Supercurrent flow with large superconductor gap in cuprates: resurrection of phonon-mediated Cooper pairs

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Abstract
We systematically explore the correctness of the Bardeen–Cooper–Schrieffer (BCS) Hamiltonian where the BCS-type electron–phonon interaction is unambiguously reinforced as the only viable attractive interaction between two electrons in cuprate superconductors because phonon-induced scattering is effectively nil for Cooper pairs (in its original form), and also phonons are not required to Bose condense. Here, we prove that (i) the Cooper-pair binding energy can be strengthened to obtain high superconductor transition temperature ($T_{sc}$) and (ii) the existence of a generalized electron–phonon potential operator that can induce the finite-temperature phase transition between superconducting and strange metallic phases. To lend support for this extended BCS Hamiltonian, we derive the Fermi–Dirac statistics for Cooper-pair electrons, which correctly captures the physics of strongly bounded Cooper-pair break up with respect to changing temperature or superconductor gap ($\Delta_{BCS}$). Finally, we further extend the BCS Hamiltonian within the ionization-energy theory formalism to prove (iii) the existence of optimal doping that has maximum $T_{sc}(x_{\text{optimum}})$ or $\Delta_{BCS}(x_{\text{optimum}})$, and (iv) that the specific heat capacity jump at $T_c$ in cuprates is due to finite-temperature phase transition. Along the way, we expose the precise microscopic reason why predicting (not guessing) a superconductor properly is a hard problem within any theory that require pairing mechanism.

Keywords: superconductivity, extended BCS theory, cuprates, specific heat capacity

(Some figures may appear in colour only in the online journal)

1. Introduction

Above zero Kelvin, phonons do not Bose condense, they never did, and consequently, phonons define the ultimate resistance to electrons or bosons flow, and this resistance does not go away until we reach absolute zero. In particular, Bose condensation is meaningless for $T = 0$ K for phonons do not exist at absolute zero, while for $T > 0$ K, Bose condensation of phonons is definitely not possible because the atoms in solids are bonded such that the atoms are not independent of each other with overlapped valence-electron distribution (or overlapped wavefunction). It is a fundamental fact that for any conducting particles or pairs of particles (namely, Cooper pairs, bipolarons, holon pairs, anyons or bosons) to superconduct, they eventually need the ‘approval’ of phonons such that the particle-phonon or paired particle-phonon scattering is completely removed. The only model Hamiltonian that properly and correctly eliminates the phonon-induced scattering is the Bardeen–Cooper–Schrieffer (BCS) Hamiltonian such that phonons are not required to Bose condense [1, 2].

BCS Hamiltonian of superconductivity on the basis of Cooper pairs [3] was not properly pursued after the discovery of cuprate superconductors (also known as the high temperature superconductors) by Bednorz and Müller [4]. The argument used to abandon the BCS Hamiltonian is that it only applies to weakly-coupled Onnes-type [5] conventional superconductors with $s$-wave pairing. Here, the notion of weak coupling refers to the strength of electron–phonon ($e$:$ph$) coupling that is responsible for the formation of Cooper pairs, which is found to be too weak (with large coherence...
length) to produce high superconductor transition temperature ($T_c$). The highest BCS transition temperature is found for Hg-based cuprate which is about 130 K [6]. Hence, other types of pairing mechanisms have been proposed, but these proposals ignore the phonon-induced scattering effect.

Unlike resistivity [5], Meissner-effect [7] and specific heat capacity ($C_v$) measurements [8], the analysis based on angle-resolved photoemission spectroscopy, tunneling and nuclear magnetic resonance measurements [9–11] cannot be used (on their own) to unambiguously deduce the existence of superconductivity, unless one is already aware that the system is a superconductor. On the other hand, the meaning of this statement—‘microscopic mechanism without internal inconsistency’ shall be explored when we revisit the BCS Hamiltonian (see equations (1)–(3)).

The Cooper-pair mechanism (in its original form) has been abandoned on the basis of the following arguments. The binding energy of Cooper pairs cannot be made large enough to transform $T^\text{BCS}_c \rightarrow T^{\text{cuprates}}_c$ because the BCS mechanism of phonon-mediated Cooper pairing is limited to s-wave pairing and also due to small $|E_k - E_{k+q}|$ where $E_k > \hslash \omega_k$, $E_{k+q} > \hslash \omega_q$ and $|E_k - E_{k+q}| \ll \hslash \omega_q$. The first two inequalities allow adiabatic approximation due to this time relation, $t_s < t_{ph}$ (an electron responds at a faster timescale compared to a phonon decay), which is crucial for the formation of Cooper pairs. Here, $|E_k - E_{k+q}| \approx k_0 T^\text{BCS}_c$ where $k_0 T^\text{BCS}_c \times \Delta^\text{BCS}$ and $\Delta^\text{BCS}$ denotes the BCS superconductor gap. The second inequality defines the attraction (if $|E_k - E_{k+q}| < \hslash \omega_q$) between two electrons such that one of the electrons has a change of energy from $E_k$ to $E_{k+q}$. While the energy of the second electron changes from $E_k$ to $E_{k+q}$ mediated by a phonon absorption and emission, respectively, with energy $\hslash \omega_q$.

BCS happened to have derived the gap equation and the $C_v$ relation based on s-wave pairing (spherical Fermi surface). But this is not a restriction for the application of BCS Hamiltonian in cuprates because their Hamiltonian permits singlet pairing for different types of Fermi surfaces, s- or p- or d- or f-wave pairing symmetry, or any combination of them. It is just a matter of finding which atoms in a given superconductor contribute to Cooper pairing. For example, light atoms may give rise to s- or p-wave singlet pairing, whereas heavier atoms may lead to d- or f-wave singlet pairing. Additionally, the types of atoms and their sequence found along the a, b or c-axis in cuprates are different. This means that, the existence of anisotropic (or quasi-two dimensional) normal state resistivity ($ab$-plane versus $c$-axis) above $T_c$ is expected because the normal state is not a free-electron or Fermi-liquid metal (in the usual sense). In particular, the normal state is a strange (Fermi) metal. But this quasi-two dimensional conductivity does not invalidate the formation of BCS-type Cooper pairs. Here, the term Cooper pair strictly refers to the original BCS-type, and we do not refer to any other types. More details on the d-wave pairing symmetry are available in [12, 13].

The existence of pseudogap for $T^* > T_c$ and doping-dependent superconductor gap ($\Delta_{\text{BCS}}$) can be made to obey the conduction mechanism of Cooper pairs by reworking the BCS attraction operator within the ionization-energy theory (IET) [14]. In fact, IET has enabled us to address the strange metallic phase and doping-dependent resistivity [15–17] above $T_c$ properly. However, we have to postpone the research on pseudogap because BCS Hamiltonian, even after extension, does not ‘uniquely’ lead us to find the origin of this gap. For example, we can always assume that preformed Cooper pairs or some forms of phonon ‘readjustment’ is the cause for this pseudogap where both can be related to BCS Hamiltonian. Warning: Cooper-pair formation is responsible for an upward (not downward) ‘jump’ in the $C_v$ data at $T_c$, and therefore, preformed Cooper pairs (if they really exist) should be detectable with a similar upward-jump (however small) in the $C_v$ measurements for $T > T_c$. Thus far, there is no such data reported.

It is worth noting that the IET introduced here is applicable for all systems that are composed of atoms, except for Fermi-liquid metals. In fact IET is a proper theory for any non-Fermi compounds with or without defects, regardless of whether these defects are arranged periodically or not (non-homogeneously distributed such that the translational symmetry is broken). Apart from superconductivity and normal state properties of cuprates, IET and the energy-level spacing renormalization group method have been successfully applied to study many important physical and physico-chemical properties. In particular, the Raman effect [18], structural phase transition [19], ion selectivity in cation channels, polymerase-β DNA replication, solidification mechanism of the Earth’s iron inner core, chemical reaction between atoms and peptide bond formation, finite-temperature phase transition in water–ice system and molten solids, water-molecule dissociation induced by electronic polarization, gas sensing mechanism, atom–substrate interaction during quantum-dot or thin-film growth, the interaction between a quantum dot and its substrate, generalized carrier-type transition for all types of semiconductors (including oxides), doping-dependent electronic transport phenomena in topological insulators, manganites and diluted magnetic semiconductors [20–22].

2. Theoretical calculations

Our strategy here is to prove the existence of a generalized potential operator such that e:ph interaction can either induce the e:e attraction via phonon exchange to give rise to a superconducting phase, or can play its role in the form of electron–ion (e:ion) attraction to activate the usual e:e coulomb repulsion. This repulsion can either produce the strange metallic phase (if the energy levels are still degenerate) or an insulator (due to Mott or band gap). Subsequently, we derive the Fermi–Dirac statistics (FDS) for Cooper pairs to understand their excitation probability below $T_c$ by counting the Cooper-pair electrons, instead of Cooper pairs. Finally, we invoke the above generalized potential operator to show that this potential allows finite-temperature phase transition (FPT) to exist, which is responsible for the phase transition between superconductor and strange metal. But before doing any of these, let us introduce the
connection between BCS attractive potential and finite-
temperature phase transition.

2.1. BCS attraction and finite-temperature phase transition

We now introduce the physics needed to reconstruct Cooper
pairs within the BCS Hamiltonian in unconventional super-
conductors. First, let us recall the BCS Hamiltonian that takes
the phonon assisted electron–electron (e:e) attraction into
account (for singlet pairing), which is given by [1]

$$H_{BCS} = \sum_{k > k_F} E_k n_{k\sigma} + \sum_{k < k_F} [E_k (1 - n_{k\sigma})]
+ H_{\text{Coulomb}} + H_{\text{Cooper}}^{\text{pair}},$$

(1)

$$H_{\text{Coulomb}} = \sum_k \frac{e^2}{\epsilon_0 (k^2 + K_i^2)},$$

(2)

$$H_{\text{Cooper}}^{\text{pair}} = \frac{1}{2} \sum_{k, k', \sigma, \sigma'} \frac{2/\omega_q |s_{k,k'}|^2 e^8(k' - q, \sigma')c(k'\sigma')c^\dagger(k + q, \sigma)c(k, \sigma)}{\langle E_k - E_{k + q}\rangle^2 - (\hbar\omega_q)^2},$$

(3)

where the first two terms in equation (1) define the non-
interacting ground state kinetic energy (or the kinetic energies
below and above the Fermi surface ($k_F$)), while equation (2) is
an operator and is not corrected for ionic screening because it
has been taken care of in $H_{\text{Coulomb}}$ by definition. The normal
metal is captured by the first three terms on the right-hand
side (rhs) of equation (1) such that the first two terms are
constants that do not play any role in the mechanism of
Cooper pairing. However, the first three terms ignore the
electron–phonon scattering where in the absence of Cooper
pairing, the fourth term in equation (1) reduces to the standard
electron–phonon interaction. Apparently, the fourth term in
equation (1)) turned the electron–phonon interaction into
Cooper pairing, but then, this particular term needs to compete
with the screened coulomb potential (which gives rise to electron–electron repulsion) to produce superconductivity.
Given this background, it should be noted that BCS did
not derive the Cooper-pair operator from the first principles,
instead, they constructed it based on the notion of Cooper-
pairing mechanism [1]. Here, we shall derive the Cooper-pair
attraction operator from the first principles. Secondly, we
shall also derive the mechanism that defines the existence of
superconducting critical temperature due to the above-said
competition.

Apart from that, $|s_{k,k'}|^2 = |\langle \psi_k | H_{\text{e:ph}} | \psi_{k'} \rangle|^2$, $H_{\text{e:ph}}$ denotes the usual e:ph interaction Hamiltonian and the crystal
momentum is conserved ($k + k' = (k + q) + (k' - q)$) as
required. Next, the symbol $n_{k\sigma}$ is the electron number
operator with spin, $\sigma$, $K_i$ denotes the Thomas–Fermi screen-
ing length, $k$ and $|k| = k$ are the respective wave vector and
wavenumber for an electron, while $q$ and $\omega_q$ are the phonon
wave vector and frequency, respectively. The screened
coulomb-Hamiltonian (see equation (2)) gives the e:e repul-
sion after factoring in the screening effect, $\hbar$ is the Planck
constant divided by $2\pi$. $\epsilon_0$ denotes the permittivity of free
space and $e$ is the electron charge. The factor $1/2$ avoids
counting the same Cooper pair twice, if $\sigma = \uparrow$ then
$\sigma' = \downarrow$, $k' = -k$ such that $k + k' = q = 0$. The last two
requirements on $\sigma' = -\sigma$ and $q = 0$ are to maximize
$|H_{\text{Cooper}}^{\text{pair}}|$ defined in equation (3), which are as they should be
if one were to determine the superconducting ground state
with efficient phonon exchange between two electrons
forming a Cooper pair. Here, $|H_{\text{Cooper}}^{\text{pair}}|$ removes the negative
sign due to electron–phonon induced electron–electron
attraction.

