BCS @ 50: DERIVATION OF GAP EQUATIONS IN DIFFERENT LATTICE GEOMETRIES

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Abstract

We rigorously derive BCS gap equations for a square, triangular and a honeycomb lattice using a two-dimensional $t-J$ model. The gap equations in all the three lattice geometries look usual, with band indices appearing and a minor modification in the separable pair potential for the (two band) honeycomb lattice. In each case, the gap equation is solved (self consistently with the number equation) at low densities assuming singlet pairing.

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I. INTRODUCTION

The behaviour of strongly correlated electrons on low dimensional lattice systems continues to intrigue interest among researchers. The discovery of the cuprate superconductors\(^1\), among a plethora of things, demanded an understanding of the link that possibly exists between the underlying band structure of a particular lattice geometry which, in turn, decides the shape of the fermi surface and the microscopic mechanism that causes superconductivity.

The other materials which could not escape the fancy of various people working in the field are inorganic compounds such as Cs\(_2\)CuCl\(_4\) and Cs\(_2\)CuBr\(_4\)\(^2,3\) where the \(s = 1/2\) Cu ions interacting antiferromagnetically form layers of anisotropic triangular lattices. Also the exotic layered organic materials \(\kappa - (ET)\(_2\)\_X\) (\(X:\) anion) attracted a great deal of attention where the \((ET)\(_2\)\) dimers are arranged in a quasi-2D anisotropic triangular lattice\(^5,6,7,8\). Further, the importance of studying triangular lattices grew with the discovery of superconductivity in hydrated Sodium Cobaltate Na\(_x\)CoO\(_2\)·yH\(_2\)O\(^9\). The Co ions, where the charge carriers reside, form a triangular lattice. Beside Cuprates, Cobaltates are the other layered transition metal oxides in which superconductivity (albeit with a low \(T_c, \sim 4K\)) has been observed. A more interesting phenomena emerges at a doping, \(x = 1/3\). The spin-0 Co\(^{3+}\) ions form a new triangular lattice with a larger unit cell and the spin-1/2 Co\(^{3+}\) ions form a half filled honeycomb lattice. Upon further doping some of the sites get doubly occupied.

Superconductivity in a honeycomb lattice is also realised experimentally in MgB\(_2\)\(^4\) which is a \(\pi\)-electron system on a layered honeycomb lattice. Thus the superconductivity is essentially two-band and constitutes the other unique thing (other than a remarkably high \(T_c\) of \(\sim 40K\)) in MgB\(_2\) which attracts increasing attention.

In a general framework, the word ‘unconventional superconductivity’ is assigned to all the three candidates mentioned above, \(e.g.\) the high-\(T_c\) superconductors, the Cobaltates and the Borides with varied degree of deviation from the conventional BCS theory. In such materials, there exists some sort of a broken symmetry (usually it is the lowering of the symmetry of the crystal point group) in addition to the spontaneously broken global gauge symmetry, \(viz.\) \(U(1)\).

In the next section we briefly introduce the \(t - J - U\) model used in the paper. Section III discusses the rigorous derivation of the BCS gap equations for a square, triangular and a two-band honeycomb lattice at low densities assuming singlet pairing and thus gain insight on the conventional superconductivity in these lattice structures with, of course, the motivation derived from the existence of real materials as described in the last few paragraphs. In section IV, we solve for the gap functions making ansatz for the orbital symmetry of the order parameter which derives motivation from experiments.
II. THE MODEL

We consider a two-dimensional $t - J - U$ Hamiltonian given by,

$$
H = -t \sum_{<ij>\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c) + J \sum_{<ij>} \langle S_i \cdot S_j - \frac{n_in_j}{4} \rangle + U \sum_i n_{i\uparrow}n_{i\downarrow} \tag{1}
$$

The first term in the Hamiltonian corresponds to kinetic energy, the second is the exchange term (that causes pairing) and the last term is the Hubbard repulsion that prohibits double occupancy. It may be noted that the limit $U \to \infty$ completely projects out the doubly occupied states from the Hilbert space and thus brings back the more familiar $t - J$ model. In fact, due to the presence of $U$, it is not mandatory to use the constrained fermion operators. Other symbols in Eq.(1) have the usual meaning and are not elaborated here.

