New "entangled" superfluid state

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We introduce a new fermionic variational wavefunction, suitable for interacting multi-species systems and sustaining superfluidity. In this frame, we also introduce a novel way for the treatment of entanglement via a new quantum index, which is related to the internal symmetry of the quantum state. This index is "ghostly", i.e. it appears only within the quantum state, but it does not appear in any observable quantity. Applications include quark matter, nuclei, neutron stars and the high temperature superconductors. Spin up and down fermions are, in principle, inequivalent. A wider class of Hamiltonians than sheer Bardeen-Cooper-Schrieffer (BCS) type, comprising interaction and hybridization between different fermion species, can be treated "exactly", as in the well known manner of BCS theory. We present the finite temperature version of the theory, and we discuss the appearance of charge and spin density wave order.

The Bardeen-Cooper-Schrieffer (BCS) wavefunction \[ |\Psi_{\text{BCS}}\rangle = \prod_{k} (u_k + v_k c_{k,\downarrow}^\dagger c_{k,\uparrow}^\dagger) |0\rangle \] has set a paradigm for the description of fermionic superfluids. The creation/annihilation operators \( c_{k,\sigma}^\dagger / c_{k,\sigma} \) describe fermions with momentum \( k \) and spin \( \sigma \), and \( |0\rangle \) is the vacuum state.

We are interested in a wavefunction for fermionic systems with two or more different species of spinful fermions, which can perform a task similar to what \( |\Psi_{\text{BCS}}\rangle \) can do.

Let the usual fermionic operators be \( c_{x,\mu} \) with \( x = \{i, k, \sigma\} \), where \( i \) denotes the fermion species/flavor.

We introduce a new quantum index, which is related to the internal symmetry of the quantum state. It serves to enumerate the "entangled" components of the quantum state as a function of both momentum and spin. Thereby we introduce the new fermionic operators \( c_{x,\mu,\delta}^\dagger / c_{x,\mu,\delta} \) obeying the anticommutators \( \{a, b\} = ab + ba \)

\[
\{c_{x,\mu,\nu}, c_{y,\nu',\delta}\} = 0 \quad , \quad \{c_{x,\mu,\nu}, c_{y,\delta,\nu'}\} = \delta_{x,y} \delta_{\mu,\nu} .
\]

Then, we write the usual \( c_{x}^\dagger / c_{x} \) as the superposition

\[
c_{x}^\dagger = \frac{1}{\sqrt{N_o}} \sum_{\delta=1}^{N_o} c_{x,\delta}^\dagger , \quad c_{x} = \frac{1}{\sqrt{N_o}} \sum_{\delta=1}^{N_o} c_{x,\delta} .
\]

The usual anticommutation relations of \( c_{x}^\dagger / c_{x} \) are preserved, while

\[
\{c_{x}, c_{y,\nu,\delta}\} = 0 \quad , \quad \{c_{x}, c_{y,\delta,\nu'}\} = \frac{\delta_{x,y}}{\sqrt{N_o}} .
\]

We also introduce

\[
A_{i,k,\delta}^\dagger = u_{i,k} c_{i,k,\uparrow,\delta}^\dagger c_{i,-k,\downarrow,\delta}^\dagger + s_{i,k,\uparrow} c_{i,k,\uparrow,\delta}^\dagger s_{i,-k,\downarrow} c_{i,-k,\downarrow,\delta}^\dagger + s_{i,k,\downarrow} c_{i,k,\downarrow,\delta}^\dagger s_{i,-k,\uparrow} c_{i,-k,\uparrow,\delta}^\dagger .
\]

\( A_{i,k,\delta}^\dagger \) is a bosonic operator, creating spin singlet pairs of fermions (for triplet pairs c.f. eq. (60) below), and \( (i,j) = \{(1,2), (2,1)\} \).

We form the following multiplet of \( A_{i,k,\delta}^\dagger \)'s

\[
M_{k}^\dagger = A_{1,k,\delta=1}^\dagger A_{1,-k,\delta=2}^\dagger A_{2,k,\delta=3}^\dagger A_{2,-k,\delta=4}^\dagger .
\]

This multiplet creates all states with momenta \( \pm k \), so we take \( N_o = 4 \), as \( N_o \) such states exist (cf. also after eq. (60) below).

The new index allows for the bookkeeping of a superposition of states of a given particle, i.e. same \( x = \{i, k, \sigma\} \), without the difficulties due to entanglement within the multiplet \( M_{k}^\dagger \); if the index were removed. In that case, the treatment of the coherence factors \( u_k, v_k, s_k \) is prohibitively complicated.
This index is "ghostly", i.e. it appears only within the state $|\Psi\rangle$ below. It does not appear in any observable quantity! (C.f. the Faddeev-Popov ghosts in gauge field theories, where the ghosts disappear from the final physical outcome.) We note that there is no change whatsoever implied in the Hamiltonian or in the representation of any observable.