Finally, the e:ph coupling constant or its matrix element
is denoted by $s_{k,k'}$, $e^8(\cdots)$ and $c(\cdots)$ are the usual electron
creation and annihilation operators, respectively. For example,
$c^\dagger(k + q, \sigma)$ creates an electron by absorbing a phonon

after annihilating the electron (prior to absorption) with $c(k, \sigma)$.
The formation of a Cooper pair requires another electron to
emit the previously absorbed phonon such that the second
electron is first annihilated, $c(k', \sigma')$, and then recreated by
emitting the absorbed phonon, $c^\dagger(k' - q, \sigma')$. Therefore,
the electron with $k + q$ and $\sigma$ is paired with the second electron
with $k' - q$ and $\sigma'$, and they form a Cooper pair.

Note this, the transition to superconducting phase is readily
achieved for $H_{\text{Coulomb}}$ < $|H_{\text{Cooper}}^{\text{pair}}|$; while preformed
Cooper pairing above $T_{sc}$ is possible if $H_{\text{Coulomb}}$ > $|H_{\text{Cooper}}^{\text{pair}}|
and $|H_{\text{Cooper}}^{\text{pair}}| > 0 \Rightarrow E_k - E_{k + q}$. If $E_k - E_{k + q} = 0$, then
$H_{\text{Cooper}}^{\text{pair}} = 0$ and consequently, Cooper-pair concentration is
zero. Moreover, physically $(E_k - E_{k + q})^2 \geq (\hbar\omega_q)^2$ is not
allowed because if we were to use ‘=’, then this would imply
perfect phonon exchange between electrons, while ‘>’ means
electrons can absorb phonons with energies larger than the
largest available phonon energy. But in any case, $H_{\text{Cooper}}^{\text{pair}}$ is
zero by definition for this second condition. Clearly, phonon
induced scattering has been eliminated because they con-
tribute to Cooper pairing, and therefore, Bose condensation
of phonons is not required. Of course, in the absence of phonons
(at absolute zero), one has maximum BCS superconductor
gap as a result of maximum number of Cooper pairs and
efficient Cooper-pair formation because lattice distortion for
$T = 0$ K originates entirely from the emission and absorption
of phonons by the Cooper-pair electrons, via the temperature-
independent e:ph interaction.

To extend BCS Hamiltonian to cuprates, one needs to
understand the origin of equation (3), which can be traced
back to the derivation of the e:ph interaction term from the
second-order perturbation theory and Landau’s approach [23].
In particular, the e·ph potential operator reads [23],

\[
V^\text{repulsion}_{k,k'} = \frac{1}{2} \left\{ \frac{2\hbar\omega_q|g_{k,k'}|^2}{(\hbar\omega_q)^2 - (E_k - E_{k'-q})^2} + \frac{2\hbar\omega_q|g_{k,k'}|^2}{(\hbar\omega_q)^2 - (E_k - E_{k'-q})^2} \right\}.
\]  

(4)

\[
\approx \frac{2\hbar\omega_q|g_{k,k'}|^2}{(\hbar\omega_q)^2 - (E_k - E_{k'-q})^2},
\]  

(5)

\[
\approx \frac{2\hbar\omega_q|g_{k,k'}|^2}{(\hbar\omega_q)^2 - (E_k - E_{k'-q})^2},
\]  

(6)

after the removal of the energy-level spacing (\(\xi\)) term, \(\exp[(1/2)\lambda(\xi - E^F_0)]\) by taking \(\lambda = (12\pi e^2/\varepsilon_0 a_B)\) where \(a_B\) is the Bohr radius and \(E^F_0\) denotes the Fermi level for \(T = 0\). Here \(V_{kk'}\) is positive because \((\hbar\omega_q)^2 > (E_k - E_{k'-q})^2\), and large e·ph interaction (or large \(E_k - E_{k'-q}\)) leads to large e·e repulsion [14], which is also inevitable from equation (6) where \(E_k\) and \(E_{k'-q}\) refer to the same electron (before and after phonon absorption). The phonon exchange based on equation (4) that produces electron–electron repulsion does not demand any unique relationship between \(k, k', q\), and \(q'\) because the same electron does not absorb or emit the same phonon such that the phonon exchanges are random and the crystal momentum is conserved.

Here, we have considered that when one of the electrons emits (equation (5)) a phonon, the other electron does not absorb (equation (6)) the same phonon, giving rise to the usual e·e coulomb repulsion where we have assumed \(q \approx q'\) on average. In addition, we can define the first and second electrons to have opposite spins. This electron interacts strongly with another electron if \(E_k = E_{k'-q}\) is large, which is implicit from equation (6). This interaction is obviously always repulsive between two different electrons, which can only be converted into an effective attraction between these electrons by switching the signs for \(+/(\hbar\omega_q)^2\) and \(-/(E_k - E_{k'-q})^2\) in the denominator of equation (6).

This sign-switch converts the repulsive interaction into an attraction because as stated earlier, \((\hbar\omega_q)^2 \leq (E_k - E_{k'-q})^2\) is physically impossible. This switch uniquely leads us to Cooper-pairing mechanism where one of the electrons interact attractively with another electron via absorption (electron 1) and emission (electron 2) of phonons. In particular, the said sign-switch in equation (6) naturally activates the formation of Cooper pairs via the following notions—'if' \(E_k = E_{k'-q}\) is true for the second electron, and 'if' \(E_k' = E_{k'-q}\) is also allowed to be true for the first electron, and 'if' these changes in energies (for both electrons) should occur faster than the phonon timescale, \(t_{ph} = 1/\omega_q\), then the formation of Cooper pairs is inevitable. Here, the electrons always respond faster than phonons \(t_{ph} = 1/\omega_q > t_c = 1/E_k\) because \(E_k > \hbar\omega_q\), \(E_{k'+q} > \hbar\omega_q\), \(E_k' > \hbar\omega_q\), and \(E_{k'-q} > \hbar\omega_q\). Implementing the above notions (the highlighted 'if's) leads one to transform equation (4) into,

\[
V^\text{attraction}_{k,k'} = \frac{1}{2} \left\{ \frac{2\hbar\omega_q|g_{k,k'}|^2}{-(\hbar\omega_q)^2 + (E_k - E_{k'-q})^2} + \frac{2\hbar\omega_q|g_{k,k'}|^2}{-(\hbar\omega_q)^2 + (E_k - E_{k'-q})^2} \right\},
\]  

(7)

\[
= \frac{2\hbar\omega_q|g_{k,k'}|^2}{-(\hbar\omega_q)^2 + (E_k - E_{k'-q})^2},
\]  

(8)

\[
= \frac{2\hbar\omega_q|g_{k,k'}|^2}{-(\hbar\omega_q)^2 + (E_k - E_{k'-q})^2}.
\]  

(9)

In this case, when one of the electrons emits (equation (8)) a phonon, the other electron absorbs (equation (9)) the same phonon, giving rise to the el·el BCS attraction where obviously \(q = q'\). After incorporating the creation and annihilation operators for both electrons, the factor 1/2, the sum to count all the occupied states in momentum space, and of course, after tacking the spin (\(\sigma\) or \(\sigma'\)) for each electron as required to form strongly bounded Cooper pairs, one can obtain equation (3) from (9). The arguments used to derive equation (3) from (6) were also exploited to construct the ‘first paragraph’ in the introduction. For example, phonon-induced scattering has been eliminated without enforcing phonons to Bose condense. Note this, much stronger Cooper pairs (large \(V^\text{attraction}_{kk'}\)) can be formed (from equation (3) or (9)) if one could further enhance the electron–ion attraction strength such that \((\hbar\omega_q)^2 \gg (E_k - E_{k'-q})^2 \rightarrow (\hbar\omega_q)^2 > (E_k - E_{k'-q})^2\). The second inequality shall lead us to a much smaller denominator, and therefore to a large \(V^\text{attraction}_{kk'}\) or \(H^\text{Cooper-pair}\). The first inequality is for conventional superconductors.

On the other hand, if the above highlighted ‘if’s are not true, then Cooper pairing is not possible, and therefore, equation (9) or (3) needs to transform in order to be superseeded by coulomb repulsion between electrons, giving rise to an insulating ground state or a strange metallic phase. In this case, equation (9) or (3) reverts to equation (6), which in turn implies the existence of finite-temperature phase transition (FPT\(^{(0)}\)), which actually follows from the competing effect that shall be captured in equation (28). Here, one is naturally led to relate this phase transition to strange metallicity to superconducting-phase transition, or more precisely, the transition from equation (6) (for \(T > T_c\)) to equation (9) (or equation (3)) below \(T_c\) we shall comeback to this point later.

Now assuming equation (3) or (9) activates the formation of weakly-coupled BCS Cooper pairs (by assuming \((\hbar\omega_q)^2 \gg (E_k - E_{k'-q})^2\)), one can surmise that \(F^\text{Cooper-pair}_{\text{screened}}\) is a constant such that \(\langle H^\text{Cooper-pair}_{\text{screened}} \rangle = \langle V_{kk'} \rangle = V' < 0\) where for convenience, \(|V'| > V > 0\) is defined to cause the attraction between electrons. Based on this approximation, BCS
moved on to construct an elegant Hamiltonian [1],

\[ H_{\text{BCS}}^{\text{reduced}} = 2 \sum_{k \neq k'} c_k^* b_k b_{k'} + 2 \sum_{k \neq k'} |c_k| b_k c_{k'}^* - V \sum_{k k'} b_k^* b_{k'}, \]  

(10)

by assuming that each Cooper pair is a boson-like particle, and these (ground state) pairs only form in the vicinity of Fermi energy (\( E_F \)). But Cooper pairs are composed of electrons, and these pairs are not bosons in a real physical sense due to Cooper-pair formation mechanism explained earlier between equations (3) and (6). This means that, a Cooper pair as an independent boson-like entity cannot obey FDS or Bose–Einstein (BES) statistics [1]. However, the electrons in Cooper pairs do obey FDS, which will also be addressed later.

In equation (10), \( b_k^* \) and \( b_k \) creates and annihilates a Cooper pair (two electrons), respectively, hence the factor 2, \( b_k^* = c_{k \uparrow}^* c_{k \downarrow}, b_k = c_{k \uparrow} c_{k \downarrow}, b_k^* = (1 - n_{k \uparrow} - n_{k \downarrow}) j_{k \downarrow}, \) where \( j_{k \downarrow} = c_{k \downarrow}^* c_{k \downarrow} \), \( [b_k, b_{k'}] = 0, \) \( [b_k, b_k^*] = 2n_{k \downarrow} b_k \), \( n_{k \downarrow} = c_{k \downarrow}^* c_{k \downarrow} \), \( \Delta_{\text{BCS}} \) is not a constant, and the attraction is uniquely between two electrons. We then go on to derive the FDS for the electrons that have formed Cooper pairs between \( T = 0 \) and \( T_{\text{sc}} \) such that these pairs are still boson-like. Finally, we prove the existence of (a) doping(\( \xi \))-dependent \( T_{\text{sc}} \), controlled by Cooper-pair (or superfluid) density \( n_{\text{pair}}(\xi)^{\text{ff}} \), and (b) \( \text{FPT}^{10 \text{K}} \) giving rise to the \( C_{\text{sc}} \) discontinuity at the critical point \( (T_{\text{sc}}) \). The above objectives shall be properly covered in the following sections.

2.2. Strongly bounded Cooper pairs

Earlier, stronger e:ph interaction is shown to have the physical capability to produce two types of e:e interactions (see equations (6) and (9)), one is the expected coulomb repulsion, while the other is due to Cooper attraction. The said repulsion and attraction between electrons refer to \( (\hbar \omega_{q}^2 - (E_k - E_{k+q})^2 > 0) \), respectively. Hence, \( V_{k k'} \) should accommodate both equations (4) and (7), which means,

\[ V_{k k'} = \left\{ \begin{array}{ll}
V_{k k'}^{\text{repulsion}} : & \text{for } \{(\hbar \omega_{q}^2 - (E_k - E_{k+q})^2 > 0)\} \\
V_{k k'}^{\text{attraction}} : & \text{for } \{-\hbar \omega_{q}^2 + (E_k - E_{k+q} - \Delta)^2 < 0\}
\end{array} \right. \]  

(12)

where stronger repulsion and attraction can be achieved by a larger magnitude of \( (E_k - E_{k+q})^2 \). Equation (12) has been constructed on the basis of these two different physical mechanisms, \( \{(\hbar \omega_{q}^2 - (E_k - E_{k+q})^2 > 0)\} \) and \( \{-\hbar \omega_{q}^2 + (E_k - E_{k+q} - \Delta)^2 < 0\} \), which implies the existence of finite-temperature phase transition—\( V_{k k'}^{\text{repulsion}} \) (normal state) \( \rightarrow V_{k k'}^{\text{attraction}} \) (superconducting state).