III. GAP EQUATIONS: A RIGOROUS DERIVATION

The symmetry of the superconducting state depends crucially on how the order parameter (OP) transforms. The OP may non-trivially depend upon the wavevector $k$ owing to the lattice symmetry or equivalently the microscopic mechanism that leads to the pairing instability and hence the superconducting state.

The identification of the orbital symmetry of the OP has remained a subject of intense investigation in materials where the superconducting transition is found to exist. Probes such as measurement of specific heat, tunneling and photoemission spectra, penetration depth, Raman spectra etc. constitute important tools to study symmetry of the OP. While reasonably robust consensus exists on a $d_{x^2-y^2}$ ($d$-wave) pairing scenario for the cuprates, an $s$-wave for MgB$_2$, the pairing symmetry for Na$_x$CoO$_2$·yH$_2$O is still under scrutiny with some experimental support for a singlet pairing for low doping evolving gradually to a triplet pairing at higher values of doping.

In the following we use a two-dimensional $t - J - U$ model and derive the celebrated BCS equation gap equation in the singlet channel for a square, triangular and a honeycomb lattice.

A. Square lattice

The ground state BCS wavefunction is written as,

$$
|\psi_{BCS}\rangle = \prod_k (u_k + v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger)|0\rangle \tag{2}
$$

where $|u_k|^2 + |v_k|^2 = 1$ implies that the probability of the pair $(k \uparrow, -k \downarrow)$ is occupied by $|v_k|^2$, while the probability that it is unoccupied is $|u_k|^2$. In general, $u_k$ and $v_k$ are complex quantities.
Now we must actually compute the unknown quantities, \(v_i u_k\) and \(v_k\). We employ a variational approach which is in the same spirit as used in the original paper of BCS\(^1\). Thus we minimize the expectation value of the Hamiltonian between the states in Eq. (2) by setting,

\[
\delta \langle \psi_{BCS} | H - \mu N_{op} | \psi_{BCS} \rangle = 0
\]

where \(N_{op} = \sum_{k\sigma} n_{k\sigma}\) is the number operator and \(\mu\) is the chemical potential that controls filling. The inclusion of \(-\mu N_{op}\) implies taking the zero of the kinetic energy to be \(\mu\) (or Fermi energy)\(^2\). The calculations are greatly simplified if we introduce Bogoliubov operators \(\alpha_k\) and \(\beta_k\), related to the \(c\)-operators by the following transformation,

\[
\alpha_k = u_k c_{k\uparrow} - v_k c_{-k\downarrow} \quad \text{and} \quad \beta_k = u_k c_{-k\downarrow} + v_k c_{k\uparrow}
\]

with \(\alpha_k\) and \(\beta_k\) satisfying,

\[
\alpha_k |\psi_{BCS}\rangle = \beta_k |\psi_{BCS}\rangle = 0
\]

Inverting Eq. (4) one gets,

\[
c_{k\uparrow} = u_k^* \alpha_k + v_k^* \beta_k^\dagger \quad \text{and} \quad c_{k\downarrow}^\dagger = u_k \alpha_k^\dagger + v_k \beta_k
\]

To evaluate Eq. (3), we consider Eq. (1) term by term. We begin by computing the on site Hubbard term,

\[
\hat{U} = U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow}
\]

The real-space raising and lowering operators are defined as,

\[
c_{i\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{ik \cdot R_i} c_{k\sigma}^\dagger \quad \text{and} \quad c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_k e^{-ik \cdot R_i} c_{k\sigma}
\]

Using the inverse transform one can write \(\hat{U}\) as,

\[
\hat{U} = \frac{U}{N} \sum_{k_1k_2q} c_{k_1-q\downarrow}^\dagger c_{k_2+q\downarrow}^\dagger c_{k_2 \uparrow} c_{k_1 \downarrow}
\]

so we have

\[
\langle \psi_{BCS} | \hat{U} | \psi_{BCS} \rangle = \frac{U}{N} \sum_{k_1k_2q} \langle \psi_{BCS} | c_{k_1-q\downarrow}^\dagger c_{k_2+q\downarrow}^\dagger c_{k_2 \uparrow} c_{k_1 \downarrow} | \psi_{BCS} \rangle
\]

