Interplay of pairing correlation and Coulomb correlation in Boson exchange superconductors

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Abstract. A theoretical methodology for exploring the conventional Bardeen–Cooper–Schrieffer (BCS) pairing instability for superconductivity from a correlated normal phase for all possible degrees of many-body correlation has been developed. The Gutzwiller projection scheme with a correlation parameter was made use of in generating the BCS pairing state. A variational scheme was thereafter implemented, leading to a self-consistent equation for superconducting gap function. This equation shows explicit dependence of the gap function on the many body correlation parameter. This ‘pairing-gap’ and the corresponding self-consistent gap equation in zero correlation limit, becomes identical in nature with those of the pure (1-well) BCS formalism, as expected and the Coulomb correlation affects the pairing significantly with the strength of correlation. The detailed consequences are being presented here.

1 Introduction

Since the discovery of superconductivity, in the early twentieth century, human endeavour has been steadily getting oriented towards attaining superconductivity at elevated temperatures with the ultimate dream of reaching room temperature superconductivity. In the recent past, a group of experimental physicists, had claimed very high conductivity (nearly vanishingly small resistance) and close to Meissner value of diamagnetism at ambient temperature in a silver-embedded gold plate [1]. Superconductors with critical temperature $T_C$, above 30 K, in general belong to high-temperature superconductors (HTSC). According to the Eliashberg theory [2,3], and its simplified version by McMillan [4], a material with very low atomic mass, generates very high frequency phonons which couple strongly to conduction electrons and thereby can produce high value of $T_C$. From this, analytically it is established that at high pressure, metallic hydrogen should be a superconductor with a very high $T_C$ around 100–240 K [5,6]. However, it is experimentally found that not pure metallic hydrogen but hydrogen saturated compounds like sulfur hydride [7] and lanthanum superhydride [8] show the superconductivity at high temperatures, viz. at 203 K and 260 K, respectively, at mega-bar pressure. Meanwhile, Dias et al. have reported a pressure driven room temperature (287 K) superconductivity in a carbonaceous sulfur hydride [9]. In cuprate system, HTSC was mainly found in the layered structure materials like La$_2-x$Sr$_x$CuO$_4$, YBa$_2$Cu$_3$O$_{7-\delta}$ [10,11]. But, in those materials, the mechanism behind observed anisotropic pairing is not fully understood yet.

The conventional isotropic (s-wave) pairing interaction for Cooper pair formation is mediated by the electron–phonon coupling and is greater in magnitude than that of the ‘suppressed’ Coulomb interaction even by an arbitrarily small amount for certain frequency range ($\omega_C$; of the order of Debye cut off frequency) in almost ideal Fermi sea (IFS). This idea of phonon-mediated pairing was initially used in the microscopic pairing mechanism of superconductivity put forward by Bardeen, Cooper and Schrieffer, which is known as the microscopic BCS theory [12,13].

Here, we aim to study the BCS pairing originating from a realistic normal state. In other words, we would like to understand that whether Coulomb correlation among the fermions is considered, how this novel phenomena of particle-pairing, gets modified and up to what extent of this correlation the system can sustain superconducting properties. This was earlier taken care of partly by considering repulsive Coulomb interaction along with the phonon mediated electron–electron interaction in the BCS theory [4,32] which in other way
can be stated as two-square well formalism of the BCS theory.

The Coulomb correlation in a system of our interest can be introduced in two different ways: (i) correlated operator algebra: correlated fermion creation, annihilation operators are defined and then dealt the system accordingly [14]; and the other is (ii) correlated variational state: variational states are defined in which Coulomb correlation is in-built along with the pairing correlation [15]. In this correlated operator approach, the commutation relations of the operators may not be exactly identical with the uncorrelated fermionic algebra but here the creation operator is indeed the complex conjugate of the annihilation operator. In the literature, the hole-doped Gossamer superconductor was studied by defining this type of correlated operators. Not only that particular Gossamer system, there are other superconducting-systems, which are handled by defining new correlated operators. Here, we would like to go for the second approach, i.e. correlated variational states and later we define two distinct way to introduce Coulomb correlation in the system.

In superfluid theory of $^3$He, pairing is observed in Coulomb correlated fermions [16], where the trial wave functions are used to investigate the pairing with a phenomenological two body potential. A similar approach has been introduced in the pairing mechanism for Coulomb correlated fermions where Gutzwiller projection operator is introduced to take care of this correlation in the system [17]. In the first case, model states for this system are developed at first by defining the Fermi sea in which correlation is already introduced, i.e. correlated variational states and later we define two distinct way to introduce Coulomb correlation in the system.

The second type of variational state is defined by the action of the pairing operator on the non-interacting FS to form the pairing state first and then the Gutzwiller operator acted on it as to block the double occupancy of a site. In other words, the Gutzwiller operator is imposed on the paired fermions state to examine how the Coulomb correlation competes with the pairing correlation. We would like to investigate characteristic upper cut-off of the Coulomb correlation in terms of the Gutzwiller parameter, below which the ‘pairing-gap’ can open up for a specified weak coupling regime in a boson exchange superconducting system.