Now we introduce the "entangled" state

$$|\Psi\rangle = \prod_{k'} M^\dagger_{k'} |0\rangle ,$$

where the prime implies that $k$ runs over half the momentum space. Note that all $A^\dagger_{i,k,\delta}$'s in $|\Psi\rangle$ commute with each other.

$|\Psi\rangle$ generalizes $|\Psi_{BCS}\rangle$ and sustains superfluidity. This wavefunction makes sense for two or more fermion species, with an interaction between different species. It can obviously be generalized for three or more fermion species. Moreover, a similar wavefunction using the new quantum index can be written in the real space representation instead of the momentum space one. At the moment, it is not possible to say how close $|\Psi\rangle$ is to experimental reality. It does represent a very promising avenue though, as can be seen from the discussion which follows.

$|\Psi\rangle$ is, in principle, relevant for the description of systems such as quark matter [2], nuclei [3, 4], superconducting grains [5], cold atoms [6, 7], graphene [8], high-temperature superconductors, i.e. both copper oxides [9, 10] and iron pnictides [11], and neutron stars [4]. It allows for inequivalence between spin up and down fermions. Plus, it allows for the "exact" variational treatment of a wider class of Hamiltonians than sheer BCS type, e.g. comprising interaction and hybridization between different fermion species, in the well known manner of the BCS-Gorkov theory [1, 12].

The normalization $\langle \Psi | \Psi \rangle = 1$ and the choice of real $v_{i,k}, v_{i,k}, s_{i,k,\uparrow}, s_{i,k,\downarrow}$ imply

$$v_{i,k}^2 + v_{i,k}^2 + s_{i,k,\uparrow}^2 + s_{i,k,\downarrow}^2 = 1 , \quad 0 \leq v_{i,k}^2, v_{i,k}^2, s_{i,k,\uparrow}, s_{i,k,\downarrow} \leq 1 ,$$

thus allowing to treat these coherence factors as $u_{i,k} = \cos(\theta_{i,k}) \cos(\phi_{i,k})$, $v_{i,k} = \sin(\theta_{i,k}) \cos(\phi_{i,k})$, $s_{i,k,\uparrow} = \cos(\delta_{i,k}) \sin(\phi_{i,k})$, $s_{i,k,\downarrow} = \sin(\delta_{i,k}) \sin(\phi_{i,k})$.

Two fermion species at zero temperature. Calculations are straightforward. E.g. for 2 fermion species with dispersions $\epsilon_{i,k,\sigma} = \epsilon_{i,-k,\sigma}$ we have

$$\sqrt{N_o} \ c_{1,k,\uparrow} M^\dagger_{k} |0\rangle = (v_{1,k} c_{1,-k,\downarrow,\delta=1}^\dagger + s_{1,k,\uparrow} c_{1,-k,\downarrow,\delta=1}^\dagger) A^\dagger_{1,-k,\delta=2} A_{2,k,\delta=3} A^\dagger_{2,-k,\delta=4} |0\rangle$$

$$- s_{2,k,\downarrow} c_{2,-k,\downarrow,\delta=3} A^\dagger_{1,k,\delta=1} A_{1,-k,\delta=2} A^\dagger_{2,-k,\delta=4} |0\rangle .$$

Then

$$\langle 0 | M_k c_{1,k,\uparrow}^\dagger c_{1,k,\uparrow} M_k^\dagger |0\rangle = \frac{1}{N_o} (v_{1,k}^2 + s_{1,k,\uparrow}^2 + s_{2,k,\downarrow}^2) .$$

Also,

$$\sqrt{N_o} \ c_{2,k,\uparrow} M^\dagger_{k} |0\rangle = (v_{2,k} c_{2,-k,\downarrow,\delta=3} + s_{2,k,\uparrow} c_{2,-k,\downarrow,\delta=3}) A^\dagger_{1,k,\delta=1} A_{1,-k,\delta=2} A^\dagger_{2,-k,\delta=4} |0\rangle$$

$$- s_{1,k,\downarrow} c_{1,-k,\downarrow,\delta=1} A^\dagger_{1,k,\delta=3} A_{2,k,\delta=3} A^\dagger_{2,-k,\delta=4} |0\rangle ,$$

which yields

$$\langle 0 | M_k c_{2,k,\uparrow}^\dagger c_{1,k,\downarrow} M_k^\dagger |0\rangle = - \frac{1}{N_o} (v_{1,k} s_{1,k,\downarrow} + v_{2,k} s_{2,k,\uparrow}) .$$