In view of equation (12), the original BCS Hamiltonian in the extended version within the framework of IET should read,

\[ H_{\text{BCS}}^{\text{extended}} = \sum_{k \neq k'} E_k n_{k \sigma} + \sum_{k \neq k'} |E_k| (1 - n_{k \sigma}) + \sum_{k k'} V_{k k'}, \]  

(13)

where \( H_{\text{BCS}}^{\text{screened}} + H_{\text{pair}}^{\text{BCS}} \) from equation (1) have been transformed into \( V_{k k'} \) (see equation (12)) such that \( H_{\text{BCS}}^{\text{screened + pair}} \rightarrow [H_{\text{BCS}}^{\text{screened}} + H_{\text{pair}}^{\text{BCS}}] \rightarrow [V_{k k'}^{\text{attraction}} + H_{\text{pair}}^{\text{BCS}}] = V_{k k'} \) for \( \text{BCS} \) Coulomb and Cooper interaction. This transformation is theoretically valid because the electrons in the extended BCS Hamiltonian are no longer Fermi liquid (weakly interacting), instead the electrons are subject to strong correlation as captured by IET. Here, \( V_{k k'} \) denotes the general renormalized screened electron–photon potential operator that captures the strange metallic phase (above \( T_{\text{c}} \)) and the superconducting phase (below \( T_{\text{c}} \)) under certain conditions.

For example, the normal electron (see equation (12)) that happen to absorb \( \hbar \omega_{q} \) may not emit the same phonon, hence, the label \( q = q' \) in \( V_{k k'}^{\text{repulsion}} \). In contrast, a Cooper electron always absorb and emit the same phonon, which carry the label \( q = q' \) in \( V_{k k'}^{\text{attraction}} \). In addition, if a particular electron (that is not part of a Cooper pair) absorbs or emits \( (E_k - E_{k+q}) \) a relatively high-energy phonon, \( \hbar \omega_{q} \), then \( (\hbar \omega_{q}^2 - (E_k - E_{k+q} - \Delta)^2 < 0) \), which readily leads to large \( V_{k k'}^{\text{repulsion}} \) where \( \hbar \omega_{q} > \hbar \omega_{q} \).

The reader should be aware of this fact—in the Hartree–Fock formalism, the exchange interaction term is given by \([20, 21],(14)\)

\[ \frac{1}{2} \sum_{i j} \int \psi_i^{HF}(\mathbf{r}_i)^* \psi_i^{HF}(\mathbf{r}_j)^x e^2 \frac{4\pi}{\varepsilon_0 |\mathbf{r}_i - \mathbf{r}_j|} \times \left[ -\psi_i^{HF}(\mathbf{r}_i) \psi_j^{HF}(\mathbf{r}_j)^x \right] d\mathbf{r}_i d\mathbf{r}_j, \]  

(14)

which decreases the Hartree–Fock total energy due to spin-exchange interaction. First, note that this exchange interaction
is not related to the repulsion energy term given in equation (6). Secondly, the negative sign in equation (14) is due to Pauli’s exclusion principle [20, 21],

$$\psi^{\text{HF}}(r_1, r_2) = -\psi^{\text{HF}}(r_2, r_1).$$  \hspace{1cm} (15)

In contrast, the negative sign in equation (9) is obtained by physically demanding one of the terms in the denominator, \((\hbar \omega_q)^2\) is larger than \((E_k - E_{k+q})^2\), which is in accordance with the second law of thermodynamics. In addition, we also have enforced that \((\hbar \omega_q)^2\) carries a negative sign, while \((E_k - E_{k+q})^2\) is positive by demanding that the phonons with energy, \(\hbar \omega_q\) is always exchanged between the electrons to form Cooper pairs. Hence, these phonons are not independent of the electrons. If these phonons are not exchanged between electrons (meaning, the phonons are free to vibrate independent of the electrons), then these phonons scatter the electrons, and the electrons themselves scatter the other neighboring electrons due to the usual electron–electron repulsion. Thus, these sign-switch mechanism has got nothing to do with Pauli’s exclusion principle. In particular, the sign-switch mechanism makes perfect sense by noting that in the repulsion term given in equation (6), if the phonons are eliminated, then \((\hbar \omega_q)^2\) is zero and \(\lim_{\omega_q \to 0} \frac{\langle \omega \rangle}{\langle \omega \rangle_{\text{renormalized}}} \leq 0\). Even though the said limit is physically false, but it provides the physical origin of the sign-switch mechanism.

In order to derive the negative sign, we first need to start from the second-order perturbation theory (similar to the derivation of \(V_{\text{repulsion}}^{\text{phonon}}\) that has a positive sign). The second-order correction to energy is given by,

$$E_{m}^{(2)} = \sum_{m=0}^{\infty} \frac{\langle \psi^{(0)}_{m} | H_{\text{el-ph}} | \psi^{(0)}_{m} \rangle^2}{E_{m}^{(0)} - E_{m}^{(0)}},$$  \hspace{1cm} (16)

which leads us to the usual repulsive interaction, and in this case, the energy denominator reads,

$$E_{m}^{(0)} - E_{m}^{(0)} = \left\{ \begin{array}{l} \frac{1}{2} \lambda(\xi - E_{m}^{(0)}) \end{array} \right\} - E_{m}^{(0)}.$$

Here, \(\psi^{(0)}_{m}\) and \(\psi^{(0)}_{m}\) are the orthonormalized (zeroth-order or unperturbed) wavefunctions, while equation (17) captures the energy difference due to phonon absorption by the electrons. On the other hand, if we were to also demand the electron to emit the absorbed phonon (as demanded by the Cooper mechanism), then the energy denominator should read,

$$E_{m}^{(0)} - E_{m}^{(0)} = \left\{ \begin{array}{l} \frac{1}{2} \lambda(\xi - E_{m}^{(0)}) \end{array} \right\} - E_{m}^{(0)}.$$

After using Landau’s approach, and after going through the energy-level spacing renormalization procedure, equations (16) and (18) would eventually lead us directly to \(V_{\text{repulsion}}^{\text{phonon}}\), with the negative sign (see the appendix for details). In particular, the exponential term that appears in equations (17) and (18) originates from the energy-level spacing renormalization that captures the interaction between a bound electron and its nucleus, which in turn influences the phonon frequency. Even though the energies in the denominator of equation (16) are bare energies, \(E_{m}^{(0)} - E_{m}^{(0)}\), however these bare energies are substituted accordingly with \(E(k), E(k)\) and \(\hbar \omega(k - k)\exp\left(\frac{1}{2} \lambda(\xi - E_{m}^{(0)})\right)\) as shown in equation (18), which are renormalized parameters. These renormalized parameters are not trivial, and for details see [23]. Secondly, other higher-order corrections are assumed to be small enough to be negligible in superconductors as a result of the energy-level spacing renormalization and the dominant Cooper-pair mechanism. Note this, the said higher-order corrections have to be negligibly small, for otherwise, superconductivity due to Cooper-pair mechanism cannot occur.

Later, we shall observe (with more details) as to why superconductivity becomes a possibility when and only when \(\langle V_{\text{repulsion}}^{\text{phonon}}\rangle > \langle V_{\text{repulsion}}^{\text{phonon}}\rangle\). Most importantly, for \(V_{\text{repulsion}}^{\text{phonon}}\) to be valid, phonons are exclusively exchanged between the electrons such that the phonons absorbed by the electrons are emitted, which are then re-absorbed by the electrons indirectly through the vibrating ions, and this process repeats. We stress here that in this process, there are no significant direct exchange of phonon energies between electrons. Direct phonon exchange between electrons shall always give rise to electron–phonon scattering due to unexchanged phonons, which shall also activate the standard coulomb repulsion between electrons.

Having said that, we can now deduce that for a Cooper electron to be strongly bounded to another Cooper electron, one also requires \(E_k - E_{k+q}\) to be large. However, an additional requirement is needed such that \(E_k - E_{k+q}\) for electron 1 should also lead to \(E_k - E_{k+q}\) for electron 2 where electron 1 and 2 form a Cooper pair. The spins can be suppressed because it is straightforward to note that \(k\) and \(k'\), refer to \(\sigma\) and \(\sigma'\), respectively, and high-energy phonon exchange between electron 1 and 2 gives rise to high binding energy for Cooper pairs, and consequently a larger \(V_{\text{repulsion}}^{\text{phonon}}\). Even if electron 1 and 2 has been considered as a single entity (boson-like) by BCS, but in our formalism, these electrons (1 and 2) are treated as individuals, as they should be. Treating each Cooper-pair electrons as an individual particle does not violate the original boson-like Cooper-pair formation mechanism (bounded due to \(V_{\text{repulsion}}^{\text{phonon}}\)), which can be shown to be valid from the following BCS identity,

$$[b_k, b_{k}^*] = (n_k \delta_{\uparrow \downarrow} - n_{-k} \delta_{\downarrow \uparrow} + \epsilon_{k} \delta_{-k} \downarrow \uparrow_{\downarrow} + \epsilon_{-k} \downarrow \uparrow_{\downarrow} \downarrow \uparrow_{k}) \delta_{kk},$$

where \(n_k\) and \(n_{-k}\) are the unpaired electron numbers, and therefore

$$[b_k, b_{k}^*] = (1 - n_k - n_{-k}) \delta_{kk},$$

after letting \(\epsilon_{k} \downarrow \uparrow_{k} = 0\) and \(\epsilon_{-k} \downarrow \uparrow_{k} = 0\) due to \(\delta_{\uparrow \downarrow} = 0\) where \(\epsilon\) and \(c\) are the respective creation and annihilation operators for individual (unpaired) electrons. Here, the number of Cooper pairs has to be \(1 - n_k - n_{-k}\) for \(k = k'\) as given in equation (20). Apparently, the creation and annihilation of Cooper pairs (\(b\) and \(b\)) require the creation and
annihilation of individual electrons such that they can be paired.

Since our Cooper pairs have large binding energies compared to conventional superconductors, one has no other option but to supersede the BCS approximation, \( \langle \omega_{k\bar{q}}^2 \rangle \gg (E_k - E_{k+q})^2 \) with \( \langle \omega_{k\bar{q}} \rangle > (E_k - E_{k+q})^2 \), which implies \( V_{kk'}^{\text{attraction}} \) can no longer be considered a constant (denoted earlier by \( V \)). Our next aim is to properly define \( V_{kk'}^{\text{attraction}} \) in such a way that it is also a function of atomic energy-level spacing, \( \xi \). We first make use of the energy-level spacing renormalization group method [23] to renormalize \( V_{kk'} \) and \( |s_{kk'}|^2 \) given in equation (6) to obtain (also after the sign-switch transformation),

\[
V_{kk'}^{\text{attraction}} = |s_{kk'}|^2 \frac{2/\hbar \omega_{k\bar{q}} e^{\frac{1}{2} (E_k - E_{k+q}^2))}}{\hbar \omega_{k\bar{q}} e^{\frac{1}{2} (E_k^2 - E_{k+q}^2))}} + \frac{1}{k} \bar{q} T_k \nabla \omega_{k\bar{q}} e^{\frac{1}{2} (E_k - E_{k+q}^2))}.
\]

(21)

(22)

where \( K_\xi \) has been defined earlier (see the text after equation (3)) and \( \Omega \) is the volume in momentum space. Our renormalization method employed here can be exactly mapped onto the Shankar’s wavenumber-dependent renormalization technique [25–27]. Now we invoke the large binding-energy condition that validates \( \langle \omega_{k\bar{q}} \rangle > (E_k - E_{k+q})^2 \) such that \( \Delta \langle \omega_{k\bar{q}} \rangle^2 \ll \Delta \langle E_k - E_{k+q}^2 \rangle \) where \( \Delta \) denotes the change in the stated variables due to temperature and doping applicable for cuprate superconductors. This inequality \((<)\) is understandable as the change in \( T_{el} \) \((\Delta T_{el})\) due to isotope effect \( \Delta \langle \omega_{k\bar{q}} \rangle \) at minute, compared to \( \Delta T_{el} \) as a result of \( \Delta \langle E_k - E_{k+q}^2 \rangle \) where \( (E_k - E_{k+q}) \approx k_B T_{el} \).

Physically, \( \hbar \omega_{k\bar{q}} e^{\frac{1}{2} (E_k - E_{k+q}^2))} \leq [E_k - E_{k+q}^2] \) is not allowed for two reasons—(i) \( \leq \rightarrow \) requires perfect phonon exchange, and on the other hand, (ii) \( \leq \rightarrow \) violates the second law of thermodynamics. Equation (21) tells us that one can increase \( T_{el} \) by increasing \( |s_{kk'}|^2 \) to be close to \( \hbar \omega_{k\bar{q}} e^{\frac{1}{2} (E_k - E_{k+q}^2))} \), which in turn implies large \( V_{kk'}^{\text{attraction}} \). To obtain large \( |s_{kk'}|^2 \) \((E_k - E_{k+q}) \), one also needs large \( |E_k - E_{k+q}| \) so as to set the stage for high Cooper-pair formation probability. Obviously, this probability can be enhanced if the density of states at the Fermi level is large, which is nothing but what is required from the BCS gap equation, equation (11) through \( N(0) \).