Expectation values of various terms and usage of Wick’s theorem yields

\[
\langle \psi_{BCS} | \hat{U} | \psi_{BCS} \rangle = \frac{U}{N} \sum_{k_1k_2} [v_{k_1}^* u_{k_1} v_{k_2} u_{k_2}^* + |v_{k_1}|^2 |v_{k_2}|^2]
\]
Next we find out the expectation value of the kinetic energy term which is written as,

$$\hat{t} = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma}$$  \hspace{1cm} (12)

here, $\varepsilon_k = \epsilon_k - \mu$ and $\epsilon_k = -2t(cos k_x + cos k_y)$. Simplification of the $\hat{t}$ term yields,

$$\langle \psi_{BCS} | \hat{t} | \psi_{BCS} \rangle = 2 \sum_k \varepsilon_k |v_k|^2$$  \hspace{1cm} (13)

Finally, we consider the interaction term $\hat{J}$. Expanding in terms of the momentum space operators yields three terms which are,

$$\hat{J}_1 = -\frac{1}{2N} \sum_{k_1 k_2 q} V(q) c_{k_1 + q}^\dagger c_{k_1} c_{k_2 + q} c_{k_2}$$  \hspace{1cm} (14)

$$\hat{J}_2 = \frac{1}{2N} \sum_{k_1 k_2 q} V(q) c_{k_1 + q}^\dagger c_{k_1} c_{k_2} c_{k_2 + q}$$

$$\hat{J}_3 = -\frac{1}{2N} \sum_{k_1 k_2 q} V(q) [c_{k_1 + q}^\dagger c_{k_2} c_{k_1 + q} c_{k_2} + c_{k_1} c_{k_2 + q} c_{k_1} c_{k_2 + q}]$$

where $V(q) = J \sum_i e^{-iq \cdot \gamma_i}$ and $\gamma_i$ refers to $\pm \hat{x}$ and $\pm \hat{y}$ which are the nearest neighbours in a square lattice. Thus,

$$V(q) = 2J [\cos q_x + \cos q_y]$$  \hspace{1cm} (15)

The expectation values of these terms between the BCS ground states are computed in the following,

$$\langle \psi_{BCS} | \hat{J}_1 | \psi_{BCS} \rangle = -\frac{1}{2N} \sum_{k_1 k_2} V(k_2 - k_1) u_{k_2} v_{k_1}^* u_{-k_1}^* v_{-k_1}$$  \hspace{1cm} (16)

$$\langle \psi_{BCS} | \hat{J}_2 | \psi_{BCS} \rangle = -\frac{1}{2N} \sum_{k_1 k_2} V(k_1 - k_2) u_{k_2} v_{k_1}^* u_{-k_1}^* v_{-k_1}$$

$$\langle \psi_{BCS} | \hat{J}_3 | \psi_{BCS} \rangle = -\frac{1}{2N} \sum_{k_1 k_2} [V(k_2 - k_1) + V(k_1 - k_2)] u_{k_2} v_{k_2}^* u_{k_1}^* v_{k_1}$$

Adding the contributions from all the terms, we now write down the expectation of the full Hamiltonian,

$$\langle \psi_{BCS} | H - \mu N_{op} | \psi_{BCS} \rangle = \frac{1}{N} \sum_k 2\varepsilon_k |v_k|^2 + \frac{1}{2N} \sum_{k_1 k_2} [2U - \{V(k_2 + k_1) + V(k_1 - k_2) \} u_{k_2} v_{k_2}^* u_{k_1}^* v_{k_1}$$

$$+ V(k_2 - k_1) + V(-k_1 - k_2)] u_{k_2} v_{k_2}^* u_{k_1}^* v_{k_1}$$

The above expression is subjected to the constraint $u_k^2 + v_k^2 = 1$ which is satisfied by letting $u_k = \sin \theta_k$ and $v_k = \cos \theta_k$. Minimizing with respect to $\theta_k$, one gets the gap equation,

$$\Delta_k = -\frac{1}{N} \sum_{k'} \frac{\Delta_{k'} V_{kk'}}{2(\varepsilon_{k'}^2 + \Delta_{k'}^2)^{1/2}} = -\frac{1}{N} \sum_{k'} \frac{\Delta_{k'} V_{kk'}}{2E_{k'}}$$  \hspace{1cm} (18)
with

\[ V(q) = J \sum_i e^{-iq \cdot \gamma_i} \]  \hspace{1cm} (19)

and

\[ V_{kk'} = \frac{U}{N} + \frac{1}{2N} \left[ V(k + k') + V(-k - k') + V(k - k') + V(k' - k) \right] \]  \hspace{1cm} (20)

At finite temperatures, Eq. (18) assumes the form,

\[ \Delta_k = -\frac{1}{N} \sum_{k'} \Delta_{k'} V_{kk'} \tanh \left( \frac{\beta E_{k'}}{2} \right) \]  \hspace{1cm} (21)

where \( \beta = 1/T \) (with \( k_B = 1 \)) is the inverse temperature.