Moreover,

$$N_o c_{2,-k,\downarrow} c_{1,k,\uparrow} M_k^\dagger |0\rangle = s_{1,k,\uparrow} A^\dagger_{1,-k,\delta=2} A_{2,k,\delta=3} A^\dagger_{2,-k,\delta=4} |0\rangle - s_{2,k,\downarrow} A_{1,k,\delta=1} A^\dagger_{1,-k,\delta=2} A^\dagger_{2,-k,\delta=4} |0\rangle ,$$

and

$$\langle 0 | M_k c_{2,-k,\downarrow} c_{1,k,\uparrow} M_k^\dagger |0\rangle = \frac{1}{N_o} (u_{1,k} s_{1,k,\uparrow} - u_{2,k} s_{2,k,\uparrow}) .$$
Using the commutativity of $A_i^{+k,\delta}$’s and generalizing the previous equations, we obtain ($\langle H \rangle = \langle \Psi | H | \Psi \rangle$)

$$n_{i,k,\sigma} = \langle c^+_{i,k,\sigma} c_{i,k,\sigma} \rangle = \frac{1}{N_o} \left( v_{i,k}^2 + s_{i,k,\sigma}^2 + s_{j,k,-\sigma}^2 \right), \quad (i,j) = (1,2), (2,1), \quad (14)$$

$$z_{k,\sigma} = \langle c^+_{i,k,\sigma} c_{j,k,\sigma} \rangle = -\frac{\text{sgn}(\sigma)}{N_o} \left( v_{1,k} s_{1,k,-\sigma} + v_{2,k} s_{2,k,-\sigma} \right), \quad (15)$$

$$g_{k,\sigma} = \langle c_{2,-k,-\sigma} c_{1,k,\sigma} \rangle = \frac{1}{N_o} \left( u_{1,k} s_{1,k,\sigma} - u_{2,k} s_{2,k,-\sigma} \right). \quad (16)$$

The general Hamiltonian for two fermion species interacting via intra-species potentials $V_{1,2}$ and via an inter-species potential $F_q$, and hybridizing via $h_k$, is

$$H = \sum_{i,k,\sigma} \xi_{i,k,\sigma} n_{i,k,\sigma} + \sum_{k,\sigma} h_k \left( c^+_{1,k,\sigma} c_{2,k,\sigma} + c^+_{2,k,\sigma} c_{1,k,\sigma} \right) \quad (17)$$

$$+ \frac{1}{2} \sum_{i,k,p,q,\sigma_\sigma'} V_{i,q} c^+_{i,k+q,\sigma'} c^+_{i,p-q,\sigma'} c_{i,p,\sigma} c_{i,k,\sigma} + \sum_{k,p,q,\sigma_\sigma'} F_{i,k,p} c^+_{i,k,\sigma} c^+_{i,p,\sigma} c_{i,p,\sigma} c_{i,k,\sigma},$$

with $i = 1,2$, $\xi_{i,k,\sigma} = \epsilon_{i,k,\sigma} - \mu_{i,\sigma}$ and $\mu_{i,\sigma}$ the chemical potential. Note that the usual BCS pairing potential is just the sub-term $\sum_{i,k,p} V_{i,k-p} c^+_{i,k,\sigma} c_{i,k+q,\sigma}$ of the single species potential.

Considering $\Psi$ above, we have for $\langle H \rangle = \langle \Psi | H | \Psi \rangle$, $a_o = 1/N_o$

$$\langle H \rangle = \sum_{i,k,\sigma} \xi_{i,k,\sigma} n_{i,k,\sigma} + \sum_{i,k,p,\sigma} h_k z_{k,\sigma} n_{i,k,\sigma} - \frac{1}{2} \sum_{i,k,p,\sigma} V_{i,k-p} n_{i,k,\sigma} n_{i,p,\sigma} + \frac{1}{2} \sum_{i,k,p,\sigma} V_{i,q=0} n_{i,k,\sigma} n_{i,p,\sigma} \quad (18)$$

$$+ a_o ^2 \sum_{i,k,p} V_{i,k-p} u_{i,k} v_{i,k} u_{i,p} v_{i,p} - \sum_{k,p,\sigma} F_{k-p} z_{k,\sigma} z_{p,\sigma} + F_{q=0} \sum_{k,p,\sigma} n_{i,k,\sigma} n_{i,p,\sigma} - \sum_{k,p,\sigma} F_{k-p} g_{k,\sigma} g_{p,\sigma},$$

with $(i,j) = \{(1,2), (2,1)\}$. The first term in the second line is exactly the usual BCS pairing term, and the last term is the equivalent inter-species pairing term due to $F_q$. Then, considering the up and down spins as equivalent, we minimize $\langle H \rangle$ with respect to the angles $\theta_{i,k}$ and $\phi_{i,k}$ respectively, obtaining

$$0 = 2U_{i,k} \sum_{\sigma} \xi_{i,k,\sigma} - \sum_{\sigma} h_k Z_{i,k,\sigma} + U_{i,k} \sum_{p,\sigma} \left\{ V_{i,q=0} - V_{i,k-p} \right\} n_{i,p,\sigma} + 2\Delta^0_{i,k} (v_{i,k}^2 - u_{i,k}^2) \quad (19)$$