Another important implication of BCS Cooper-pair formation with respect to equation (21) (with or without extension) is the existence of a proper supercurrent-flow mechanism [1] such that the scattering rates \( (1/\tau) \), induced by the electron–phonon \((1/\tau_{e-ph})\), electron–electron \((1/\tau_{e-e})\) and spin–disorder \((1/\tau_{sc})\) scattering processes are literally zero. As explained earlier, \( E_{k+\bar{q}} - E_{k+q} \rightarrow E_{k+\bar{q}} - E_{k+q} \) for the first electron require the second electron to satisfy \( E_{k+\bar{q}} - E_{k+q} \), which imply \( 1/\tau_{e-ph} = 0 = 1/\tau_{e-e} \) because the Cooper-pair formation mechanism obviously requires these systematic changes in momenta, \( k' \rightarrow k' - q \) and \( k \rightarrow k + q \), and also due to \( V_{kk'}^{\text{attraction}} \). Here, we do not need \( \nu_{k\bar{q}}^{\text{repulsion}} \) to obtain \( 1/\tau_{e-e} = 0 \) because the e:e and e:ph scattering processes are entirely responsible for the above stated momentum-change in the first and second electrons.

Now, \( 1/\tau_{sc} \) is also zero because the first electron with spin, \( \sigma \) do not scatter the second electron with spin, \( \sigma' \) if these two electrons momenta change in this way, \([k', \sigma' \rightarrow k' - q; \sigma', \sigma'] \) and \([k, k \rightarrow k + q, \sigma] \) for \( \sigma \) and \( \sigma' \) respectively. In other words, the above scattering processes are not zero, but they are entirely responsible to initiate the required phonon-mediated momentum-change for Cooper-pair formation, and therefore, these scattering processes do not cause resistance, which means, \( 1/\tau_{sc} = 0 = 1/\tau_{e-ph} \). The above exposition also applies to triplet pairing symmetry where we just need to allow an additional criterion, \( \sigma = \sigma' \) for such pairing.

The above arguments on the supercurrent flow were constructed from the extended BCS theory within IET. These arguments by themselves do not prove the existence of supercurrent flow in superconductors because such a proof is available in [1]. But in any case, our supercurrent flow arguments at least agree with the original formalism of BCS theory such that the extended theory presented here does not ignore this essential requirement, \( 1/\tau_{e-ph} = 0 = 1/\tau_{e-e} = 1/\tau_{sc} \) as it should be for superconductivity. We also did not require the spins to fluctuate in order to induce electron-pair formation because in such a case, we are left puzzled as to the reason why and how the spin-disorder scattering, \( 1/\tau_{sc} \) can be zero. The details on \( 1/\tau_{sc} \) within the transport theory of ferromagnets can be found in [28]. Therefore, alternative theories should first settle the primary issues of superconductivity with respect to (a) supercurrent-flow mechanism, (b) Meissner effect, (c) specific heat capacity jump at the critical temperature and (d) doping-dependent critical temperature and resistivity for \( T > T_c \).

Apart from that, magnetic interaction can and should exist in one form or another in cuprates or other unconventional superconductors because cuprates are antiferromagnets (with different types of atoms arranged in different sequences in \( ab \)-plane compared to \( c \)-axis), and moreover, Cooper-pair binding energy also depends on the electron’s spin (see equations (3), (19) and (20)). But, as we have said many times now, and as unambiguously shown above, the magnetic interaction is unlikely to be the cause for electron pairing. Another point to note here is that even though phonons are responsible for superconductivity, but this does not mean that phonons in general enhance the \( T_c \) in superconductors. What this means is that—only phonons that contribute to Cooper-pair formation \((V_{kk'}^{\text{attraction}})\) enhances \( T_{el} \), while the phonons that do not involve in Cooper pairing contribute to \( 1/\tau_{e-ph} = 0 \) (due to \( V_{kk'}^{\text{repulsion}} \)), which in turn reduces \( T_{el} \). Hence, the energy exchanged between an electron and a phonon is always conserved such that the phonons responsible for Cooper pairing is of different energy scale than that of the phonons that give rise to electron scattering and retain the electron–electron repulsion. In other words, the energy exchanged between an electron and a phonon to form Cooper pair is conserved, while the exchanged energy in the absence of pairing that gives rise to electron–phonon scattering is also...
independently conserved. The energy scale for the Cooper-pair formation and for the electron–phonon scattering had to be independently conserved because they originate from two different and independent physical processes (as already invoked earlier in equations (6) and (9)). See also the appendix for the derivation of attractive interaction.

In summary, even though BCS Hamiltonian is not perfect, but its correctness and consistency on the basis of well established microscopic physics are unparalleled (compared to other alternatives), even when the Cooper-pair binding energy is made to be large by replacing the BCS condition $(\hbar\omega_q)^2 > (E_k - E_{k+q})^2$ with $(\hbar\omega_q)^2 > (E_k - E_{k+q})^2$. Hence, one should be convinced by now that the BCS Hamiltonian can handle high $T_c$ materials, as well as other unconventional superconductors.

The theory of Eliashberg-Migdal reviewed in [29–31] has considered the effect of strongly bound Cooper pairs by allowing some additional effects (known as the retardation effects) that could be used to convert the weaker electron–phonon interaction into a stronger one. Indeed, Eliashberg-Migdal theory goes beyond BCS theory in a sense that it incorporates the so-called retardation effects, which also give rise to anisotropic superconductor gap, mass enhancement, and the correct value, $2\Delta_{BCS}/k_B T_c = 4.5$ for Pb, which is closer to the experimental value. In contrast, BCS theory gives a smaller universal value, $2\Delta_{BCS}/k_B T_c = 3.53$. However, the said theory made exclusive use of the usual Landau’s Fermi-liquid theory (with quasiparticle picture remains intact) within Gorkov’s Green-function formalism [32]. Hence, despite the said improvement with retardation effects, Eliashberg-Migdal theory is still a weak coupling theory that relies on the weakly-interacting electrons with Fermi energy as the dominant energy. In summary, Eliashberg-Migdal and the extended BCS theory within IET do complement each other. However, the primary difference is—our formalism provides the missing links to explain the strange metallic phase, the doping-dependent effects and the finite-temperature phase transition from the normal-to-superconducting state (see the conclusions) within the strongly coupled unconventional systems, whereas, the Eliashberg-Migdal theory improves the BCS theory within the weakly-coupled conventional systems.

2.3. FDS for Cooper-pair electrons

In the preceding sub-section, we have proven that the BCS attraction operator is a special case (see equation (12)) that allows the formation of Cooper pairs, composed of two individual electrons, coupled attractively by means of emission and absorption of phonons. This picture of looking at each Cooper-pair electrons individually shall allow us to derive the FDS for both Cooper-pair and unpaired electrons. In particular, each Cooper pair is not considered as a single boson-like entity (because it is neither a boson nor a two-fermion entity in a real physical sense), but as two individual electrons with changes in energies, $E_{k_1} - E_{k_1'}$ and $E_{-k_1} - E_{-k_1'}$ such that they are coupled attractively due to phonon exchange. Additionally, Cooper-pair formation satisfies the conservation of crystal momentum where $k + (-k) = k' + (-k') = k + q + (-k - q) = 0$.

As a consequence of the above picture, one can readily exploit the FDS to understand the excitation probability of Cooper pairs. Here, the excitation of Cooper-pair electrons simply means breaking up of Cooper pairs. The restrictive conditions for both unpaired and Cooper-pair electrons are given by,

$$\sum_{i=1}^{\infty} n_i = N,$$

where $n_i$ counts each electron, $i = 1, 2, \cdots, N$. $N$ denotes the total number of electrons, including Cooper-pair electrons, and the factor $1/2$ in equation (24) avoids counting $|\langle V_{kk'}^{\text{attraction}} \rangle|$ twice because it takes two to activate the attraction. Moreover, $E > |\langle V_{kk'}^{\text{attraction}} \rangle|$, or at least $E > 0$ is always true physically because not all electrons can form Cooper pairs—it would be physically unacceptable if we were to assume that localized core electrons can and will form Cooper pairs. If $T \rightarrow T_c$, then $|\langle V_{kk'}^{\text{attraction}} \rangle| \rightarrow 0$ and at the same time $E \rightarrow E_{\text{FDS}}$ phase where $E_{\text{FDS}}$ is the total energy in the non-superconducting phase (above $T_c$).

The BCS dispersion relation, $E_{k^{\uparrow}} = \sqrt{\epsilon_k^2 + \epsilon_0^2}$ differs from equation (24) because the said dispersion is only valid for energies near the Fermi level [1] such that $E_{k^{\uparrow}} + E_{k^{\uparrow}} = 2\epsilon_0 = 2\Delta_{BCS}$ because $\epsilon_{k} \rightarrow 0$ and $\epsilon_{k'} \rightarrow 0$ where $E_{k^{\uparrow}} = \sqrt{\epsilon_k^2 + \epsilon_0^2}$. The limit $\epsilon_{k} \rightarrow 0$ implies all electrons near Fermi level are paired. In addition, if $k^{\uparrow}$ and $-k^{\uparrow}$ are unoccupied, then $k^{\uparrow}$ and $-k^{\uparrow}$ are occupied. In other words, the BCS dispersion relation only considers electrons that will form Cooper pairs near Fermi level. Anyway, after following the standard procedure [33] using equations (23) and (24), one should be able to derive the sought-after statistics for both Cooper-pair- and unpaired-electrons,

$$f_{\text{FDS}}^{\text{Cooper}} = \frac{1}{e^{E_{\text{FDS}}(\{V_{kk}\}^{\text{attraction}}) - E_{\text{FDS}}}/k_B T + 1},$$

where $E_{\text{FDS}} = \sum_{i=1}^{\infty} E_{FDS}^i$.

As anticipated, the above statistics correctly guides us to this fact—the probability for breaking up Cooper-pair electrons ($f_{\text{FDS}}^{\text{Cooper}}$) is diminished (as it should be) for decreasing $T$ or increasing $|\langle V_{kk}^{\text{attraction}} \rangle|$. Above $T_c$, $|\langle V_{kk}^{\text{attraction}} \rangle| \rightarrow 0$, $E \rightarrow E_{\text{FDS}}$ phase and therefore $f_{\text{FDS}}^{\text{Cooper}} \rightarrow f_{\text{FDS}}^{\text{standard}}$. Here, $f_{\text{FDS}}^{\text{standard}}$ can also be written as a function of $E_{\text{FDS}} = E' + |\langle V_{kk}^{\text{repulsion}} \rangle|$, where $E'$ denotes the non-interacting energy, which correctly points to the fact that large $e-e$ repulsion increases the energy-level spacing, leading to smaller excitation probability, $f_{\text{FDS}}^{\text{standard}}$ for the usual (unpaired) electrons. Hence, the above transformation, $f_{\text{FDS}}^{\text{Cooper}} \rightarrow f_{\text{FDS}}^{\text{standard}}$ is physically valid such that $f_{\text{FDS}}^{\text{Cooper}}$ is not only unique for Cooper-pair electrons, but it is also not ad hoc.
3. Results and discussion

3.1. Ionization-energy approximation

The origin of $T_{sc}$ has been exposed earlier (beyond equation (11)) on the basis of $V_{kk'}$ defined in equation (12) such that equation (3) is a special case. The phase transition from $V_{repulsion}^{kk'}$ to $V_{attraction}^{kk'}$ or vice versa is activated by FPT at 0 K. We also have extended the BCS Hamiltonian to capture cuprate superconductors by allowing the Cooper pairs to be strongly bounded (by requiring $(\hbar \omega_q)^2 > (E_k - E_{k+q})^2$).

In the subsequent sub-sections, we shall make the microscopic origin for the existence of FPT due to $V_{repulsion}^{kk'} \rightarrow V_{attraction}^{kk'}$ transformation explicit. This result should help us to understand the doping-dependent $T_{sc}$ effect. This notorious effect shall be tackled with the IET connotation on the basis of IET is that it cannot be used to predict $T_{sc}$ for a given material because the analysis is at best abstract at the lowest (or operator) level, which is already apparent from our analysis presented earlier. It so happens that, regardless of the approach employed, one cannot predict $T_{sc}$ microscopically, which shall be exposed on the fly later.

In addition, we should note that IET does not rely on wavefunctions, which means that IET does not require the knowledge on wavefunctions in order to compute the dynamical variables such as doping-dependent carrier density, specific heat capacity as well as the doping-dependent pairing interaction potential operator. Therefore, we are not able to compute the wavefunction-dependent variables, namely, the paired and the unpaired Fermi surfaces, and also the symmetry of the superconductor gap function. The said disadvantages are due to the defects found intrinsically within the energy-level spacing renormalization group method employed, and not of the theory of unconventional superconductivity and its mechanism derived here.