**B. Triangular lattice**

Triangular lattice is a bravais lattice which can be thought of as three identical interlacing sublattices (tripartite lattice). Three of the six nearest neighbours are given by, \( \hat{\gamma}_1 = -\frac{1}{2} \hat{x} - \frac{\sqrt{3}}{2} \hat{y}, \) \( \hat{\gamma}_2 = -\frac{1}{2} \hat{x} + \frac{\sqrt{3}}{2} \hat{y} \) and \( \hat{\gamma}_3 = \hat{x} \). Exactly the same calculation, as shown for the square in the previous subsection, follows for the triangular lattice as well. So we arrive exactly at the same gap equation as it appears in Eq. (21) with the electronic and spin-wave dispersions modified as,

\[ \epsilon_q = -2t \left[ \cos q_x + 2 \cos \frac{q_x}{2} \cos \frac{\sqrt{3}}{2} q_y \right] \]  \hspace{1cm} (22)

\[ V(q) = 2J \left[ \cos q_x + 2 \cos \frac{q_x}{2} \cos \frac{\sqrt{3}}{2} q_y \right] \]

**C. Honeycomb lattice**

Here we discuss our next candidate, viz the honeycomb lattice. It consists of two interleaved triangular lattices, i.e. it has two sites per unit cell. We denote the two sites by \( A \) and \( B \) and each site is uniquely represented by \((R_i, \alpha)\) where \( R_i \) is the position vector of the \( i \)-th unit cell and \( \alpha \) is either \( A \) or \( B \). The three neighbours of a \( A \) site at \((R_i, A)\) are given by \((R_i + \gamma_j, B)\), where \( \gamma_1 = (0, 0), \gamma_2 = (-\frac{1}{2}, -\frac{\sqrt{3}}{2}) \) and \( \gamma_3 = (\frac{1}{2}, -\frac{\sqrt{3}}{2}) \). So the BCS wavefunction written earlier in Eq. (2) needs to be generalized to account for the presence of two different sites that lead to the existence of two bands. The ground state including the band index may be written as,

\[ |\psi_{BCS}\rangle = \prod_{k\eta} (u_{k\eta} c_{k\eta} + v_{k\eta} \eta_{k\eta} c_{-k\eta}) |0\rangle \]  \hspace{1cm} (23)

where \( \eta = (A/B) \) is the band index. It may be noted here that we are only concerned with intraband pairing, whereas interband transition is possibly too expensive and also it will lead to
a second (spurious) transition temperature. Again the variational procedure leading to the gap
equation requires a calculation of the expectation values of the $H - \mu N_{op}$ operator within the BCS
state. The Coulomb term is written as,

$$\hat{U}^A = U \sum_{R \in A} c_{R\sigma}^{A\dagger} c_{R\sigma}^A c_{R\sigma}^{A\dagger} c_{R\sigma}^A$$  \hspace{1cm} (24)

In terms of the band indices the fermion operators are written as,

$$c_{R\sigma}^{A\dagger} = \frac{1}{\sqrt{2N}} \sum_k e^{i k \cdot R} (c_{k\sigma}^{+\dagger} + c_{k\sigma}^{-\dagger}) \quad \text{and} \quad c_{R\sigma}^B = \frac{1}{\sqrt{2N}} \sum_k e^{i k \cdot R} h^*(k)(c_{k\sigma}^{+\dagger} - c_{k\sigma}^{-\dagger})$$  \hspace{1cm} (25)

where $h(k) = \frac{\nu(k)}{\eta(k)}$. Thus Eq. [24] becomes,

$$\hat{U}^A = \frac{U}{4N} \sum_{k_1 k_2 q_1 q_2 \eta_1 \eta_2} c_{k_1 + q_1}^{\eta_{1\dagger}} c_{k_2 - q_1}^{\eta_{1\dagger}} c_{k_2}^{\eta_{2\dagger}} c_{k_1}^{\eta_{2\dagger}}$$  \hspace{1cm} (26)

