta \Omega_A/2) + th(\beta \Omega_B/2)}{-iE + \Omega_A + \Omega_B} \delta_{ABA'B'} + U^{-1}_{ABA'B'}, \]

\[ \Omega_A = \omega_p - \mu. \]

To remove the denominator in the first term and the inverse power of the interaction operator \( U \), one has to make the following substitution of variables in the functional integral (4): \( U^{-1}\psi \rightarrow \psi, \psi_{AB}^* \cdot (iE\Omega_A - \Omega_B) \rightarrow \psi_{AB}^* \). This procedure leads to the partition function in the form:

\[ Z = \int D\psi^* D\psi \exp\{ \sum_{ABA'B'E} \psi_{AB}^*(-D_{ABA'B'} + iE\delta_{ABA'B'})\psi_{A'B'} \}, \]

where

\[ D_{ABA'B'} = (\Omega_A + \Omega_B)\delta_{ABA'B'} + W_{ABA'B'}, \]

\[ W_{ABA'B'} = \frac{1}{4} \cdot \left( th\frac{\beta \Omega_A}{2} + th\frac{\beta \Omega_B}{2} \right) U_{ABA'B'}. \]
Now we have to diagonalize the quadratic form of the exponent, that is to solve the equation:

$$\sum_{A'B'} D_{AB,A'B'} u^{(n)}_{A'B'} = \lambda_n u_{AB}^{(n)}.$$  \hfill (8)

Complex index \(n\) numerating the eigenstates of the system will be shown to include quasimomentum of the local pair, its spin and a band number. The eigenvalues \(\lambda_n\) obey the secular equation:

$$\text{Det}(D_{AB,A'B'} - \lambda_n \delta_{AA'} \delta_{BB'}) = 0.$$  \hfill (9)

The eigenfunctions are chosen to be orthonormal:

$$\sum_{AB} u_{AB}^{(n)*} u_{AB}^{(n')} = \delta_{nn'}.$$  \hfill (10)

The final step consists of introducing new variables \(C_n(E)\) in the integral (5):

$$\psi_{AB} = \sum_n C_n(E) u_{AB}^{(n)}, \quad \psi_{AB}^* = \sum_n C_n^*(E) u_{AB}^{(n)*}.$$  \hfill (11)

This leads to the expression:

$$Z = \prod_n \int DC_n DC_n^* \exp\{C_n^*(iE - \lambda_n)C_n\}.$$  \hfill (11)

This form of the partition function clarifies the meaning of the new variables \(C_n, C_n^*\) as the wave functions of bosonic excitations of energy \(\lambda_n\). It will be shown below that \(u_{AB}^{(n)}\) functions describing the internal structure of the bound state must be taken into account in the analysis of the pair interaction with an external field. Eq. (9) is the only one we need to calculate bosonic - type spectra excitations. The pair energy depends on its quasimomentum and spin projection. Quasimomentum and spin conservation can be accounted for in the form of interaction term:

$$W_{AB,A'B'} = \frac{1}{4} w_{AB,A'B'} \delta(A + B - A' - B').$$  \hfill (12)

Index \(A = (p_A, s_A)\) includes both the momentum \(p_A\) and the spin projection \(s_A\) of the fermion. Let variables \(R = A + B, R' = A' + B'\) characterize the momentum and spin projection of the coupled state as a whole. One can easily find from Eqs. (12), that matrix \(D\) is diagonal in indices \(R, R'\). Several energy bands may exist and we specify them by additional index \(\alpha\). It means that the complex index \(n\) in the expression (11) should incorporate the quasimomentum \(p_K\) of the 2-particle state as well as its spin projection \(\sigma_K = 0, \pm 1\), united in
the common index $K = (p_K, \sigma_K)$, and eigenfunctions of the matrix $D$ should have the form:

$$u_{A'B}^{(\alpha)} = u_{RA}^{(\alpha)} = v_{RA} = \delta_{K,R}x_{KA}^{(\kappa,\alpha)},$$

where $\kappa = 0(1)$ corresponds to singlet (triplet) case. The substitution of expression (13) into Eq.(8) along with the normalization condition term (10) lead to:

$$[\Omega_A + \Omega_{K-A} - \lambda_\alpha(K)]x_{KA}^{(\kappa,\alpha)} + \frac{1}{4} \sum_{A'} w_{A,K-A,K-A',A'}x_{KA'}^{(\kappa,\alpha)} = 0,$$

and

$$\sum_A x_{KA}^{(\kappa,\alpha)}* x_{KA}^{(\kappa',\alpha')} = \delta_{\kappa\kappa'} \delta_{\alpha\alpha'}.$$