Apart from that, we should also be aware that wavefunctions shall always remain as guessed functions with adjustable parameters that cannot be used to prove a physical mechanism. This last statement should explain why the BCS operators renormalized within IET are used directly to construct the pairing mechanism and other doping-dependent variables (resistivity and heat capacity) by completely side-stepping the need to guess the wavefunctions. In particular, it is a scientific fact that can be deduced from the guessed-wavefunction methodologies that the wavefunction-dependent methods developed thus far (since the discovery of quantum mechanics) cannot be used to discover nor to explain the doping-dependent effects unambiguously such as the doping-dependent resistivity, doping-dependent specific heat capacity and the precise mechanism for the doping-dependent finite-temperature phase transition.

The advantage of using IET is profound as our analysis are not only microscopically precise, unambiguous and consistent (with no adjustable parameters), but can also be used to discover (i) exactly where does $V_{attraction}^{kk'}$ originate from (see equation (12)), (ii) that the Cooper-pair formation is indeed the correct mechanism for superconductivity in cuprates (see the analysis between equations (6) and (9)), and (iii) the possibility to pin down the precise microscopic mechanism for doping-dependent $T_{sc}$, which is controlled by $\eta_{Cooper}^{xx}$. Apart from these points ((i)-(ii)), one should also note this—only the lowest-level analysis can unequivocally prove whether a theory is free of any internal inconsistency.

We now briefly introduce IET. More details on IET and its formalism in different context have been reported in [14–17, 23, 34–39]. The term ionization energy ($\xi$) in IET is precisely the energy-level spacing ($\xi$) of a given system where $\xi_{system}$ varies systematically if one carries out a systematic substitutional doping. Here, the ionization-energy approximation can be employed to determine $\xi_{system}$ from its constituent atoms where the approximation reads [16, 17],

$$\xi_{system} = \sum_{j} \sum_{i} \frac{1}{z_{ij}} \xi_{ij}(x_{ij}^{ou}),$$  \hspace{1cm} (27)

where each $x_{ij}$ represents a particular atom in a given system such that $j > 1$ implies that there are more than one type of atoms, while $i$ counts the valence electrons for each type of constituent atoms. Here, $\xi_{ij}(x_{ij}^{ou})$ denotes the energy-level spacing for constituent atom, $x_{ij}^{ou}$ and its energy-level spacing or ionization energy values can be directly obtained from any validated databases listed in [40, 41]. Even though atomic energy-level spacing is known to exist since the early days of quantum mechanics, but its rigorous connection to energy-level spacing in condensed matter (composed of atoms) is not known to exist. We have proved this connection to be a physical law via the ionization-energy based FDS [16], IET Hamiltonian [14] and the renormalization group transformation [23].

If a system is made up of free electrons (Fermi gas) or weakly-interacting fermions (Fermi liquid), then IET or its approximation is literally useless because $\xi$ is either zero or it is a nonzero constant ($\xi = \xi_{irr} = 0$). In semiconductors and insulators however, $\xi$ is neither zero nor a constant, and it is known as the trivially relevant energy-level spacing (or $\xi_{irr} = 0$), and it can refer to a band or Mott-Hubbard or molecular gap. In the early days of our investigation [16], we have discovered that the strange metallic phase in cuprates above $T_{sc}$ has an anomalous gap, which turned out to be a nontrivial energy-level spacing, $\xi_{non} \neq 0$ [15]. It is nontrivial because the energy levels are degenerate (gapless) and yet, $\xi_{non} \neq 0$, and therefore, $\xi_{non}$ determines the electron transition probability between different orthogonal and degenerate wavefunctions [15]. Our immediate aim now is to formally incorporate $\xi_{non}$ into equation (9), and then analyze FPT at 0 K with respect to doping (or changing chemical composition).

3.2. Finite-temperature (quantum) phase transition

The quantum phase transition discussed herein is not based on the standard zero Kelvin quantum phase transition. In particular, the finite-temperature quantum phase transition exploited here has been rigorously proven to exist (with unequivocal experimental supports) in [20, 34–38, 42]. To
avoid unnecessary confusion (because QPT is originally defined to occur only for zero Kelvin), we shall call our phase transition as the finite-temperature phase transition. We do not call this phase transition as thermal phase transition because the said transition is caused by quantum mechanical processes that occur at a finite temperature or at a constant-temperature critical point. The microscopic origin for the existence of finite-temperature phase transition is depicted in equations (28) and (29) where the superconductor transition temperature is defined to exist due to the competition between the electron–phonon induced Cooper attraction and the electron–electron repulsion. Therefore, we know exactly which two microscopic interaction operators responsible for the entire ensemble of electrons and phonons that need to compete to produce the superconducting or the strange metallic phase. Hence the finite-temperature phase transition discussed here is not a mere assumption.

Having said that, we can now invoke $\xi_{\text{fin}}$ by realizing that these normalized wavefunctions, $\psi_{k,\sigma}$, $\psi_{k',\sigma'}$, $\psi_{k+q,\sigma}$, and $\psi_{k'-q,\sigma'}$ are orthogonal to each other by definition and they can be degenerate. The existence of strange metallic phase in cuprates above $T_c$, necessitates one to write $[E_k - E_{k+q}] = \xi_{\text{fin}} = \xi$ and $[E_k - E_{k'-q}] = \xi'$ following [15] where $\xi = \xi'$ if $q = q'$. From here onwards, our notation for $\xi_{\text{fin}}$ reverts to $\xi$ for convenience because we focus only on cuprates. Introducing this substitution into equations (6) and (9) gives us the large effective Cooper attraction between electrons,\n
$$\langle V_{\text{attraction}}^{\text{ib}} \rangle + \langle V_{\text{repulsion}}^{\text{ib}} \rangle = \frac{2\hbar\omega_q |\langle \psi_{k,\sigma} | \psi_{k',\sigma} \rangle|^2 e^{\frac{\xi^2}{\hbar\omega_q}}}{-\hbar\omega_q e^{\frac{\xi^2}{\hbar\omega_q}} + \xi^2} + \frac{2\hbar\omega_q |\langle \psi_{k+q,\sigma} | \psi_{k'-q,\sigma'} \rangle|^2 e^{\frac{\xi'^2}{\hbar\omega_q}}}{\hbar\omega_q e^{\frac{\xi'^2}{\hbar\omega_q}} - \xi'^2}$$

$$= \langle \psi_{k'-q,\sigma} | H_{\text{pair}}^{\text{ib}} | \psi_{k,\sigma} \rangle + H_{\text{screened}}^{\text{ib}}$$

(28)

where $\xi_{q-q}$ and $\xi'_{q-q}$ denote the different phonon exchange processes in the superconducting and in the normal phase, respectively, where $\xi$ in the exponential term refers to doping-dependent energy-level spacing such that $\xi^2 = \xi_{q-q}^2 = \xi_{q-q}'$. In addition, $H_{\text{screened}}$, defined in equation (23) in the absence of very large effective mass effect. One should be able to note that the two terms on the rhs of equation (28) do not cancel each other for all $\xi$ because these two terms originated from two different physical processes and phonon energy scales. In particular, one term (see equation (28) with $\xi_{q-q}'$ in the denominator) is responsible for the attraction between two electrons (see also equation (9)), while the other term (see equation (28) with $\xi_{q-q}'$ in the denominator) is due to the standard electron–electron repulsive interaction (see also equation (6)). Therefore, the averaged energy of phonons responsible for Cooper pairing is of different energy scale than that of the averaged energy of phonons, which gives rise to phonon scattering, which leaves the repulsion between electrons intact. Recall also that \(\hbar\omega_q e^{\frac{\xi^2}{\hbar\omega_q}} \leq \xi\) is physically not permitted as justified earlier, which explains why the denominator in the two terms on the rhs of equation (28) cannot be independently zero for any temperature nor for any physical system. Recall that this substitution is not applicable for conventional superconductors because the normal state of BCS superconductors satisfy Fermi gas ($\xi = 0$) or Fermi liquid ($\xi \rightarrow \xi_{\text{Fermi}} = 0$). In other words, the electron transition probability between the wavefunctions defined in equation (28) for BCS superconductors is always one because there is no energy barrier to cross over. In any case, we have gotten what we needed, namely, equation (28), which is in a suitable form to extract the necessary information on FPT $\sim 0.5K$.

It is straightforward to deduce the following features from equation (28). In the strange metallic phase, $\langle V_{\text{attraction}}^{\text{ib}} \rangle = 0$ and $\langle V_{\text{repulsion}}^{\text{ib}} \rangle$ is maximum, and for $T = T_c$, FPT $\sim 0.5K$ is activated such that FPT $\sim 0.5K$ when $\langle V_{\text{attraction}}^{\text{ib}} \rangle = 0$ and $\langle V_{\text{repulsion}}^{\text{ib}} \rangle > \langle V_{\text{repulsion}}^{\text{ib}} \rangle$. Interestingly, we may have preformed Cooper pairs for $T > T_c$ and only if $\langle V_{\text{attraction}}^{\text{ib}} \rangle < 0$ and $\langle V_{\text{attraction}}^{\text{ib}} \rangle < \langle V_{\text{repulsion}}^{\text{ib}} \rangle$ where $n_{\text{pair}}$ is not sufficiently high to activate FPT $\sim 0.5K$. In addition, the existence of preformed Cooper pairs does not imply that FPT $\sim 0.5K$ or the transition to superconducting phase is inevitable. For $T < T_c$ and when $T \rightarrow 0$, $\langle V_{\text{attraction}}^{\text{ib}} \rangle$ should approach zero, while $\langle V_{\text{attraction}}^{\text{ib}} \rangle \rightarrow 0$ maximum when $\langle V_{\text{repulsion}}^{\text{ib}} \rangle$ can be zero because both $\langle V_{\text{attraction}}^{\text{ib}} \rangle$ and $\langle V_{\text{repulsion}}^{\text{ib}} \rangle$ refer only to electrons (near Fermi level) that can form Cooper pairs. In contrast, the restrictive condition given in equation (28) counts all the electrons in a given system, and therefore, $E > 0$ is mandatory because of core electrons contribution where $E$ here is the total energy (see equation (24)) of both Cooper and all the normal (or unpaired) electrons. Hence, the total energy, $E$ does not solely capture the electrons (both paired and unpaired) near the Fermi level.

Let us now discuss the consequence of changing $\xi$ (due to doping) on $\langle \xi_{\text{repulsion}}^{\text{ib}} \rangle$ and $\langle \xi_{\text{attraction}}^{\text{ib}} \rangle$. The effect of varying $\xi$ that comes from an exponential term in the numerator is more or less canceled by the same term in the denominator (see equation (28)). Whereas, $|\langle \psi_{k,k} |\rangle$ (defined in equation (22)) is proportional to $\xi$, which is as it should be because increasing $\xi$ should results in the amplification of $\langle \xi_{\text{attraction}}^{\text{ib}} \rangle$ (see equation (28)). This repulsion is also further enhanced if $\xi_{q-q}'$ in the denominator becomes large provided that $\hbar\omega_q e^{\frac{\xi^2}{\hbar\omega_q}} \leq \xi^2$ increases slower than $\xi^2$ or $\Delta / \hbar\omega_q e^{\frac{\xi^2}{\hbar\omega_q}} < \Delta \xi^2$. Another essential point here is that the repulsion do not require a second electron to emit ($k - \mathbf{q}$) the absorbed phonon by the first electron (see equation(3)), and this leads to a maximum repulsion.

In contrast, the relationship between $\xi$ (due to doping) and $\langle \xi_{\text{attraction}}^{\text{ib}} \rangle$ is not so straightforward because $\xi$ does not determine the formation of Cooper pairs, or $\xi$ is not the cause for superconductivity. As explained earlier, superconductivity occurs if the second electron happens to emit the phonon absorbed by the first electron. If this scenario (systematic emission and absorption of phonons) occurs exclusively for large number of electrons, then (and only then), $\langle \xi_{\text{attraction}}^{\text{ib}} \rangle$
becomes relevant in such a way that these Cooper pairs shall lead to FPT\(_{sc}\), provided that \(\langle V_{\text{attraction}}^{s} \rangle > \langle V_{\text{repulsion}}^{s} \rangle\).

This means that, predicting a superconducting material is a hard problem because the source for the existence of \(V_{\text{attraction}}^{s}\) is not predictable by definition, even within the BCS Hamiltonian. For example, we do not know exactly what observable (or measurable) parameter causes (or induces) this scenario—when one electron absorbs a phonon, the second electron happens to emit an identical phonon (note this point). What we know (from BCS Hamiltonian) is that we need large \(N(0)\) to increase \(T_{sc}\), but it is not responsible for superconductivity. This is similar to \(\xi\), which is also not responsible for superconductivity. This means that, if a particular system is a superconductor, then we can invoke \(\xi\) to evaluate the changes to \(\langle V_{\text{attraction}}^{s} \rangle\) or \(T_{sc}\) with respect to doping.