Similarly for the $B$-band,

$$\hat{U}^B = \frac{U}{4N} \sum_{k_2 k_4 q_3 q_4 \eta_3 \eta_4} c_{k_1 + q_4}^{\eta_{3\dagger}} c_{k_2 - q_4}^{\eta_{3\dagger}} c_{k_2}^{\eta_{4\dagger}} c_{k_1}^{\eta_{4\dagger}}$$  \hspace{1cm} (27)

where $\eta_i$’s are dummy band indices. Combining the above equations one gets,

$$\hat{U} = \frac{U}{4N} \sum_{k_1 k_2 q_1 q_2 \eta_1 \eta_2} (1 + \eta_{1\eta_2 \eta_3 \eta_4}) c_{k_1 + q_1}^{\eta_{1\dagger}} c_{k_2 - q_1}^{\eta_{1\dagger}} c_{k_2}^{\eta_{2\dagger}} c_{k_1}^{\eta_{2\dagger}}$$  \hspace{1cm} (28)

The expectation value of the Coulomb term for states in Eq. 23 yields,

$$\langle \psi_{BCS} | \hat{U} | \psi_{BCS} \rangle = \frac{U}{2N} \sum_{k_1 k_2 q_1 q_2} \left| v_{k_1}^{q_1} \right|^2 \left| v_{k_2}^{q_2} \right|^2 + \left| u_{k_1}^{q_1} u_{k_2}^{q_2} \right|^2$$  \hspace{1cm} (29)

Similarly the kinetic energy term is written as,

$$\langle \psi_{BCS} | \hat{t} | \psi_{BCS} \rangle = \sum_{k \sigma \eta} \epsilon_k^{\eta} c_{k\sigma}^{\eta\dagger} c_{k\sigma}^\eta$$  \hspace{1cm} (30)

The expectation value of the kinetic energy is computed as,

$$\langle \psi_{BCS} | \hat{t} | \psi_{BCS} \rangle = 2 \sum_{k \eta} \epsilon_k^{\eta} \left| v_k^{(\eta)} \right|^2$$  \hspace{1cm} (31)

Next the exchange term is written in terms of band indices as,

$$\hat{J} = \frac{J}{2} \sum_{\langle R, R' \rangle} (c_{R\sigma}^{A\dagger} c_{R\sigma}^{B\dagger} c_{R'\sigma}^B + c_{R\sigma}^{A\dagger} c_{R\sigma}^B c_{R'\sigma}^{B\dagger} - c_{R\sigma}^{A\dagger} c_{R\sigma}^B c_{R'\sigma}^B - c_{R\sigma}^{A\dagger} c_{R\sigma}^{B\dagger} c_{R'\sigma}^B)$$  \hspace{1cm} (32)
Fourier transformation of the above leads to,

\[ \hat{J} = -\frac{1}{8N} \sum_{k_1k_2m_1n_1n_2n_3n_4} [\eta_3\eta_4J(q)h(q)]c_{k_1+q_1}^{n_1\dagger}c_{k_1}^{n_2\dagger}c_{k_2-q_1}^{n_3\dagger}c_{k_2}^{n_4} \]

\[ \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad (33) \]

\[-\frac{1}{8N} \sum_{k_1k_2m_1n_1n_2n_3n_4} [\eta_3\eta_4J(q)h(q)]c_{k_1+q_1}^{n_1\dagger}c_{k_1}^{n_2\dagger}c_{k_2-q_1}^{n_3\dagger}c_{k_2}^{n_4} \]

\[ + \frac{1}{8N} \sum_{k_1k_2m_1n_1n_2n_3n_4} [\eta_3\eta_4J(q)h(q)]c_{k_1+q_1}^{n_1\dagger}c_{k_1}^{n_2\dagger}c_{k_2-q_1}^{n_3\dagger}c_{k_2}^{n_4} \]

\[ + \frac{1}{8N} \sum_{k_1k_2m_1n_1n_2n_3n_4} [\eta_3\eta_4J(q)h(q)]c_{k_1+q_1}^{n_1\dagger}c_{k_1}^{n_2\dagger}c_{k_2-q_1}^{n_3\dagger}c_{k_2}^{n_4} \]

\[ = \hat{J}_1 + \hat{J}_2 + \hat{J}_3 + \hat{J}_4 \]