These equations determine the pair structure $x_{KA}^{(\kappa,\alpha)}$ and the excitation spectra $\lambda_{\kappa,\alpha}(K)$. The previous analysis shows that for $\kappa = 0$ the solution is antisymmetrical in the fermion spin indices ($x_{KA}^{(0,\alpha)} = -x_{K,K-A}^{(0,\alpha)}$) while it is symmetrical for $\kappa = 1$. It confirms the notation $\kappa = 0$ for the singlet pairs and $\kappa = 1$ for the triplet ones.

### 2.2 Equations for triplet and singlet states

Cooper pairs in the BCS theory are singlets. There are many reasons to think that in HTSC – materials triplet pairs exist along with singlet ones [22]. Both of these possibilities are included in the system of equations (14) and the task is to write down the equations for the singlet and triplet states separately. It is convenient to redefine the wave functions of the coupled states and the interaction term $w$ by extracting the spin variables, that are included in the indices $A, A'$ and so on:

$$x_{s,s}^{(\kappa,\alpha)}(k, p) \equiv x_{KA}^{(\kappa,\alpha)},$$
$$w_{s,s,-s,-s'}(p, k - p, k - p', p') \equiv w_{A,K-A,K-A',A'}.$$
and singlet states. Accordingly, one obtains the system of two equations:

\[ \kappa \text{ should describe triplet states. We marked it by setting } \kappa = 1. \]

This equation is apparently symmetrical in the spin indices and its solution should describe triplet states. We marked it by setting \( \kappa = 1 \).

The case \( \sigma = 0 \) is more complex, because of the contributions from triplet and singlet states. Accordingly, one obtains the system of two equations:

\[
[\Omega_p + \Omega_{k-p} - \lambda_\alpha(K)]x^{(1,\alpha)}_{1,\frac{1}{2}}(k, p) \\
+ \frac{1}{4} \sum_{p'} w_{\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}}(p, k - p; k - p', p') x^{(1,\alpha)}_{1,\frac{1}{2}}(k, p') = 0. \tag{16}
\]

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The case \( \sigma = 0 \) is more complex, because of the contributions from triplet and singlet states. Accordingly, one obtains the system of two equations:

\[
[\Omega_p + \Omega_{k-p} - \lambda_\alpha(K)]x^{(\kappa,\alpha)}_{0,\frac{1}{2}}(k, p) \\
+ \frac{1}{4} \sum_{p'} [w_{\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}}(p, k - p; k - p', p') x^{(\kappa,\alpha)}_{0,\frac{1}{2}}(k, p') + \\
w_{\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}}(p, k - p; k - p', p') x^{(\kappa,\alpha)}_{0,-\frac{1}{2}}(k, p')] = 0,
\]

\[
[\Omega_p + \Omega_{k-p} - \lambda_\alpha(K)]x^{(\kappa,\alpha)}_{0,-\frac{1}{2}}(k, p) \\
+ \frac{1}{4} \sum_{p'} [w_{\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}}(p, k - p; k - p', p') x^{(\kappa,\alpha)}_{0,-\frac{1}{2}}(k, p') + \\
w_{\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}}(p, k - p; k - p', p') x^{(\kappa,\alpha)}_{0,\frac{1}{2}}(k, p')] = 0. \tag{17}
\]

A nontrivial solution to this system exists only if both equations are equivalent. This equivalence is guaranteed by antisymmetrical properties of the \( x \) and \( w \) functions:

\[
x^{(\kappa,\alpha)}_{0,\frac{1}{2}}(k, p) = -x^{(\kappa,\alpha)}_{0,-\frac{1}{2}}(k, k - p);
\]

\[
w_{s,s',s''}^{s'''}(p, p'; p''', p''') = -w_{s,s',s''}^{s'''}(p, p'; p''', p''') = -w_{s,s',s''}^{s'''}(p, p'; p''', p''').
\]

For this reason we consider only the first equation of the system \([17]\) in the following.