Similar to the relationship between \(\langle V_{\text{attraction}}^{s} \rangle\) and \(\xi\), one can also amplify \(\langle V_{\text{attraction}}^{s} \rangle\) by increasing \(\xi\), again provided that \(\Delta\left[\frac{\mu_{r}}{\epsilon_{r}} - \frac{1}{2\epsilon_{r}}E_{f}^{2}\right] \leq \Delta\varepsilon \xi^{2}\). Consequently, both \(\langle V_{\text{attraction}}^{s} \rangle\) and \(\langle V_{\text{repulsion}}^{s} \rangle\) are proportional to \(\xi\) but due to Cooper-pair formation, \(\langle V_{\text{attraction}}^{s} \rangle\) becomes the dominant interaction below \(T_{sc}\), and therefore, one can immediately predict an interesting outcome here—increasing \(\xi\) does not indefinitely increases \(\langle V_{\text{attraction}}^{s} \rangle\). In other words, there exists an optimal doping or \(\xi_{\text{optimum}}\) with maximum \(\langle V_{\text{attraction}}^{s} \rangle\) or \(T_{sc}\) controlled by \(n_{\text{pair}}\). As we have pointed out earlier, it is not possible to determine why \(n_{\text{pair}}\) changes with doping, namely, why \(n_{\text{pair}}\) is maximum for \(\xi_{\text{optimum}}\), and otherwise for \(\xi < \xi_{\text{optimum}}\) or \(\xi > \xi_{\text{optimum}}\). For example, large \(\xi\) is required to obtain high \(T_{sc}\) (due to strongly bounded Cooper pairs), but large \(\xi\) is not responsible for the formation of Cooper pairs, for the same reason large \(N(0)\) is required to increase \(T_{sc}\), but large \(N(0)\) is not the cause for superconductivity. But never mind, at least, we now know exactly what one cannot know within BCS Hamiltonian, with or without extension.

In summary, we have extended the BCS Hamiltonian to be applicable to cuprates without internal inconsistency (by means of operator-level analysis), explained why and how \(T_{sc}\) can be high (due to Cooper-pair formation in the presence of large \(\xi\)), and have shown the existence of finite-temperature phase transition (denoted by FPT\(_{sc}\)) and optimal doping concentration (\(\xi_{\text{optimum}}\)). Here, FPT\(_{sc}\) and \(\xi_{\text{optimum}}\) exist due to temperature-and doping-dependent \(n_{\text{pair}}\), and also because of the competition between \(\langle V_{\text{attraction}}^{s} \rangle\) and \(\langle V_{\text{repulsion}}^{s} \rangle\) (see equation (28)). Finally, we have established that predicting a superconductor material is next to impossible because we do not even know what parameter induces the formation of Cooper pairs.

### 3.3. Specific heat capacity at the critical point

Earlier, we have shown that a Cooper-pair binding energy can be large if the pair is formed in the presence of large \(\xi\), provided the energy levels are still degenerate and \(\langle V_{\text{attraction}}^{s} \rangle > \langle V_{\text{repulsion}}^{s} \rangle\). However, the role played by \(\xi\) when \(\langle V_{\text{attraction}}^{s} \rangle > \langle V_{\text{repulsion}}^{s} \rangle\) remains ambiguous or hidden (see equation (28)), and therefore, experimentally not verifiable because unlike \(n_{\text{pair}}\), \(\xi\) is not responsible for superconductivity, at least not directly. This means that, we need to find a way to show that \(\xi\) is indeed responsible for strongly bounded Cooper pairs. To achieve this, we make use of the finite-temperature phase transition theory developed in [42] to address FPT\(_{sc}\) in cuprates. In particular, we require \(\xi\) to be unequivocal in determining the reason why \(C_{v}\) is discontinuous at \(T_{sc}\), as well as why \(C_{v}\) jumps up (not down) such that \(C_{v}^{\text{paired}}(T_{sc}) > C_{v}^{\text{unpaired}}(T_{sc})\) where ‘paired’ and ‘unpaired’ refer to Cooper pairs and unpaired electrons, respectively.

We stress that the validity and correctness of \(\xi\) above \(T_{sc}\) in cuprates are irrefutable [15, 16], and we will not reproduce them here. Briefly though, \(\xi\) has been proven to give unambiguous microscopic explanations on the doping-dependent electrodynamics above \(T_{sc}\). Here in this last sub-section before we wrap up, we shall attempt to provide a direct evidence that \(\xi\) also plays a leading role in the phase transition from the normal-to-superconducting state by associating \(\xi\) to the notion of FPT\(_{sc}\). This evidence implies that \(\xi\) is indeed responsible for the formation of strongly bounded Cooper pairs. Recall here that \(\xi\) is either zero or denotes an irrelevant constant in conventional superconductors where ‘irrelevant’ means \(\xi\) does not play any role on the electrodynamics of a given solid [23].

Above \(T_{sc}\), the specific heat capacity is given by \(C_{v}^{\text{unpaired}}(T > T_{sc})\), while \(C_{v}^{\text{paired}}(T < T_{sc})\) is obviously valid below \(T_{sc}\). At the critical point (for \(T = T_{sc}\)) however, both \(C_{v}^{\text{unpaired}}(T > T_{sc})\) and \(C_{v}^{\text{paired}}(T < T_{sc})\) are invalid as already proven in [42] by studying the solidification and melting processes. In particular, when \(T = T_{sc}\), Cooper-pair formation gives rise to FPT\(_{sc}\), such that \(\langle V_{\text{repulsion}}^{s} \rangle\) is no longer a constant (because \(\langle V_{\text{repulsion}}^{s} \rangle > \langle V_{\text{attraction}}^{s} \rangle\) and \(\langle V_{\text{attraction}}^{s} \rangle\) is no longer a constant). This transformation is only possible if we allow \(\xi\) to change significantly at \(T_{sc}\).

Note this carefully, unlike solidification or melting process [42], the change in \(\xi\) at \(T_{sc}\) in cuprates does not (in any way) refers to changing \(|E_{k} - E_{k+q}| = \xi\) or \(|E_{k} - E_{k+q}| = \xi\), but refers to increasing or decreasing \(i\) in \(\sum_{i} E_{k} - E_{k+q} = \sum_{i} \xi\), or \(\sum_{i} E_{k} - E_{k+q} = \sum_{i} \xi\). The summation here counts the number of unpaired electrons that controls the magnitude of \(\langle V_{\text{repulsion}}^{s} \rangle\). Actually, we have the option to choose either to count the unpaired or the paired electrons (Cooper pairs), but we prefer to count the unpaired electrons because we know exactly how to relate \(\xi\) to \(C_{v}^{\text{unpaired}}(T > T_{sc})\) as already proven in [23, 42]. Thus, we have no other choice but to avoid counting the paired electrons because we do not know the relation between \(\xi\) and \(C_{v}^{\text{paired}}(T < T_{sc})\) that determines \(\langle V_{\text{attraction}}^{s} \rangle\). Warning: if the change in \(\xi\) is due to doping, then one requires the energy-level spacing itself, namely, \(|E_{k} - E_{k+q}| = \xi\) to change as discussed earlier and in [42].

Having explained that, we can now exploit equation (28) derived in [42] such that the specific heat change right at the critical point during the transformation from non-superconducting (sc or unpaired) to superconducting (sc or paired) state is given by the non-equilibrium specific heat
capacity,
\[
C\ell(T_{sc}, t)^{\text{nom}} = C\ell(T_{sc}) \exp \left[ -\frac{3}{2} \lambda \sum_i J_i^{\text{unpair}} \xi_{\text{nsc}} \right], \tag{30}
\]
where \(C\ell(T_{sc}, t)^{\text{nom}}\) is also the dynamic (or time-dependent) specific heat at a constant temperature, \(T_{sc}\). \(\sum_i J_i^{\text{unpair}}\) sums the decreasing unpaired electron density that measures the ‘strength’ of \(\xi_{\text{nsc}}\), which is a constant for each electron. The strength of \(\xi_{\text{nsc}}\) is maximum if all electrons are unpaired (\(\sum_i J_i^{\text{unpair}} = 1\)). Furthermore, we have \(C\ell(T_{sc})\) that can either transform into \(C\ell(T_{sc})\) if \(T\) is increased from \(T < T_{sc}\) to \(T > T_{sc}\), or \(C\ell(T_{sc}) \rightarrow C\ell(T)\) if one reduces the temperature from \(T > T_{sc}\) to \(T < T_{sc}\).

To construct equation (30), we need to start from the renormalized specific heat capacity that is valid for \(T\) above \(T_{sc}\) (or above any critical point), which is given by [23],
\[
\tilde{C}\ell(T) = [\text{Constants}] \exp \left[ -\frac{3}{2} \lambda \xi \right]. \tag{31}
\]
Here, the tilde indicates it is a renormalized parameter (due to the exponential term) and the term ‘Constants’ denotes a collection of numbers, physical constants, \(\pi\) and temperature. When a system (for a given temperature) obeys equation (31) is substitutionally doped with another chemical element, then the energy-level spacing of that particular system changes too. Here, the energy-level spacing refers to the energy-level difference between the ground state energy level (or the Fermi level) and its first excited-state energy level. Such changes can be readily captured by \(\xi\), which is nothing but the average energy-level spacing of the atom that is being substituted compared to that of the substituting atom [15, 16].

However, the superconductor transition temperature that starts to occur at \(T = T_{sc}\) cannot be due to changing \(\xi\) due to doping because the chemical composition stays the same when the temperature is lowered (from \(T > T_{sc}\)) or increased (from \(T < T_{sc}\)). Therefore, the change to the specific heat capacity at the critical point (for \(T = T_{sc}\)) of a superconductor has to be due to changing concentration of Cooper-pair electrons below \(T_{sc}\). In particular, unlike the unpaired electrons above \(T_{sc}\), we have to demand \(\xi = 0\) for the Cooper-pair electrons because these Cooper electrons that superconduct do not need to overcome any energy obstacle for superconductivity. Therefore, the specific heat capacity at the superconductor critical point can be constructed to look like equation (30). More detailed analysis are given below.

For the first transformation (sc to nsc), one has,
\[
C\ell(T_{sc}, t)^{\text{nom}} = C\ell(T_{sc}) \exp \left[ -\frac{3}{2} \lambda \sum_i (1 - J_i) \xi_{\text{nsc}} \right], \tag{32}
\]
where
\[
\sum_i J_i^{\text{unpair}} = \sum_i \frac{N_{\text{unpaired electron}}}{N_{\text{total}}}, \sum_i J_i^{\text{pair}} = \sum_i \frac{N_{\text{paired electron}}}{N_{\text{total}}}, \tag{33}
\]
and \(\sum_i (1 - J_i)\) counts the decreasing number of paired electrons such that \(\sum_i (1 - J_i) = 1\) if all electrons are unpaired. For paired electrons, we still count them individually. It is now straightforward to observe (see figure 1) that when nsc transforms into sc, \(\sum_i J_i^{\text{unpair}} \rightarrow 0\) or \(\sum_i J_i^{\text{pair}} \rightarrow 1\) and \(C\ell(T_{sc}) \rightarrow C\ell(T)\) gives rise to a divergent specific heat based on classical thermodynamics. The solid line (\(C\ell(T_{sc}, t)^{\text{nom}}\)) is obtained from the quantum thermodynamical approach formulated in [42].

Hence, solely on the basis of BCS Hamiltonian extended within IET formalism, we have proven that \(C\ell(T)\) jumps up at \(T_{sc}\) if we approach \(T_{sc}\) from \(T > T_{sc}\) to \(T < T_{sc}\). On the other hand, \(C\ell(T)\) jumps down at \(T_{sc}\) if one reaches the normal state from the superconductor phase by increasing the temperature. These jumps refer to the same measured discontinuity in \(C\ell(T)/T\) at \(T_{sc}\), which has been sketched in figure 1 following [45] for proper visualization. Note this, the specific heat capacity depicted in figure 1 is found to jump upward at \(T_{sc}\), determined entirely from the first principles, which is in agreement with experimental data reported by Loram et al [45].

In contrast, for conventional superconductors, BCS theory in its original form has been used to correctly derive the specific heat jump for \(T = T_{sc}\) by calculating the difference in free energies (see equation (36.9) on page 306 in [46]). In particular, the said jump can be understood from this relation, \(C\ell(T_{sc}) = C\ell(T_{sc}) + \alpha T_{sc}\) where \(C\ell(T_{sc}) > C\ell(T_{sc})\), and
\( \alpha \) here symbolically represents a collection of constants [46]. However, the transition from \( C_\text{el}^\alpha(T_{\text{sc}}) \) to \( C_\text{em}^\alpha(T_{\text{sc}}) \) or vice versa that defines the existence of \( C_\text{v}(T_{\text{sc}}, T_{\text{um}}^\text{phon}) \) remains unknown within the original BCS theory because we do not know the explicit function for \( \Delta_{\text{BCS}}(T_{\text{sc}}, T) \), thus, the jump is always assumed to be discontinuous on the basis of Landau phase transition theory [46].