Computation of expectation values of each of these terms yield,

\[ \langle \psi_{BCS}|\hat{J}_1|\psi_{BCS}\rangle = -\frac{1}{8N} \sum_{k_1k_2n_1n_2} V^{n_1n_2}(k_2-k_1)|v_{n_1}^{k_1}||u_{n_2}^{k_2}|^2 - u_{n_2}^{k_2}v_{n_1}^{k_1}u_{n_1}^{k_1}v_{n_2}^{k_2} \]

\[ \langle \psi_{BCS}|\hat{J}_2|\psi_{BCS}\rangle = -\frac{1}{8N} \sum_{k_1k_2n_1n_2} V^{n_1n_2}(k_2-k_1)|v_{n_1}^{k_1}||u_{n_2}^{k_2}|^2 - u_{n_2}^{k_2}v_{n_1}^{k_1}u_{n_1}^{k_1}v_{n_2}^{k_2} \]

\[ \langle \psi_{BCS}|\hat{J}_3|\psi_{BCS}\rangle = \frac{V_0}{8N} \sum_{k_1k_2n_1n_2} |v_{n_1}^{k_1}|^2 |v_{n_2}^{k_2}|^2 + \frac{1}{8N} \sum_{k_1k_2n_1n_2} V^{n_1n_2}(k_2-k_1)u_{n_1}^{k_1}v_{n_1}^{k_2}u_{n_2}^{k_2}v_{n_2}^{k_2} \]

\[ \langle \psi_{BCS}|\hat{J}_4|\psi_{BCS}\rangle = \frac{V_0}{8N} \sum_{k_1k_2n_1n_2} |v_{n_1}^{k_1}|^2 |v_{n_2}^{k_2}|^2 + \frac{1}{8N} \sum_{k_1k_2n_1n_2} V^{n_1n_2}(k_2-k_1)u_{n_1}^{k_1}v_{n_1}^{k_2}u_{n_2}^{k_2}v_{n_2}^{k_2} \]

where \( V_0 \) is \( V(q = 0) \) and is independent of the band index, \( \eta \). Finally, after simplifying we have,

\[ \langle \psi_{BCS}|H - \mu N_v|\psi_{BCS}\rangle = 2 \sum_{k_1n_1} c_{v_{k_1}}^{(n_1)}|v_{n_1}^{k_1}|^2 + \sum_{k_1k_2n_1n_2} \left[ \frac{U}{2N} + \frac{1}{8N} \{ V^{n_1n_2}(k_2-k_1) \right. \]

\[ + V^{n_1n_2}(k_1-k_2) + V^{n_1n_2}(k_2+k_1) + V^{n_1n_2}(-k_1-k_2) \} |u_{n_1}^{k_1}v_{n_1}^{k_2}u_{n_2}^{k_2}v_{n_2}^{k_2} | \]

Again \( u_k^\eta \) and \( v_k^\eta \) are subjected to the constraint \( |u_k^\eta|^2 + |v_k^\eta|^2 = 1 \) for all \( k \) and \( \eta = (A/B) \). Thus imposing \( u_k^\eta = \sin \theta_k^\eta \) and \( v_k^\eta = \cos \theta_k^\eta \) and minimizing with respect to \( \theta_k^\eta \) we obtain,

\[ \Delta_k^\eta = -\frac{1}{N} \sum_{k'\eta'} \frac{\Delta_{k'}^{\eta'} \Delta_k^\eta v_{k'}^{\eta'} v_{k}^{\eta}}{2(c_k^2 + \Delta_k^\eta)^{1/2}} \]

\[ \Delta_k^\eta = -\frac{1}{N} \sum_{k'\eta'} \frac{\Delta_{k'}^{\eta'} \Delta_k^\eta v_{k'}^{\eta'} v_{k}^{\eta}}{2E_k^{k'}} \text{tanh} \left( \frac{\beta E_{k'}^{\eta'}}{2} \right) \]

where,

\[ V_{k_1k_2}^{n_1n_2} = \frac{U}{2N} + \frac{1}{8N} \left( V^{n_1n_2}(k_2-k_1) + V^{n_1n_2}(k_1-k_2) + V^{n_1n_2}(k_2+k_1) + V^{n_1n_2}(-k_1-k_2) \right) \]

with

\[ V_{n_1n_2}(q) = \eta_1\eta_2 J(q) h(q) \]