$$+ 2F_{q=0} U_{i,k} \sum_{p,\sigma} n_{i,p,\sigma} + 2 \sum_{p,\sigma} F_{k-p} Z_{i,k,\sigma} z_{p,\sigma} - 2a_o \sum_{p,\sigma} F_{k-p} v_{i,k} \sum_{p,\sigma} F_{k-p} s_{i,k,\sigma} (u_{i,p} s_{i,p,\sigma} - u_{j,p} s_{j,p,-\sigma});$$

and

$$0 = 2W_{i,k} \sum_{\sigma} \xi_{i,k,\sigma} - \sum_{\sigma} h_k Y_{i,k,\sigma} + W_{i,k} \sum_{p,\sigma} \left\{ V_{i,q=0} - V_{i,k-p} \right\} n_{i,p,\sigma} + \Delta^0_{i,k} \sin(2\theta_{i,k}) \sin(2\phi_{i,k}) \quad (20)$$

$$+ 2F_{q=0} W_{i,k} \sum_{p,\sigma} n_{i,p,\sigma} + 2 \sum_{p,\sigma} F_{k-p} Y_{i,k,\sigma} z_{p,\sigma} + 2a_o \cos(\theta_{i,k}) \frac{\cos^2(\phi_{i,k})}{\sin(\phi_{i,k})} \sum_{p,\sigma} F_{k-p} s_{i,k,\sigma} (u_{i,p} s_{i,p,\sigma} - u_{j,p} s_{j,p,-\sigma});$$

with

$$U_{i,k} = u_{i,k} v_{i,k}, \quad Z_{i,k,\sigma} = \text{sgn}(\sigma) u_{i,k} s_{i,k,-\sigma}, \quad \Delta^0_{i,k} = -a_o \sum_{p} V_{i,k-p} u_{i,p} v_{i,p},$$

$$W_{i,k} = \frac{\sin(2\phi_{i,k})}{4} \left\{ 1 - 2\sin^2(\theta_{i,k}) \right\}, \quad Y_{i,k,\sigma} = \text{sgn}(\sigma) \cos(\theta_{i,k}) \frac{\cos^2(\phi_{i,k})}{\sin(\phi_{i,k})} s_{i,k,\sigma},$$

and $(i,j) = \{(1,2), (2,1)\}$. $\Delta^0_{i,k}$ is the usual BCS gap. Equations $19-21$ can be solved numerically (this will appear elsewhere). For the number operator $n_{i,p,\sigma} = c_{i,p,\sigma}^+ c_{i,p,\sigma}$, $i \partial_\tau n_{i,p,\sigma} = [n_{i,p,\sigma}, H] = h_p (c_{i,p,\sigma}^+ c_{j,p,\sigma} + c_{j,p,\sigma}^+ c_{i,p,\sigma})$, and $\langle \partial_\tau n_{i,p,\sigma} \rangle = 0$.