In order to derive \( \Delta_{\text{BCS}}(T_{\text{sc}}, T) \), we need to find the parameter that controls the Cooper-pair formation. For example, we need to discover the parameter that is responsible for this phenomenon—when one electron absorbs a phonon, the second electron happens to emit an identical phonon that has been pointed out earlier. Within IET formalism, we can ignore \( \Delta_{\text{BCS}}(T_{\text{sc}}, T) \), and instead, one can construct the function, \( C_\text{v}(T_{\text{sc}}, T_{\text{um}}^\text{phon}) \) (see equations (30), (32) and (33)) to expose that the transition to superconducting phase is a continuous process, which is as it should be from quantum thermodynamics point of view [42]. This means that, our lack of knowledge on the function, \( \Delta_{\text{BCS}}(T_{\text{sc}}, T) \) does not imply that it does not exist, for the same reason we cannot assume \( C_\text{v}(T_{\text{sc}}, T_{\text{um}}^\text{phon}) \) does not exist just because \( C_\text{v}(T) \) measurement do not indicate any continuous process at \( T_{\text{sc}} \) [47]. Unfortunately, IET is by definition not applicable for conventional superconductors because their normal states satisfy Fermi-liquid metallic properties, and therefore, \( \Delta_{\text{BCS}}(T_{\text{sc}}, T) \) cannot be approximated from IET.

We shall now predict the superconductor’s normal state specific heat, which is expected to follow (from equation (30))

\[
\tilde{C}_\text{v}(T > T_{\text{sc}}) = C_\text{v}(T > T_{\text{sc}}) \exp \left[ \frac{3}{2} \lambda \tilde{\xi}_\text{em} \right],
\]

(34)

where \( \tilde{C}_\text{v}(T > T_{\text{sc}}) \) is known as the renormalized normal state specific heat, while the term, \( \sum_i \tilde{D}_i^\text{em} \) originally from equation (30) is equal to one for \( T > T_{\text{sc}} \), thus it does not appear in equation (34).

The specific heat capacity versus temperature curves for the cuprate, La\(_2\)−\(x\)Sr,CuO\(_4\) are depicted in figure 6 of [48], and the Sr concentration \( (x) \) is changed from 0.03 to 0.45 (3% to 45%). The said experimental specific heat were obtained by Loram et al [45, 48] where the electron specific heat coefficient, \( \gamma(T) \) for La\(_2\)−\(x\)Sr,CuO\(_4\) is plotted against temperature for increasing Sr content \( (x) \). They found that the coefficient, \( \gamma(T) \) curve shifts up with increasing Sr content for up to \( x = 24\% \), while \( \gamma(T) \) curve shifts down for \( x > 24\% \) (\( x = 27\% \) to 45%). Here, we should also note that \( \gamma(T) \propto C_\text{el}(x, T) = C_\text{v}(T > T_{\text{sc}}) \). The variable \( \gamma(T) \) is known as the electronic specific heat coefficient, and it is connected to \( C_\text{v} \) via the formula,

\[
\gamma(T) = \frac{C_\text{el}^\text{v}}{T} = \frac{C_\text{v}(T > T_{\text{sc}})}{T},
\]

(35)

where \( C_\text{el}^\text{v} \) is the electronic specific heat capacity at constant volume. The renormalized \( C_\text{el}^\text{v} \) is nothing but equation (34).

It is clear that we can anticipate for \( C_\text{v}(T > T_{\text{sc}}) \) curve to shift up systematically with Sr content \( (x) \) because \( \xi_{\text{Sr}}(x) < \xi_{\text{La}}(x) \). From these curves, the maximum \( T_{\text{sc}} \)s follow \( x \) between \( x = 15\% \) and \( x = 17\% \). Below \( T_{\text{sc}} \), the drop in the coefficient is rather sharp compared to \( \gamma(T) \) in the normal state (above \( T_{\text{sc}} \)). From figure 6 in [48], we can further deduce that indeed \( C_\text{el}^\text{v}(x, T) \) (in the normal state of course) have shifted up for \( x \) between 3% and 24% as predicted by equation (34). On the contrary, for \( x > 24\% \), between 24% and 45%, the said heat capacity curve has shifted down, which is due to defects (that induce the changes in the valence states of multivalent chemical elements) that have been explained earlier [17, 28, 49, 50] for the doping-dependent resistivity-curve shifts.

### 4. Conclusions

Even though BCS Hamiltonian is an idealized model of superconductivity, but it has been properly extended and generalized here to capture the physics of cuprate superconductors without any internal inconsistency. Anisotropic resistivity, \( d \)-wave pairing, doping-dependent superconductor gap or \( T_{\text{sc}} \) and the pseudogap above \( T_{\text{sc}} \) do not rule out the formation of Cooper pairs in its original form. The microscopic mechanism presented here is valid for zero electric and magnetic fields \( (E = 0 = B) \) supercurrent flow below \( T_{\text{sc}} \) without demanding the phonons to Bose condense in one form or another, and it does not neglect the phonon-induced scattering.

For example, the phonon-induced scattering mechanism between phonons and paired polaron, spin-induced electron pairs, spinons and holons were not properly eliminated in these alternative supercurrent-flowing mechanisms (see the first paragraph in introduction). On the contrary, Cooper pairs and its conduction mechanism below \( T_{\text{sc}} \) and for \( E = 0 = B \) are well-defined in such a way that phonons play an active role by directly mediating the formation of Cooper pairs, and therefore, the e-ph scattering effect is readily and properly eliminated. In addition, these phonons are not required to Bose condense, even below \( T_{\text{sc}} \). Rightly so, we have decided to extend the well thought-out BCS Hamiltonian, in its original form, to cuprate superconductors with a much stronger Cooper pairs regardless of their coherence lengths. Also note this, sufficient operator-level analysis at the critical point is missing in these alternative theories.

Here, we have developed a comprehensive microscopic physics of superconductivity for cuprates based on the BCS Hamiltonian, which also allowed us to invoke FPT\(^{100}\) to explain the existence of \( T_{\text{sc}} \) and the possibilities of phonon readjustment and preformed Cooper pairs above \( T_{\text{sc}} \). Most importantly, our approach is entirely based on first principles such that we did not resort to any guessed functions or fitting-parameter tactics to justify the validity and correctness of BCS Hamiltonian in cuprates. Hence, it is not an exaggeration to claim that BCS Hamiltonian is applicable to all types of superconductors due to its unambiguous superiority in taming phonons, and in handling Cooper-pair formation and supercurrent flow microscopically and consistently at the operator level in accordance with the most relevant and important experiments.
The relevant experiments are associated to (1) isotope effect, (2) dissipationless supercurrent flow below Tc, including the Meissner effect, (3) specific heat below Tc (Cv(T)), (4) doping- and temperature-dependent superconductor gap (on the basis of equations (26) and (28)), (5) doping-dependent normal state resistivity above Tc (see [16]), (6) the existence of strange metallic phase above Tc (see [15]), and (7) the discontinuous specific heat capacity at Tc (see equations (30), (32) and (33)). This specific heat discontinuity due to FPT opens up the path to stretch the energy-level spacing influence in the strange metallic phase to the superconducting state. Bardeen, Cooper and Schrieffer have already addressed points (1) to (3) decades ago, while the extended BCS Hamiltonian within IET has been used to tackle points (4) and (7).

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Appendix

Here, we provide additional explanations so as to avoid possible confusion. Additional notes I and II (given below) discuss different complicated aspects that are still not captured by the extended BCS theory within the ionization-energy formalism. The detailed derivation for the BCS electron–electron attraction operator is given in the final subsection, after the additional notes.

A.1. Additional notes I

The different sequences found along the crystal structure axes (a, b and c) in cuprates can be further manipulated (by doping) to control the transition from n- to p-type normal states where n- and p-types refer to electrons and holes, respectively, as dominant charge carriers. Hence, cuprates are also known as polar cuprates similar to alkali halides [51]. In this case, when the holes are self-trapped in a deformable lattice, it may assist the formation of large polarons [52].

In IET however, the formation of holes is due to the relative polarizability of electrons of one chemical element compared to the next-nearest neighbor [49]. In addition, the hole conductivity itself refers to the electron conductivity in the valence band. Therefore, we can readily exploit IET to evaluate the doping-dependent resistivity and specific heat capacity data of cuprates without the need to differentiate whether the charge carriers are holes or electrons [37]. Doping-dependent resistivity data both above and below the Curie temperature for manganites and diluted magnetic semiconductors [28] also support the above deduction.

Since the notion of energy-level spacing stays the same, regardless of whether the charge carriers are holes or electrons (as explained above), then the Cooper pairs can be applied to both hole pairs and electron pairs. For example, hole conduction is equivalent to electron conduction in the valence band such that the sign is switched from negative (\(\varepsilon\)) to positive (\(\varphi\)) such that the mechanism of conductivity is the same for holes and electrons [37]. Otherwise, we have to exclude the original BCS theory for the Fermi-liquid metal, Al, which is a superconductor with holes as charge carriers, and its Tc is about 1 K. Given these facts, we can deduce that the extended BCS theory within IET formalism presented here can be applied to underdoped, optimally doped and overdoped cuprates where such applications are available in [16, 17, 21], which can be readily applied to recent materials studied in [53].

Unconventional electron–phonon interaction by means of polaronic effect has been suggested to contribute significantly in complicated situations, namely, in the pseudogap phase above Tc, as well as in the formation of the strange (Fermi and Bose) metallic phases [54, 55]. The extended BCS Hamiltonian exploited in [54, 55] with real-space pairing of polarons (bipolarons), which is a type of BCS Cooper pairing has been proposed as the origin of pseudogap phase for \(T^* > T_c\) in momentum space. Here, \(T^*\) is the characteristic temperature to identify the onset of pseudogap phase above \(T_c\).

In other words, the above extended BCS Hamiltonian (after taking the polaronic effect into account) [54, 55] allows one to find the origin of the pseudogap appearing in the normal state at \(T^* > T_c\) of underdoped cuprates. In contrast, on the basis of IET, the electron–phonon interaction in cuprates (for all doping) is unconventional in a sense that the normal state is a strange metal, which does not satisfy the usual Fermi-liquid theory. This strange metallic phase is fully captured by IET as explained in the earlier sections, and is available in [15]. However, the pseudogap phase has been excluded because the origin of this pseudogap phenomenon remains ambiguous in our analysis. But the primary reason to exclude it is that the pseudogap is never a prerequisite for the formation of superconducting phase.

Based on [56], the superconducting mechanism of Cooper pairs in underdoped, optimally doped and moderately overdoped cuprates is due to bipolarons. Therefore, the \(T_c\) in these doping ranges is assumed to be not predictable from the BCS-like relation as given in equation (11). But the said deduction is based on the assumption that polarons can form bipolarons such that the scattering caused by phonons has been ignored. The BCS gap equation from our extended version should read (from equations (11) and (29)),

\[
T_c \propto \Delta_{BCS} \propto \exp \left( \frac{1}{N(0) \left\langle V_{\text{attraction}} \right\rangle} \right),
\]

where \(N(0)\) is the density of states near the Fermi level that conveniently ignores the required symmetry of the
bandstructure at the Fermi level. This fact has also been pointed out indirectly when we claimed that we do not know why the first and second electrons happened to exchange the same phonon in the momentum space to form a Cooper pair. The exchange of the same phonon between two Cooper electrons is very much depend on the symmetry of the bandstructure or the crystal structure in real space, which makes the determination of $T_{sc}$ a hard problem. If we have enough parameters to adjust, of course, we can find a trend with a good fit between $T_{sc}$ and different types of superconductors, but this approach cannot lead us to find the cause for the phonon-mediated Cooper pairs. But in any case, the formula for $T_{sc}$ from BCS-IET formalism is given in equation (36), which is valid for underdoped, optimally doped and overdoped cases.

The onset of our $T_{sc}$ occurs when $|\langle V_{kk'}^{\text{attraction}} \rangle| = \langle V_{kk'}^{\text{repulsion}} \rangle$, which shall lead us to state (from equation (29)),

$$
\xi_{q-q'}^2 = |\hbar\omega q e^{i\lambda(-E_F)}|^2 > |\hbar\omega q e^{i\lambda(-E_F)}|^2 = \xi_{q=q'}^2,
$$

where the term on the left-hand side (lhs) tells us that the electrons absorb and emit the phonons accordingly, giving us the Cooper attraction by eliminating the electron–electron scattering, and this lhs term is equal to the rhs term with random absorption and emission of phonons that gives rise to electron–phonon scattering, which also automatically activates the electron–electron coulomb repulsion.

Just above $T_{sc}$, equation (37) should read,

$$
\xi_{q-q'}^2 = |\hbar\omega q e^{i\lambda(-E_F)}|^2 > |\hbar\omega q e^{i\lambda(-E_F)}|^2 = \xi_{q=q'}^2,
$$

where in the presence of preformed Cooper pairs, equation (38) can be valid for $T > T_{sc}$. In the case when $T$ is just above $T_{sc}$, the lhs term has to satisfy,

$$
\xi_{q-q'}^2 < |\hbar\omega q e^{i\lambda(-E_F)}|^2.
$$

Whereas, the RHS needs to obey,

$$
\xi_{q-q'}^2 > |\hbar\omega q e^{i\lambda(-E_F)}|^2.
$$

The conditions stated in equations (39) and (40) are needed so that equation (38) and the inequality, $|\langle V_{kk'}^{\text{attraction}} \rangle| < \langle V_{kk'}^{\text{repulsion}} \rangle$ can stay true.