(39)
Using $J(q) = J \sum_i e^{-i q \cdot \gamma_i}$ and $h(q) = \frac{\tau(q)}{|t(q)|}$ where $t(q) = -t \sum_i e^{-i q \cdot \gamma_i}$ in Eq. (39) ($\gamma_i$'s refer to the nearest neighbours), the interaction term can be rewritten as,

$$V_{\eta_1 \eta_2}(q) = \eta_1 \eta_2 J |r(q)|$$

(40)

where $r(q) = \sum_i e^{i d \cdot \gamma_i}$. Finally Eq. (38) becomes,

$$V_{\eta_1 \eta_2} = \frac{U}{2N} - \frac{J}{4N} \left[ \eta_1 \eta_2 |r(k_1 - k_2)| + \eta_1 \eta_2 |r(k_1 + k_2)| \right]$$

(41)

It may be noted that even if the structure of the gap equation is indistinguishable from that of the square and triangular lattices, due to Eq. (40), dictates that the interaction term is separable in a non-trivial way, i.e. it depends on the modulus of the form factor.

IV. RESULTS

In this section we present the results for the solution of the gap equations derived in the previous section.

A. Square lattice

The irreducible representation of the $C_{4v}$ point group appropriately represents the pairing symmetry of the gap function (since the interaction term, $J(k)$ is separable in terms of those) for a square lattice. In the singlet channel ($\Delta_k = \Delta_{-k}$), the relevant symmetry functions are: (i) on-site $s$-wave (constant), (ii) extended-$s$-wave ($\cos k_x + \cos k_y$) and (iii) $d$-wave ($\cos k_x - \cos k_y$). With reference to the cuprate superconductors, strong on-site Coulomb repulsion between the $Cu$ ions is fatal for on-site $s$-wave pairing to exist. However an extended-$s$ wave is an acceptable proposition. Further, suggestions for the pairing mechanism mediated via spin fluctuations assigns superconductivity in the $d$-wave channel as a natural choice. So, in general, we assume the order parameter to be a linear combination of functions that correspond to extended-$s$-wave and $d$-wave channel and is written as,

$$\Delta = \Delta_s [\cos k_x + \cos k_y] + \Delta_d [\cos k_x - \cos k_y]$$

(42)

where $\Delta_s$ and $\Delta_d$ are gap functions in extended $s$ and $d$-wave channels respectively and are considered here as real. Putting Eq. (42) into Eq. (21), one gets the following coupled equations for $\Delta_s$ and $\Delta_d$.

$$\Delta_s = \frac{J}{N} \left[ \Delta_s \sum_k \frac{f^2_s(k)}{2E_k} \tanh \left( \frac{\beta E_k}{2} \right) + \Delta_d \sum_k \frac{f_s(k) f_d(k)}{2E_k} \tanh \left( \frac{\beta E_k}{2} \right) \right]$$

(43)

$$\Delta_d = \frac{J}{N} \left[ \Delta_s \sum_k \frac{f_s(k) f_d(k)}{2E_k} \tanh \left( \frac{\beta E_k}{2} \right) + \Delta_d \sum_k \frac{f^2_d(k)}{2E_k} \tanh \left( \frac{\beta E_k}{2} \right) \right]$$
The above equations are solved self consistently for \( \Delta_s \) and \( \Delta_d \) alongwith the number equation,

\[
n = 1 - \frac{1}{N} \sum_k \left( \varepsilon_k - \mu \right) \tanh \left( \frac{\beta E_k}{2} \right)
\]  

(44)

The results for parameter values \( J/t = 2 \) and electron density, \( n = 0.2 \) are presented in Fig. 1.

![Graph](image)

**FIG. 1**: The dependence of extended s-wave gap function on temperature (both in units of hopping integral \( t \)) is shown for \( J/t = 2 \) and electron density, \( n = 0.2 \). Note that the d-wave amplitude is vanishingly small for the choice of parameters used here and hence not shown.