Our approach is much more general and complete than the works of Moskalenko [13] and of Suhl, Matthias, and Walker [14], which can treat strictly BCS-type inter-species and intra-species interactions only.
The finite temperature dependence of the theory can be derived through the equations of motion formalism for the Green’s functions \[ (\partial_\tau c_i(\tau) = [H, c_i(\tau)]) \] . We consider the Green’s functions
\[
G_{i,\sigma}(p, \tau - \tau') = \langle T_{\tau} c_{i,p,\sigma}(\tau) c_{i,p,\sigma}^\dagger(\tau') \rangle ,
\]
\[
G_{I,j,\sigma}(p, \tau - \tau') = \langle T_{\tau} c_{I,j,p,\sigma}(\tau) c_{I,j,p,\sigma}^\dagger(\tau') \rangle ,
\]
\[
F_{I,i,\sigma}(p, \tau - \tau') = \langle T_{\tau} c_{I,i,p,\sigma}(\tau) c_{I,j,-p,\sigma}(\tau') \rangle ,
\]
\[
F_{I,I,j,\sigma}(p, \tau - \tau') = \langle T_{\tau} c_{I,I,j,p,\sigma}(\tau) c_{I,j,-p,\sigma}(\tau') \rangle ,
\]
with \((i, j) = \{(1, 2), (2, 1)\} \) and \(T_\tau\) denoting imaginary time ordering. We obtain the exact coupled equations
\[
\delta(\tau - \tau') = - (\partial_\tau + \xi_{i,p,\sigma} G_{i,i,\sigma}(p, \tau - \tau') + \sum_{k,q,\sigma'} V_{i,q} (T_{\tau} c_{i,k,q,\sigma'}(\tau) c_{i,k,\sigma'}(\tau) c_{i,p,\sigma}(\tau) c_{i,p,\sigma}(\tau')) ,
\]
\[
- h_p G_{j,i,\sigma}(p, \tau - \tau') + \sum_{k,q,\sigma'} V_{i,q} (T_{\tau} c_{i,k,q,\sigma'}(\tau) c_{j,k,\sigma'}(\tau) c_{i,p,\sigma}(\tau) c_{i,p,\sigma}(\tau')) ,
\]
\[
0 = (\partial_\tau + \xi_{j,p,\sigma} F_{j,i,\sigma}(p, \tau - \tau') + \sum_{k,q,\sigma'} V_{j,q} (T_{\tau} c_{j,k,q,\sigma'}(\tau) c_{j,k,\sigma'}(\tau) c_{j,p,\sigma}(\tau) c_{j,p,\sigma}(\tau')) ,
\]
\[
+ h_p F_{j,i,\sigma}(p, \tau - \tau') + \sum_{k,q,\sigma'} V_{j,q} (T_{\tau} c_{j,k,q,\sigma'}(\tau) c_{j,k,\sigma'}(\tau) c_{j,p,\sigma}(\tau) c_{j,p,\sigma}(\tau')) ,
\]
\[
0 = (\partial_\tau + \xi_{j,p,\sigma} F_{j,i,\sigma}(p, \tau - \tau') + \sum_{k,q,\sigma'} V_{j,q} (T_{\tau} c_{j,k,q,\sigma'}(\tau) c_{j,k,\sigma'}(\tau) c_{j,p,\sigma}(\tau) c_{j,p,\sigma}(\tau')) ,
\]
\[
- h_p F_{i,i,\sigma}(p, \tau - \tau') + \sum_{k,q,\sigma'} V_{j,q} (T_{\tau} c_{i,k,q,\sigma'}(\tau) c_{i,k,\sigma'}(\tau) c_{j,p,\sigma}(\tau) c_{j,p,\sigma}(\tau')) ,
\]
\[
0 = (\partial_\tau + \xi_{j,p,\sigma} F_{j,i,\sigma}(p, \tau - \tau') + \sum_{k,q,\sigma'} V_{j,q} (T_{\tau} c_{j,k,q,\sigma'}(\tau) c_{j,k,\sigma'}(\tau) c_{j,p,\sigma}(\tau) c_{j,p,\sigma}(\tau')) ,
\]
\[
+ h_p F_{j,i,\sigma}(p, \tau - \tau') + \sum_{k,q,\sigma'} V_{j,q} (T_{\tau} c_{j,k,q,\sigma'}(\tau) c_{j,k,\sigma'}(\tau) c_{j,p,\sigma}(\tau) c_{j,p,\sigma}(\tau')) .
\]
Within the Hartree-Fock-Bogoliubov approximation \( \langle c_i c_j c_k c_m \rangle = \langle c_i c_j \rangle \langle c_k c_m \rangle - \langle c_i c_j \rangle \langle c_k c_m \rangle - \langle c_i c_k \rangle \langle c_j c_m \rangle \), and after Fourier transforming with respect to \( \tau \), we obtain the following system of equations at finite temperature \( T \)
\[
1 = (i \epsilon_n - \xi_{1,k,\sigma}) G_{1,\sigma}(k, \epsilon_n) + A_1 G_{1,\sigma}(k, \epsilon_n) + B_1 F_{1,\sigma}(k, \epsilon_n) + C_1 G_{2,\sigma}(k, \epsilon_n) + D_1 F_{1,\sigma}(k, \epsilon_n) ,