The equation for the symmetrical in spin indices solution \((x^{(1,\alpha)}_{1,\frac{1}{2}}(k, p') = x^{(1,\alpha)}_{0,-\frac{1}{2}}(k, p'))\), has the form:

\[
[\Omega_p + \Omega_{k-p} - \lambda_\alpha(K)]x^{(1,\alpha)}_{1,\frac{1}{2}}(k, p) \\
+ \frac{1}{4} \sum_{p'} [w_{\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}}(p, k - p; k - p', p') + \\
w_{\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}}(p, k - p; k - p', p') x^{(1,\alpha)}_{1,\frac{1}{2}}(k, p')] = 0 \tag{18}
\]

Eqs.\([16]\) and \([18]\) describe the triplet states with different spin projection. It will be shown below that these equations are equivalent.
The equation for the antisymmetrical in spin indices solution to the system (17) \( x_{0, s}^{(0, \alpha)}(k, p') = -x_{0, -s}^{(0, \alpha)}(k, p') \) describes the singlet states:

\[
\sum_{\alpha} \left[ \Omega_p + \Omega_{k-p} - \lambda_{\alpha}(K) \right] x_{0, \frac{s}{2}}^{(0, \alpha)}(k, p) + \frac{1}{4} \sum_{p'} \left[ w_{\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}}(p, k-p; k-p', p') - w_{\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}}(p, k-p; k-p', p') \right] x_{0, \frac{s}{2}}^{(0, \alpha)}(k, p') = 0
\]

(19)

It is useful to express the interaction matrix \( w \) in Eqs. (16), (18) and (19) in terms of the Hamiltonian parameters. In a more detailed form the Hamiltonian in the site representation may be written as:

\[
H = \frac{1}{4} \sum_{mnmn'} U_{mn,mn'}^{(1)} c_m^+ c_{m,n}^+ c_{n,m'}^+ c_{n',s}^+ + \frac{1}{4} \sum_{mnmn'} U_{mn,mn'}^{(2)} (c_m^+ c_{m,n}^+ c_{m',s}^+ c_{n',s}^+ + c_{m',-s}^+ c_{m,n,s}^+) - \frac{1}{4} \sum_{mnmn'} U_{mn,mn'}^{(3)} (c_m^+ c_{m,n}^+ c_{m',-s}^+ c_{n',s}^+ - c_{m',-s}^+ c_{m,n,s}^+), \quad s = \frac{1}{2}.
\]

(20)

The first two terms are responsible for the triplet interaction (matrices \( U_{mn,mn'}^{(1)}, U_{mn,mn'}^{(2)} \) are antisymmetrical) whereas the third term describes the singlet interaction (matrix \( U_{mn,mn'}^{(3)} \) is symmetrical). A comparison of the two equivalent expressions for the Hamiltonian (15), (21) gives:

\[
U_{m,s;n,s';m',s;n',s} = U_{m,-s;n,-s;m',-s';s,n'} = U_{mn,mn'}^{(1)};
U_{m,s;n,-s;m',s';n',s} = U_{m,s,n,m';-s',s} = U_{mn,mn'}^{(2)} + U_{mn,mn'}^{(3)};
U_{m,-s;n,m';s';n',s} = U_{m,-s,n,m',s',-s} = U_{mn,mn'}^{(2)} - U_{mn,mn'}^{(3)}.
\]

(21)