### B. Triangular lattice

The symmetry of the gap function for the triangular lattice compound Na\(_x\)CoO\(_2\)·H\(_2\)O has yet to be ascertained.\(^{14}\) A number of experiments point towards a triplet pairing scenario (\( p \) and \( f \)-wave), following Baskaran and others,\(^{15-17}\) the winner at low densities seem to be the \( d_x^2-y^2+id_{xy} \)-wave pairing symmetry. So we postulate the gap function to have the following symmetry\(^{16}\),

\[
\Delta_k = \Delta \left[ \cos k_x + e^{i\theta} \cos (k_x/2 + \sqrt{3}k_y/2) + e^{i\phi} \cos (k_x/2 - \sqrt{3}k_y/2) \right]
\]  

(45)

\[
\Delta_k = \Delta \left[ f_1(k) + e^{i\theta} f_2(k) + e^{i\phi} f_3(k) \right]
\]

For simplicity \( \Delta \) is taken to be the same for all bonds. No phase is assumed for the neighbour along the \( x \)-direction, \( \theta \) and \( \phi \) phases are assumed for the other two neighbours which are at \( \pi/3 \) and \( 2\pi/3 \) directions. Plugging this into the gap equation (Eq. (21)), the solutions for \( \Delta \), \( \theta \) and \( \phi \) are given by the following coupled equations,

\[
\Delta = \frac{2J}{N} \Delta \sum_k \left[ f_1^2(k) + e^{i\theta} f_1(k) f_2(k) + e^{i\phi} f_1(k) f_3(k) \right] / E_k
\]  

(46)

\[
e^{i\theta} \Delta = \frac{2J}{N} \Delta \sum_k \left[ f_1(k) f_2(k) + e^{i\theta} f_2^2(k) + e^{i\phi} f_2(k) f_3(k) \right] / E_k
\]

\[
e^{i\phi} \Delta = \frac{2J}{N} \Delta \sum_k \left[ f_1(k) f_3(k) + e^{i\theta} f_2(k) f_3(k) + e^{i\phi} f_3^2(k) \right] / E_k
\]
The results for one particular choice of $\theta$ and $\phi$ are presented in Fig. 2.

![Graph](image)

FIG. 2: The gap function vs temperature for $(\theta, \phi) = (2\pi/3, 2\pi/3)$ is shown for a triangular lattice. Again $J/t = 2$ and $n = 0.2$.

C. Honeycomb lattice

MgB$_2$, an example of a honeycomb lattice geometry, has an unusually high transition temperature of $\sim 40K$ and an isotope effect$^{18}$ that indicates phonon mediated pairing mechanism at work. The specific heat$^{19,20}$ and Photoemission$^{21}$ data provide robust support. A close introspection of Eq. (40) leads to the following ansatz for the gap function,

$$\Delta_k^\eta = \eta |r(k)| \Delta$$

Again putting it in Eq. (37), one gets,

$$\Delta = \frac{J}{12N} \sum_{k\eta} \frac{|r(k)|^2}{E_k^\eta} \tanh \left( \frac{\beta E_k^\eta}{2} \right)$$

The results are presented in Fig. 3.

A simple calculation of $2\Delta(0)/T_c$ ($k_B = 1$) with $T_c$ being the transition temperature and $\Delta(0)$ being the value of the gap at $T = 0$ can be represented in the Table I. It shows that the triangular lattice with the largest coordination number ($z = 6$) hosts the maximum value for $2\Delta(0)/T_c$, while the honeycomb lattice ($z = 3$) has the least. It should be kept in mind that computations of the gap equations are carried out over a finite-$k$ mesh, hence attempts to find out any correlation (if at all it exists) between the quantity $2\Delta(0)/T_c$, which is considered to have a universal value of $\sim 3.52$ for a BCS superconductor and coordination number (equivalently the lattice geometry), will be premature. However experiments can be made guide to probe into issues such as this.
FIG. 3: The gap function vs temperature is shown for a honeycomb lattice for $J/t = 2$ and $n = 0.2$.

TABLE I: $2\Delta(0)/T_c$ for a square, triangular and a honeycomb lattice for exchange interaction $J/t = 2$ and $n = 0.2$

<table>
<thead>
<tr>
<th>lattice geometry</th>
<th>coordination number, $z$</th>
<th>$2\Delta(0)/T_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>square</td>
<td>4</td>
<td>2.5</td>
</tr>
<tr>
<td>triangular</td>
<td>6</td>
<td>3.2</td>
</tr>
<tr>
<td>honeycomb</td>
<td>3</td>
<td>1.4</td>
</tr>
</tbody>
</table>

V. CONCLUSIONS

In this paper we presented an elaborate discussion on the derivation of BCS gap equations for a square, triangular and a honeycomb lattice. Even though the physics of the experimentally realized materials are important closer to half filling, and BCS theory is qualitatively correct for low electron densities, still some important consequences regarding pairing correlations, gap symmetry etc. are likely to emerge from these calculations.

References