\]
\[
0 = (i \epsilon_n + \xi_{1,k,\sigma}) F_{1,\sigma}(k, \epsilon_n) + A_2 G_{1,-\sigma}(k, \epsilon_n) + B_2 F_{1,-\sigma}(k, \epsilon_n) + C_2 G_{2,\sigma}(k, \epsilon_n) + D_2 F_{1,\sigma}(k, \epsilon_n) ,
\]
\[
0 = (i \epsilon_n + \xi_{2,k,\sigma}) G_{2,\sigma}(k, \epsilon_n) + A_3 G_{1,\sigma}(k, \epsilon_n) + B_3 F_{2,\sigma}(k, \epsilon_n) + C_3 G_{2,\sigma}(k, \epsilon_n) + D_3 F_{2,\sigma}(k, \epsilon_n) ,
\]
\[
0 = (i \epsilon_n + \xi_{2,k,\sigma}) F_{2,\sigma}(k, \epsilon_n) + A_4 G_{1,\sigma}(k, \epsilon_n) + B_4 F_{1,\sigma}(k, \epsilon_n) + C_4 G_{2,\sigma}(k, \epsilon_n) + D_4 F_{2,\sigma}(k, \epsilon_n) ,
\]
and also the equivalent set with the indices 1 and 2 interchanged. The Matsubara energies are \( \epsilon_n = (2n + 1)\pi T \), and we suppressed the labels \((k, \sigma)\) from \( A_m, B_m, C_m, D_m, m = 1 - 4 \). Here
\[
A_1 = \sum_{p,q,\sigma'} V_{1,q} \{ - \delta_{q,0} \langle c_{1,p,\sigma}^\dagger c_{1,p,\sigma} \rangle + \delta_{\sigma,\sigma'} \delta_{k,p} \langle c_{1,k,q,\sigma}^\dagger c_{1,-k,q,\sigma} \rangle \} - F_{q=0} \sum_{p,\sigma'} \langle c_{2,p,\sigma}^\dagger c_{2,p,\sigma} \rangle ,
\]
\[
B_1 = - \sum_{q} V_{1,q} \langle c_{1,-k,q,-\sigma} c_{1,k,q,-\sigma} \rangle ,
\]
\[
C_1 = - h_k + \sum_{q} F_{q} \langle c_{1,k,-q,-\sigma} c_{2,k,-q,-\sigma} \rangle ,
\]
\[
D_1 = \sum_{q} F_{q} \langle c_{2,k,q,-\sigma} c_{1,k,-q,-\sigma} \rangle ,
\]
\[
A_2 = B_1^\dagger ,
\]
\[
B_2 = - A_1 ,
\]
\[
C_2 = - F_{q=0} \langle c_{1,k,-q,k,-\sigma} \rangle ,
\]
\[
D_2 = h_k + \sum_{q} F_{q} \langle c_{2,k,q,\sigma} c_{1,k,q,\sigma} \rangle ,
\]
\[
A_3 = - D_2 ,
\]
\[
B_3 = \sum_{q} F_{q} \langle c_{1,k,q,-\sigma} c_{2,k,q,-\sigma} \rangle ,
\]
\[
C_3 = \sum_{q} V_{2,q} \{ - \delta_{q,0} \langle c_{2,p,\sigma}^\dagger c_{2,p,\sigma} \rangle + \delta_{\sigma,\sigma'} \delta_{k,p} \langle c_{2,k,q,\sigma}^\dagger c_{2,k,-q,\sigma} \rangle \} - F_{q=0} \sum_{p,\sigma'} \langle c_{2,p,\sigma}^\dagger c_{1,p,\sigma} \rangle ,
\]
\[
A_4 = - F_{q=0} \langle c_{2,k,\sigma}^\dagger c_{1,k,-\sigma} \rangle ,
\]
\[
B_4 = C_1 ,
\]
\[
C_4 = D_3^\dagger ,
\]
\[
D_4 = C_3 .
\]
Also, for $\xi_{i,k,\sigma} = \xi_{i,k,\sigma}$, $B_3 = -D_1$ and $A_4 = -C_2$.
We have
\begin{align}
A_1 &= \sum_{p,q,\sigma'} V_{1,q} \left\{ -\delta_{q,0} n_{1,p,\sigma} + \delta_{\sigma,\sigma'} \delta_{k,p} n_{2,k-q,\sigma} \right\} - F_{q=0} \sum_{p,\sigma'} n_{1,p,\sigma'}, \\
B_1 &= -a_0 \sum_q V_{1,q} u_{1,k-q} v_{1,k-q} = \Delta_{1,k}^0, \\
C_1 &= -h_k + a_0 \sum_q F_q \left\{ v_{1,k-q} s_{1,k-q,-\sigma} + v_{2,k-q} \left[ s_{1,k-q,\sigma} + s_{2,k-q,-\sigma} \right] \right\}, \\
D_1 &= \sum_q F_q g_{k-q,\sigma}, \quad C_2 = F_{q=0} g_{k,\sigma}, \quad D_2 = 2h_k + C_1, \\
C_3 &= \sum_{p,q,\sigma'} V_{2,q} \left\{ \delta_{q,0} n_{2,p,\sigma} - \delta_{\sigma,\sigma'} \delta_{k,p} n_{1,k-q,\sigma} \right\} + F_{q=0} \sum_{p,\sigma'} n_{1,p,\sigma'}, \\
D_3 &= a_0 \sum_q V_{2,q} u_{2,k-q} v_{2,k-q} = -\Delta_{2,k}^0.
\end{align}