Finally, for $T < T_{sc}$, we have $|\langle V_{kk'}^{\text{attraction}} \rangle| > \langle V_{kk'}^{\text{repulsion}} \rangle$ and apparently, equation (37) becomes,

$$
\xi_{q-q'}^2 = |\hbar\omega q e^{i\lambda(-E_F)}|^2 < |\hbar\omega q e^{i\lambda(-E_F)}|^2 = \xi_{q-q'}^2.
$$

In superconducting phase, the lhs term obeys,

$$
\xi_{q-q'}^2 < |\hbar\omega q e^{i\lambda(-E_F)}|^2.
$$

Whereas, the rhs needs to obey,

$$
\xi_{q-q'}^2 > |\hbar\omega q e^{i\lambda(-E_F)}|^2.
$$

Equations (42) and (43) are the conditions that keep equation (41) and the inequality, $|\langle V_{kk'}^{\text{attraction}} \rangle| > \langle V_{kk'}^{\text{repulsion}} \rangle$ intact.

From the above inequalities and conditions, the superconducting transition temperature is controlled by the competition between the activation of Cooper attraction and the coulomb repulsion between electrons. At $T = T_{sc}$, the random exchange of phonons between electrons is matched by the proper exchange of phonons between many Cooper electrons, which induces the onset of $T_{sc}$. If the Cooper-pair formation is further enhanced, then the superconducting phase prevails, which is the case when the temperature-induced phonons are significantly and systematically reduced by decreasing the temperature. Here, the temperature-induced phonons contribute to the randomly-exchanged phonons between electrons that enhances coulomb repulsion and resistivity.

Recall that IET and the energy-level spacing renormalization group method are deliberately developed to be independent of wavefunctions because these are guessed functions. However, it is possible to guess a BCS-type wavefunction because BCS-IET formalism allows it. In this approach, the effect of energy-level spacing ($\xi$) need not be introduced into the BCS wavefunction such that the coupling constant and the electron–phonon attraction operator may stay intact because $\xi$ is also an eigenvalue. This means that, it would be redundant to carry out such additional calculations because the end result or the physics of superconductivity would be exactly as derived here in this report. We should not be falsely led to believe that a proper wavefunction can be imagined, which is a function of $\xi$ or any other suitable parameters to evaluate cuprate superconductors. Such a wavefunction (or any trial wavefunction) cannot be proper and cannot lead us to any meaningful result (other than to study the wavefunction symmetry, namely, s-, p- or d-wave symmetry) due to the following fact—the pairing mechanism of Cooper electrons (or any other pairing) has got nothing to do with wavefunctions. In particular, wavefunctions cannot be, (i) made to eliminate electron–phonon scattering and (ii) made to cause electron pairing.

Apart from that, having the ability to guess the trial wavefunction and make the relevant variational calculations do not, and cannot lead us to any new effect, new understanding or accurate prediction of $T_{sc}$ mainly because (and as we have stated earlier) we do not know why the first and second electrons have to exchange the same phonon in the momentum space to form a Cooper pair. One of the implications (not stated earlier) from the IET-BCS theory to evaluate the said phonon exchange is that in cuprate superconductors, the strength of temperature-induced phonon amplitude becomes negligible or much smaller below $T_{sc}$, compared to electron-induced. Consequently, the distortion to phonon amplitude is made to be large and is dominated by the electron–phonon attraction mechanism such that any cuprate that does not satisfy this phenomenon, cannot become superconductors. I suspect that the same phenomenon is true for BCS superconductors because BCS theory does not
invalidate the said phenomenon or condition by requiring that \( T_{\text{c}} \) is proportional to \( N(0) \) (see equation (36)).

It is to be noted here that the Josephson effect [57] and the London penetration depth [58, 59] are macroscopic phenomena that are independent of the microscopic electron-pairing mechanism. Despite this fact, these effects can indeed be useful to evaluate the parameters that can destroy superconductivity, which then can be used to crosscheck whether the same parameters can be used to destroy (or to dissociate) the Cooper pairs. One such example is that Bardeen, Cooper and Schrieffer themselves have made use of the Meissner effect [7] and the London penetration depth in formulating the original BCS theory. For example, BCS have made use of the fact that magnetic field can be applied to dissociate Cooper pairs.

### A.2. Additional notes II

It has been reported that there is an observable discrepancy between the theoretical alternative current (ac) Josephson effect and the measured data due to spin contribution [60]. Hence, the observed effect has been reported to be incompatible with the one predicted by Josephson [60, 61]. We do acknowledge the said discrepancy. Apart from the pseudogap effect (mentioned above and in [62]), the Josephson effect in cuprates are not fully captured by the BCS theory, and these developments actually imply that the extended BCS theory presented here is still incomplete to handle the said complicated situations, which is indeed the case.

However, these ignored complications do not cast any doubt on the extended Cooper-pairing mechanism such that the said ignorance means that the extended BCS Hamiltonian within IET needs further modification with suitable interaction terms to account for the said effects without disturbing the Cooper-pair mechanism. For example, the BCS-IET formalism has been proved to be able to reproduce the changes to doping-dependent resistivity curve of all cuprates (underdoped, optimally doped and overdoped) [15–17], as well as the changes to the specific heat capacity curve (see figure 6 in [48]), unambiguously and without requiring any adjustable parameters.

Based on these reports [60–62], it should be obvious that the discrepancy is due to an effect coming from the electron’s spin. But this discrepancy does not imply, in any way, that the pairing is now spin-induced because spin-induced pairing always ignores the phonon-induced scattering and it is not known how spin-induced pairing can cause the discontinuity in the specific heat data at the critical point. In one of our recent work, we have proved that the spin exchange interaction cannot cause fermion pairing (between electrons or between \(^3\)He atoms) [63] after re-evaluating the real cause for \(^3\)He pairing, which is required to form superfluid. In particular, the cause for superfluidity in \(^3\)He refers to the identification of the Ramachandran attraction term that initiates the \(^3\)He pairing, in the presence of the known contribution from the composite integer neutron spin states (to form bosonic states) and the Leggett’s spontaneously broken spin-orbit symmetry for certain temperature and pressure ranges.

Indeed, the original BCS theory explains how \( T_{\text{c}} \) is determined for conventional superconductors, which is based on Fermi-liquid theory, which is not sufficient for cuprates. Therefore, we have extended the BCS theory within IET so that the extended BCS-IET formalism can be readily applied to handle the strange metallic phase in the normal state of cuprates. In this extended version, the \( T_{\text{c}} \) and the energy gap equation is given by equation (36) that is suitable for the superconducting transition from strange metal to unconventional superconductivity below \( T_{\text{c}} \). This phase transition is microscopically captured by the transition from the repulsive coulomb interaction to a phonon-mediated attraction. See the derivation in the following section that proves the existence of an attractive potential between electrons, mediated by phonons.

The strange metallic phase above \( T_{\text{c}} \) is not a simple band metal that satisfies Fermi-liquid theory as already reported in [15] on the basis of IET. An alternative proposal is given in [64] that claims the energy gap formation is due to the so-called stabilization temperature of loop currents with a size of coherence length. This is just one of many alternative proposals such that this stabilization temperature does not invalidate the extended BCS theory formulated here. The above-mentioned facts indicate that the normal state electric conductivity is well captured by BCS-IET formalism with experimental supports, except for the pseudogap phase and the spin effects in Cooper-pairing mechanism at certain doping ranges (known as the underdoped superconductors). Nevertheless, the extended formalism devised here transcends the original BCS theory that is based entirely on the usual Fermi-liquid metals.

The current generation mechanism developed based on Anderson’s Resonating-Valence-Bond theory [65–70], and another mechanism due to the spin-vortex-induced loop current [71, 72] are also available to explain the possibility of supercurrent in cuprates. But as I have stated earlier in the first paragraph in the Introduction, the persistent current generation can only be properly produced by eliminating all the scattering mechanisms that can generate resistivity, and the most difficult scattering to eliminate is the phonon-induced scattering. However, by ignoring the contribution made by the phonons, or in a system that has no phonons, one can generate persistent current due to spin-interaction [71, 72] or in the presence of a phase variable that enables the current to flow without a voltage drop [73].

### A.3. The derivation of the attractive potential with a negative sign

First, we recall the second-order perturbation theoretical result given earlier, which is given in equation (17) that reads,

\[
E_n^{(2)} = \sum_{m=n} \frac{|\langle \psi_n^{(0)} | H_{\text{el-ph}} | \psi_m^{(0)} \rangle|^2}{E_n^{(0)} - E_m^{(0)}},
\]

where the first-order correction,

\[
E_n^{(1)} = \langle \psi_n^{(0)} | H_{\text{el-ph}} | \psi_m^{(0)} \rangle = 0.
\]
Next, we note that we are dealing with phonon-absorption and emission, hence, the zeroth-order energy denominator in equation (44) should read,

$$E_{m}^{(0)} - E_{n}^{(0)} = \left( E(k') - \hbar \omega(k - k') \exp \left[ \frac{1}{2} \lambda(\xi - E_{F}^{0}) \right] \right) - E(k).$$

(46)

after enforcing the ionization-energy renormalization. Recall here that the exponential term that appears in equation (46) originates from the energy-level spacing renormalization that captures the interaction strength between a bound electron and its nucleus, which influences the phonon frequency. In view of equation (46), the second-order correction can now be rewritten as,

$$E_{m}^{(2)}(k, k') = \sum_{k,k':k = k'} \sum_{k''} n_{k}(1 - n_{k}) \frac{[\langle \psi_{0}^{(0)} | H_{el:ph} | \psi_{0}^{(0)} \rangle]^{2}}{E(k) - E(k') + \hbar \omega(k - k') \exp \left[ \frac{1}{2} \lambda(\xi - E_{F}^{0}) \right]}.$$

(47)

where,

$$|g_{k,k'}| = |\langle \psi_{0}^{(0)} | H_{el:ph} | \psi_{0}^{(0)} \rangle|.$$ 

(48)

Here, following Landau, we have multiplied the occupation numbers,

$$\sum_{k,k':k = k'} n_{k}(1 - n_{k}) = n_{k'}(1 - n_{k'}),$$

(49)

that count the respective \( \psi_{0}^{(0)} \) and \( \psi_{0}^{(0)} \) states, and these occupation numbers of course satisfy the standard and the renormalized BES such that,

$$n_{k} = (1 - n_{k})$$

(50)

$$n_{k'} = (1 - n_{k'}).$$

(51)

because the number of phonons are not conserved. However, the crystal momentum is conserved and it requires \( q = k - k' \). Using Landau’s approach, we can derive the electron-phonon interaction potential,

$$V_{el:ph}(k, k') = \frac{\partial^{2} E_{m}^{(2)}(k, k')}{\partial n_{k} \partial n_{k'}}.$$

(52)

$$= \frac{\partial^{2} E_{m}^{(2)}(k, k')}{\partial n_{k} \partial n_{k'}} \sum_{k,k':k = k'} n_{k}(1 - n_{k}) \frac{[\langle \psi_{0}^{(0)} | H_{el:ph} | \psi_{0}^{(0)} \rangle]^{2}}{E(k) - E(k') + \hbar \omega(k - k') \exp \left[ \frac{1}{2} \lambda(\xi - E_{F}^{0}) \right]}$$

(53)

$$= |g_{k,k'}|^{2} \frac{\partial^{2}}{\partial n_{k} \partial n_{k'}} \sum_{k,k':k = k'} n_{k}(1 - n_{k}) \frac{[\langle \psi_{0}^{(0)} | H_{el:ph} | \psi_{0}^{(0)} \rangle]^{2}}{E(k) - E(k') + \hbar \omega(k - k') \exp \left[ \frac{1}{2} \lambda(\xi - E_{F}^{0}) \right]}$$

(54)

After making use of this relation,

$$\hbar \omega(k - k') = \hbar \omega(k' - k),$$

(57)

we should be able to get,

$$V_{el:ph}(k, k') = |g_{k,k'}|^{2} \frac{\partial^{2}}{\partial n_{k} \partial n_{k'}}$$

(58)

$$= \frac{1}{E(k) - E(k') + \hbar \omega(k - k') \exp \left[ \frac{1}{2} \lambda(\xi - E_{F}^{0}) \right]}$$

(59)

$$= \frac{1}{E(k) - E(k') + \hbar \omega(k' - k) \exp \left[ \frac{1}{2} \lambda(\xi - E_{F}^{0}) \right]}$$

(60)

$$= \frac{1}{E(k) - E(k') + \hbar \omega(k - k') \exp \left[ \frac{1}{2} \lambda(\xi - E_{F}^{0}) \right]}$$

(61)
As introduced above, $[\delta, k, \ell]$ is the el–ph coupling constant and $v_{el,ph}(k, \ell)$ is nothing but the attractive electron–phonon potential discussed in the text.

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