Here the site and spin indices are shown separately for the sake of clarity. It seems reasonable to suppose that the form of the interaction depends only on the spin of a 4-fermion state, rather than on its spin projection. It leads to an equality \( U_{mn,mn'}^{(1)} = U_{mn,mn'}^{(2)} \), that, being not very important, makes calculations more easy. Using Eqs. (5), (12) in the momentum representation we insert the Hamiltonian parameters (i.e. matrixes \( U_{mn,mn'}^{(1)}, U_{mn,mn'}^{(2)} \) and \( U_{mn,mn'}^{(3)} \)) into Eqs. (16), (18) and (19) instead of the function \( w \). After some transformations one obtains the equation for the singlet states:

\[
\sum_{\alpha} \left[ \Omega_p + \Omega_{k-p} - \lambda_{\alpha}(K) \right] x_{0, \frac{s}{2}}^{(0, \alpha)}(k, p) + \frac{1}{2} \left( \frac{\hbar \Omega_p}{2} + \frac{\hbar \Omega_{k-p}}{2} \right) \sum_{p'} U_{p,k-p,k-p',p'}^{(3)} x_{0, \frac{s}{2}}^{(0, \alpha)}(k, p') = 0, \quad s = \pm \frac{1}{2}.
\]

(22)
Both of equivalent Eqs. (16), (18) for the triplet states may be transformed to:

\[
\left[\Omega_{p} + \Omega_{k-p} - \lambda_{1,\alpha}(k)\right] x_{\sigma,s}^{(1,\alpha)}(k, p) + \\
\frac{1}{2} \left( \text{th} \frac{\Omega_{p}}{2} + \text{th} \frac{\Omega_{k-p}}{2} \right) \sum_{p'} U_{p,k-p,p',p}^{(1)} x_{\sigma,s}^{(1,\alpha)}(k, p') = 0, \ \sigma = 0, \pm 1.
\] (23)

Equations (24), (23) may be solved numerically though they are too complicated yet. As it will be shown below, the account of the finite number of sites in the interaction parameters \(U^{(1)}, U^{(2)}, U^{(3)}\) permits to simplify the calculations significantly. An example of such a model is discussed in the next section.

2.3 Spectra of 2-particle excitations. 1 – 2 model

Let us fix up the form of the fermion – fermion interaction. It takes into account the interaction on the same or neighboring sites (1 – 2 model). The interaction parameters \(U^{(1)}, U^{(2)}, U^{(3)}\) (see expression (20)) in the momentum representation have the form:

\[
U_{p,p-k,k-p',p'}^{(1)} = U_{p,p-k,k-p',p'}^{(2)} = \delta_{kk'} U_{12} \sum_{l} [\cos(p - p', 1) - \cos(k - p - p', 1)] \]

\[
U_{p,p-k,k-p',p'}^{(3)} = \delta_{kk'} \{U_{s1} + U_{s2} \sum_{l} [\cos(p - p', 1) + \cos(k - p - p', 1)]\},
\]

where \(U_{12}\) is the interaction energy of the fermions in the triplet state and \(U_{s2}, U_{s1}\) are the intersite and onsite interaction of the fermions in the singlet state; \(l\) is a lattice vector. Substituting these expressions into Eqs. (24), (23) one can obtain:

\[
x_{\sigma,s}^{(1,\alpha)}(k, p) - 2L_{kp} U_{12} \sum_{l} \sin(\frac{1}{2} k - p, 1) \sum_{p'} \sin(\frac{1}{2} k - p', 1) x_{\sigma,s}^{(1,\alpha)}(k, p') = 0
\] (24)

- for the triplet state and

\[
x_{0,s}^{(0,\alpha)}(k, p) - L_{kp} \sum_{p'} \{U_{s1} + 2U_{s2} \sum_{l} [\cos(\frac{1}{2} k - p, 1)\cos(\frac{1}{2} k - p', 1)] x_{0,s}^{(0,\alpha)}(k, p') = 0
\] (25)

- for the singlet one. Here the notations are:

\[
L_{kp} = \frac{1}{2} \frac{\text{th} (\beta \Omega_{p}/2) + \text{th} (\beta \Omega_{k-p}/2)}{\lambda_{(\kappa,\alpha)}(k) - \Omega_{p} - \Omega_{k-p}}, \ \Omega_{k} = \omega_{k} - \mu = t \sum_{l} \cos(kl) - \mu,
\]
\( \mathbf{p} \) is the internal momentum variable and the hopping integral is supposed to be \( t(\mathbf{m} - \mathbf{n}) = t \neq 0 \) only if \( \mathbf{m} = \mathbf{n} \pm \mathbf{l} \). These equations obviously lead to the following \( \mathbf{p} \) – dependence of the pair wave function:

\[
x^{(1,\alpha)}(\mathbf{k}, \mathbf{p}) = L_{kp} \sum_{l=1}^{dim} A_l^{(t)}(\mathbf{k}) \sin \left( \frac{1}{2} \mathbf{k} - \mathbf{p}, \mathbf{l} \right),
\]

\[
x^{(0,\alpha)}(\mathbf{k}, \mathbf{p}) = L_{kp}[A_0^{(s)}(\mathbf{k}) + \sum_{l=1}^{dim} A_l^{(s)}(\mathbf{k}) \cos \left( \frac{1}{2} \mathbf{k} - \mathbf{p}, \mathbf{l} \right)],
\]

where index \( l = 1 \) for \( \mathbf{l} = (l_x, 0, 0) \), \( l = 2 \) for \( \mathbf{l} = (0, l_y, 0) \), \( l = 3 \) for \( \mathbf{l} = (0, 0, l_z) \) and \( \text{dim} \) stands for the dimensionality of the system. The lattice vector \( \mathbf{l} \) numerates in a natural way the triplet bands and therefore the number of the triplet bands is equal to the space dimensionality. The coefficients \( A_0^{(s)}(\mathbf{k}), A_l^{(s)}(\mathbf{k}) \) \( A_l^{(t)}(\mathbf{k}) \) are determined by substitution of these functional forms into Eqs.(24, 25) for the wave functions. The equation describing the triplet pairs appears to be diagonal after this substitution and is transformed into linear independent algebraic equations for the functions \( A_l^{(t)}(\mathbf{k}) \):

\[
[1 - 2U_{12}H_l(\mathbf{k})]A_l^{(t)}(\mathbf{k}) = 0, \quad l \leq \text{dim}
\]

where \( H_l = \sum_p L_{kp} \sin^2 \left( \frac{1}{2} \mathbf{k} - \mathbf{p}, \mathbf{l} \right) \).

The excitation spectra are obtained from the equations:

\[
1 - 2U_{12}H_l(\mathbf{k}) = 0,
\]

while the coefficients \( A_l^{(t)}(\mathbf{k}) \) are derived from the normalization condition (13) which is now written as

\[
\sum_{\mathbf{p}, \sigma} x^{(1,\alpha)}(\mathbf{k}, \mathbf{p}) x^{(1,\alpha')}_{\sigma,s}(\mathbf{k}, \mathbf{p}) = \delta_{\alpha,\alpha'}.
\]

With the account of Eq.(26) one obtains:

\[
A_l^{(t)} = \left( \sum_p L_{kp}^2 \sin^2 \left( \frac{1}{2} \mathbf{k} - \mathbf{p}, \mathbf{l} \right) \right)^{-1/2}.
\]

As a result of the diagonalisation the triplet wave functions (26) appear to be rather simple:

\[
x^{(1,\alpha)}(\mathbf{k}, \mathbf{p}) = L_{kp} A_l^{(t)}(\mathbf{k}) \sin \left( \frac{1}{2} \mathbf{k} - \mathbf{p}, \mathbf{l} \right)
\]

The singlet pair case is more complicated. Nevertheless one can obtain a linear algebraic system of 4 equations on the coefficients \( A_0^{(s)}(\mathbf{k}), A_l^{(s)}(\mathbf{k}) \) by substituting expression (27) into Eq.(25):

\[
(\hat{\mathbf{1}} - \hat{\mathbf{N}}) \begin{pmatrix} A_0 \\ A_1 \\ A_2 \\ A_3 \end{pmatrix} = 0,
\]

\( 11 \)
where $\hat{M}$ is the matrix of rank 4:

$$
\hat{M} = \begin{pmatrix}
U_{s1}I_0 & U_{s1}I_1 & U_{s1}I_2 & U_{s1}I_3 \\
2U_{s2}I_1 & 2U_{s2}I_{11} & 2U_{s2}I_{12} & 2U_{s2}I_{13} \\
2U_{s2}I_2 & 2U_{s2}I_{21} & 2U_{s2}I_{22} & 2U_{s2}I_{23} \\
2U_{s2}I_3 & 2U_{s2}I_{31} & 2U_{s2}I_{32} & 2U_{s2}I_{33}
\end{pmatrix}
$$