We solve these equations for the case of equivalent up and down spin $\xi_{i,k,\sigma} = \xi_{i,k,\sigma} = \xi_{i,k}$ for both fermion species.

\begin{align}
G_1(k, i\epsilon_n) &= \frac{Z_1(k, i\epsilon_n)}{D(k, i\epsilon_n)}, \quad F_1^\dagger(k, i\epsilon_n) = \frac{X_1(k, i\epsilon_n)}{D(k, i\epsilon_n)}, \quad G_21(k, i\epsilon_n) = \frac{Z_{21}(k, i\epsilon_n)}{D(k, i\epsilon_n)}, \quad F_{12}^\dagger(k, i\epsilon_n) = \frac{X_{12}(k, i\epsilon_n)}{D(k, i\epsilon_n)},
\end{align}

and likewise for $G_2(k, i\epsilon_n), F_2^\dagger(k, i\epsilon_n), G_{12}(k, i\epsilon_n)$ and $F_{21}^\dagger(k, i\epsilon_n)$. Here
\begin{align}
Z_1 &= -i\epsilon_n^2 - \epsilon_n^2 \left\{ (1 - A_1) + i\epsilon_n \left\{ D_3^2 - C_3^2 - C_3 A_2 - C_2 A_1 - C_2 \left( 2C_3 + \xi_{2,k} \right) \right\} + A_1 [C_2^3 - D_3^2 + \xi_{2,k} (2C_3 + \xi_{2,k})] \right\}
- C_2 \left\{ D_3^2 - C_2 A_1 - C_2 \left( 2C_3 + \xi_{2,k} \right) \right\}, \\
X_1 &= -B_1 \epsilon_n^2 + 2i\epsilon_n C_2 D_2 + D_3 (C_2^2 - D_2^2) + B_1 [D_3^2 - C_3^2 - \xi_{2,k} (2C_3 + \xi_{2,k})], \\
X_{12} &= \epsilon_n C_3 + i\epsilon_n \left\{ A_1 C_2 - B_1 C_1 + C_2 (C_3 + \xi_{2,k} - \xi_{1,k}) \right\} + D_1 (B_1 D_1 - A_1 D_2) + (C_3 + \xi_{2,k}) (B_1 C_1 - A_1 C_2) + C_2 (C_2 D_1 - C_1 D_2 + \xi_{1,k} \xi_{2,k} + \xi_{1,k} D_2 D_3.
\end{align}

The denominator is
\begin{equation}
D(k, \epsilon) = \epsilon^4 + Q \epsilon^2 + S \epsilon + Y,
\end{equation}

with $Q = B_1^2 - A_1^2 - 2C_1 D_2 - 2C_2 D_1 - C_3^2 + D_2^2 + \xi_{1,k} (2A_1 - \xi_{1,k}) - \xi_{2,k} (2C_3 + \xi_{2,k})$, $S = 2B_1 (C_2 D_2 - C_1 D_1) + 2D_3 (D_1 D_2 - C_1 C_2)$, and $Y = [(\xi_{1,k} - A_1)^2 - B_1^2]/(\xi_{2,k} + C_3)^2 - D_3^2 + (C_1 D_2 - C_2 D_1)^2 + 2(C_1 D_2 - C_2 D_1) (A_1 - \xi_{1,k}) (\xi_{2,k} + C_3)$.

Then $D(k, E_k) = 0$ yields four solutions for the quasiparticle energies $E_k$. Setting $K = 27S^2 - 72YQ + 2Q^3, L = 12Y + Q^2, N = K - \sqrt{K^2 - 4L^3}$ and $W = \{ -2Q + L(2/N)^{1/3} + (N/2)^{1/3} \}/3$ we have
\begin{align}
E_{(1,2),k} &= \pm 1 \sqrt{W} \pm 1 \sqrt{-W - 2Q - 2S/\sqrt{W}}, \quad E_{(3,4),k} = -\pm 1 \sqrt{W} \pm 1 \sqrt{-W - 2Q + 2S/\sqrt{W}}.
\end{align}

For $V_1, V_2 \to 0$
\begin{align}
E_{1,k} &= -E_{4,k} + O(V_1, V_2)^2, \quad E_{2,k} = -E_{3,k} + O(V_1, V_2).
\end{align}
They depend implicitly on the temperature $T$ through the factors $u_{i,k}(T), v_{i,k}(T), s_{i,k,\sigma}(T)$. The latter can be calculated by noting that

$$G_{i,\sigma}(k, \tau = 0) = \langle c_{i,k,\sigma}^\dagger c_{i,k,\sigma} \rangle = T \sum_{\epsilon_n} G_{i,\sigma}(k, \epsilon_n) ,$$

(54)

$$F_{i,\sigma}^+(k, \tau = 0) = \langle c_{i,k,\sigma}^\dagger c_{i,-k,-\sigma} \rangle = T \sum_{\epsilon_n} F_{i,\sigma}^+(k, \epsilon_n) ,$$

(55)

and through the use of eqs. (10). For $T \leq T_c$, the critical temperature, $F_{i,\sigma}^+(k)$ become non-zero.

The superconducting gap in a physical system is probed through various experimental techniques, and it is usually extracted from a fitting procedure to some specific theoretical models, including purely phenomenological ones. E.g. for the high temperature superconductors these techniques include angle-resolved photoemission (ARPES), tunneling, NMR, Raman scattering etc. As far as the BCS theory is concerned, things are pretty straightforward. In our theory, one needs to calculate the precise spectral response in terms of the microscopic parameters of $\Psi$ for any "gap"-probing experiment, and fit appropriately the data [16].

**Charge and spin density wave (CDW/SDW) order** can appear in a natural manner, via a simple extension of $\Psi$. Namely, by allowing the total momentum of pairs to be finite, which is expected to be favored by the finite interspecies potential $F_q$.