(31)

and

$$
I_0 = \sum_p L_{kp}; \quad I_l = \sum_p L_{kp} \cos(\frac{1}{2}k - p, l);
$$

$$
I_{lm} = \sum_p L_{kp} \cos(\frac{1}{2}k - p, l) \cdot \cos(\frac{1}{2}k - p, m).
$$

The matrix $\hat{M}$ is written for the 3-dimensional system. The same matrix for the 2-dimensional system may be obtained by omitting the last column and the last line. For a 1-dimensional system this simple procedure must be repeated.

The spectra of the singlet states are found by equating the determinant of the system (30) to zero:

$$
\text{Det}(\hat{1} - \hat{M}) = 0,
$$

(32)

whereas the structure coefficients $A_0^{(s)}(k), A_l^{(s)}(k)$ describing the wave function of the singlet pair (27) are found from Eq. (30) and the normalization condition:

$$
\sum_{p,s} x_{0,s}^{(0,0)}(k,p) x_{0,s}^{(0,0')} (k,p) = \delta_{\alpha,\alpha'}.
$$

Now we have to find the excitation spectra of the local pairs by utilizing formulae (28) – (32). The numerical calculations have been done in the units: $D_{pol} = 4$. The results are represented in Fig.1 for the interaction value of $U_{s1} = +8$ (repulsive onsite interaction term); $U_{s2} = -6.8, U_{t2} = -6.5$ (attractive intersite terms for both the singlet and triplet states).

Here the most interesting case is considered: onsite repulsion (Coulomb force predominance) and intersite attraction. The concrete value of onsite repulsion has only a small effect on the character of band structure. The explanation is clear: two coupled fermions are placed on neighbor sites mostly where attraction dominates and "don’t feel" onsite repulsion. On the contrary, the value of the intersite attraction is important for the determination of low-lying bands. This situation has been analyzed in detail in [6]. The authors argued that the gap between the local pair band and the polaron band, that is placed above, increases with the coupling constant when considering onsite attractive Hubbard model. The substitution of the onsite attraction by the intersite one does not affect this qualitative result. Fig.1 represents band structure of the singlet and triplet pairs at definite values of s-wave and p-wave attraction. The choice of
the attraction value $U_{s2} = -6.8$ and $U_{t2} = -6.5$ gives reasonable mass of local pairs.

It becomes evident that the band structure is not as simple as in the standard 1-site attractive Hubbard model. There are additional gaps between the singlet and triplet bands, along with large ordinary gap. Each of the singlet and triplet band in its turn is splitted into two subbands. This could explain those contradictions that seem take place in determination of the gap value from different experiments. A one–particle (polaron) band is lying higher with the energy of its bottom being equal 0.97. It is necessary now to normalize our relative units. An appropriate value of a polaron bandwidth is about 50-100meV. The undimensional polaron bandwidth is equal 4 in the units that were used throughout the paper. It means that our energy unit is about 20meV, The chosen value of the intersite attraction is $136meV(6.8 \cdot 20meV)$, that seems reasonable. The value of the gap between the lowest local pair energy and lowest polaron energy depends strictly on the sort of pairing. Thus, in the case presented in Fig.1, the gapwidth between polaron band and s-pair band is about $20meV(0.97 \cdot 20meV)$

Another interesting conclusion concerns a mass of the local pairs. According to the wide-spread point of view the local pair mass should be large enough this being considered as a shortcoming of local pair theories. Our calculations demonstrate (see Fig.1), that the situation is more favorable: the width of the lowest singlet band is only 3-4 times smaller, than the width of the fermion band. It gives the mass of the local pair $m^{**} \simeq 3 \div 4m^*$, where $m^*$ is the effective fermion mass. One can notice finally, that the triplet pairs appear to be several times heavier than the singlet ones for this set of parameters.

3 Local pairs in external fields

The excitation spectra and the local pair structure studied above may be used for theoretical investigation of thermodynamic and kinetic properties of the systems with the strongly interacting electrons. On the other hand there are many experiments dealing with the interaction of HTSC materials with different external fields. For the theoretical explanation of these experiments one has to know the form of the interaction of the pairs with the external fields. The corresponding vertex functions should be obviously dependent on the internal structure of the coupled state. The interaction of the fermion with the external field presented in Eq.(1) for the Hamiltonian is of rather general form. It includes, for example, the interaction with neutrons and electromagnetic field. By integrating over the grassman variables in the same way as it was done before, one can obtain the action in the form (4), with the matrix $Y$ depending on the
Y_{PP'} = \begin{pmatrix} (r_{PP'} + i\epsilon\delta_{PP'})\delta_{\epsilon\epsilon'} + B(\epsilon - \epsilon')_{PP'} & \psi(\epsilon + \epsilon')_{PP'} \\ \psi^* (\epsilon + \epsilon')_{PP'} & -(r_{PP'} + i\epsilon\delta_{PP'})\delta_{\epsilon\epsilon'} - B(\epsilon - \epsilon')_{PP'} \end{pmatrix}. \tag{33}

In Eq. (33) all matrices are written in the momentum representation and an imaginary "time" Fourier transformation is assumed. Expanding this expression up to the second order in the fields \(\psi, \psi^*\) and to the first order in the (weak) field \(B\), one can obtain the effective action for the local pairs in the external field:

\[ Z = \int DC^* DC \exp S(C^*, C), \]

\[ S(C^*, C) = C_{\sigma}^{(\kappa\alpha s)}(k, E) (iE - \lambda_{\kappa\alpha}(k)) C_{\sigma'}^{(\kappa\alpha)}(k, E) \]

\[ + C_{\sigma}^{(\kappa\alpha s)}(k, E) \Gamma_{s\sigma}^{(\kappa\alpha', \kappa\alpha')}(k, E, k', E') C_{\sigma'}^{(\kappa\alpha')}(k', E'). \]

Here the summation on the repeated indices is assumed. Eq. (14) and the orthonormal basis (13) were used in the derivation of this equation. The vertex \(\Gamma\) has the form:

\[ \Gamma_{s\sigma}^{(\kappa\alpha', \kappa\alpha'}(k, E, k', E') = 2 \sum_s B_{\sigma' - s, \sigma - s}(k - k', E - E') F_{\sigma s}^{(\kappa\alpha, \kappa\alpha')}(k - k'). \tag{34} \]

Here the formfactor depends only on the structure of the coupled state. The external field is written in the more convenient form – with the spin index extracted and translational invariance taken into account: \(B_{PP'}(E) \equiv B_{s, s'}(p - p', E).\) As it was mentioned above, the vertex of the interaction of pairs with the external field depends on the frequency, the wave vector of the external field and the wave functions of the fermion pairs. One can see that the slowly varying field is not sensitive to the pair structure. A simple test shows that in this case the vertex of the singlet local pair interaction with the external field equals to zero. For the triplet pairs it is twice the interaction of the fermion with the field. The behavior of formfactor (35) plays a significant role in the theoretical explanation of experiments on the scattering of particles on the local pairs. For example, at low temperatures and small transferred momenta the transitions appear to be suppressed. The reason is quite obvious: at the low temperature the local pairs being bosons are condensed at the lowest level with the momenta \(k = 0\). The transitions into the
upper bands with approximately the same momentum are suppressed due to the orthogonality of the wave functions with different energies: \( F(k - k' = 0) = 0 \).

The typical formfactors of the transitions from the lowest singlet band to the upper singlet or triplet one are presented in Fig.2. There is also the formfactor describing the transitions inside the lowest singlet band. The transitions into the second triplet band are forbidden for chosen transferred momenta \( k = (k_x, 0) \) due to the orthogonality of the wave functions. The evident momentum dependence of the formfactor confirms its importance in the interpretation of experiments.

4 Conclusion

The mathematics of the local pair theory was developed. The ad hoc calculation of band structure of the local pairs and their interaction with external fields are presented here. It is shown that numerical calculations based on analytical formulas and being relatively simple lead to exact qualitative predictions. The method can be easily generalized. The momentum dependency of the vertex is essential for theoretical explanation of experiments.

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