For example, we may consider

$$A_{i,k,\delta} = u_{i,k} + v_{i,k} c_{i,k,\delta}^\dagger c_{i,k,\delta} + v_{i,k} P(k)^{\uparrow} c_{i,k,\delta}^\dagger P(k)^{\downarrow} + v_{i,-k,-P(k)^{\downarrow}} c_{i,-k,\delta}^\dagger C_{i,-k,\delta} + v_{i,-k,-P(k)^{\uparrow}} c_{i,-k,\delta}^\dagger C_{i,-k,\delta}$$

(56)

$$+ s_{i,k,\delta} c_{j,-k,-\delta}^\dagger s_{i,k,\delta} c_{j,-k,-\delta} + s_{i,k,\delta} c_{j,-k,-\delta}^\dagger s_{i,k,\delta} c_{j,-k,-\delta} + s_{i,k,\delta} c_{j,-k,-\delta}^\dagger s_{i,k,\delta} c_{j,-k,-\delta}$$

just for a finite set of momenta $k = \pm k_1, \pm k_2, \ldots, \pm k_N$. $k_i$ in this set is correlated with some other $k_j = P(k_i)$, and $k_i = P(k_i)$, $(i,j=1-N)$, and so are their opposite momenta $-k_i$ and $-k_j$. To fix the ideas further, considering a 2-D system with tetragonal symmetry $C_4$, we may take $N=4$, and the correlated pairs as $(k_1, k_2), (k_3, k_4)$ and $(-k_1, -k_2), (-k_3, -k_4)$. In this case $N_0 = 8 (= 4 + 4)$. In principle, the new index could be a continuous variable, instead of an integer, if a continuous range of momenta would be correlated with a given $k$. This seems to be the actual physical case. We might consider in addition the correlations $(k_1, -k_2), (-k_1, k_2), (k_3, -k_4), (-k_3, k_4)$ etc.

For a pair of such correlated momenta $(k, p)$ we obtain

$$\langle c_{i,-k,\sigma}^\dagger c_{i,p,\sigma} \rangle = \frac{1}{N_0} \left\{ - \text{sgn}(\sigma) [v_{i,k} s_{i,k,p,\sigma} + v_{i,p} s_{i,p,k,\sigma} + v_{i,k} v_{i,k,p,\sigma} + v_{i,p} v_{i,p,k,\sigma}] + s_{j,k,p,\sigma} s_{j,k,-\sigma} + s_{j,p,k,\sigma} s_{j,p,-\sigma} \right\} ,$$

(57)

$$\langle c_{i,-k,\sigma}^\dagger c_{j,p,\sigma} \rangle = \frac{1}{N_0} \left\{ - 2 \text{sgn}(\sigma) [v_{i,k} s_{i,k,p,\sigma} + v_{i,p} s_{j,p,k,\sigma}] + s_{j,k,-\sigma} v_{j,k,p,\sigma} + s_{j,p,-\sigma} v_{i,p,k,\sigma} \right\} ,$$

(58)

$$\langle c_{i,-k,\sigma}^\dagger c_{j,-p,\sigma} \rangle = \langle c_{i,-k,\sigma}^\dagger c_{j,-p,\sigma} \rangle = 0 .$$

(59)

We may further introduce spin-triplet pairing terms such as

$$u_{i,k,\sigma} c_{i,k,\sigma,\delta}^\dagger P(k,\sigma,\delta) + t_{i,k,\sigma} c_{i,k,\sigma,\delta}^\dagger P(k,\sigma,\delta) ,$$

(60)

e tc. in $A_{i,k,\delta}$, which also contribute to CDW/SDW order, yielding

$$\langle c_{i,-k,\sigma}^\dagger c_{i,p,\sigma} \rangle = \frac{1}{N_0} \left\{ s_{j,k,-\sigma} t_{j,k,p,\sigma} + s_{j,p,k,\sigma} t_{j,p,k,\sigma} + \text{sgn}(\sigma) [v_{i,p} w_{i,k,p,\sigma} - v_{i,k} w_{i,k,p,\sigma}] \right\} ,$$

(61)

$$\langle c_{i,-k,\sigma}^\dagger c_{j,p,\sigma} \rangle = \frac{1}{N_0} \left\{ s_{j,k,-\sigma} w_{j,k,p,\sigma} + s_{j,p,k,\sigma} w_{j,p,k,\sigma} + \text{sgn}(\sigma) [v_{j,p} t_{j,p,k,\sigma} - v_{i,k} t_{i,k,p,\sigma}] \right\} .$$

(62)

We note that *in principle* it is possible to have non-zero expectation values for charge and spin density $\langle c_{i,k,Q,\sigma} c_{i,k,\pm \sigma} \rangle$ - with both $i = j$ and $i \neq j$ - for some $Q$-range [17], while the anomalous propagators $F_i = 0$. This regime could correspond to the pseudogap phase of the copper oxide superconductors [18].

In [15, 16] (treating different models though!) the coexistence of charge and spin density wave order with superconductivity was explored. We emphasize that, as far as we can currently see, this coexistence is not compulsory, though possible, in our approach.
The relevance of the BCS states to the calculation of $T_c$ for the multilayer copper oxide superconductors provided a motivation for this work.

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