This paper is configured as follows: In Sect. 2, we introduce our model system along with the possible variational states. The variational correlated Bardeen–Cooper–Schrieffer (BCS) states can be described in two different ways and we first briefly demonstrate that one of those specified states is more physical than the other. In Sects. 3 and 4, we elaborate on mathematical calculations and discuss our results. In Appendix 1 and Appendix 1, the normalization of the CBCS state and the total energy expectation expression are derived, respectively.

## 2 Model system

The Hamiltonian for the conventional superconducting system is described by the zero temperature reduced BCS Hamiltonian [12,19]

$$H = \sum_k 2\epsilon_k b_k^+ b_k + \sum_{k,l} V_{k,l} b_k^+ b_l,$$

where $b_k^+ (b_k)$ is the electron pair creation (annihilation) operator in the momentum states $k \uparrow$ and $-k \downarrow$,

$$b_k^+ = c_{k\uparrow}^+ c_{-k\downarrow}^+; b_k = c_{k\downarrow} c_{-k\uparrow},$$

$\epsilon_k$ is the single particle energy in the momentum state $k$, as measured from the Fermi energy, whereas $V_{k,l}$ is a interaction matrix element connecting two paired momentum states $k$ and $l$.

We start with this Hamiltonian and then introduce electronic Coulomb correlation in terms of the correlated variational states. This correlated variational states can be formed in two different ways, as discussed below.

**Case I (a).** In this case, the correlated state is defined as the correlated fermion pairing state that is formed using the Gutzwiller projected out states with doubly occupied sites from the non-interacting filled Fermi sea (FS) ground state and it is given as

$$| \Psi \rangle_{\text{CBCS}} = P_{\text{BCS}} \otimes P_{\text{G}} | \text{FS} \rangle,$$

where $P_{\text{BCS}}$ is the BCS pairing operator as defined for the construction of the microscopic BCS pairing state and $P_{\text{G}}$ is the Gutzwiller partial projection operator. For the time being, we are not defining these two operators in great details; however, in the subsequent sections, we will discuss in details about those two operators.

**Case I (b)** The effect of Coulomb correlation on pairing phenomena has also been studied for a Cooper’s one pair problem, using a variational wave function in the first quantized form, i.e. Jastrow geminal augmented wave function [20,21]. In this formulation, the relative distance ($\rho$) between two electrons carries the effect of Coulomb correlation and the effect will be maximum when the distance is zero, i.e. the electrons are on the same site. Accordingly, there is a kink in the two-electron wave function for $\rho = 0$ and the effect of correlation weakens off gradually with the increase in separation. However, the so-called bound state energy for the electron pair is affected significantly due to the Jastrow factor. Here, because of this Jastrow correlator, a repulsive matrix element will appear in the calculation of two-body interaction which plays an important role in the calculation of the bound state energy [22]. In fact, a two-well scheme involving an attractive well arising from a boson-mediated pairing interaction and a repulsive well due to Coulomb interaction was implemented for Cooper’s one pair problem as well [23].
Thereafter, we proposed the variational state (see Eq. (3)) in case I (a), in the second quantized form, to study the effect of correlation in 2D interacting systems. Here in this approach, we are first applying the Gutzwiller projection operator on the FS state to define the correlated FS (CFS) state. Then we apply BCS pairing operator on the CFS states to form the correlated BCS (CBCS) states. The Gutzwiller partial projection operator is used to exclude the doubly occupied states for the HTSC antiferromagnetic cuprate superconducting system like La$_2$-Sr$_x$CuO$_4$ and YBa$_2$Cu$_3$O$_7$ [24,25].

**Case II** The second approach for the correlated state is defined as follows:

(i) first we define a BCS pairing state, i.e. BCS pairing operator ($P_{BCS}$) acting on the filled FS state and then (ii) we operate Gutzwiller projection operator ($P_\alpha$) on the pairing states

$$|\Psi\rangle_C = P_\alpha \otimes P_{BCS} |FS\rangle. \quad (4)$$

Here, the projection operator is blocking the electrons to sit on the same site and this blocking is controlled by a variational parameter ‘a’ ($\alpha$ varies from 0 to 1, where $\alpha = 0$ denotes the usual BCS like pairing ground state, whereas $\alpha = 1$ represents the complete projecting out of all the doubly occupied sites).

So, in the paired ground state with general $\alpha$, one has a fermionic pairing from a metallic correlated state.

In the first approach (case I (a)), our derived results do not exactly match with that of the uncorrelated BCS formalism even when we consider $\alpha = 0$. Again, in the strongly correlated regime, i.e. $\alpha \geq 0.6$, the pairing gap increases slowly with the tuning parameter $\alpha$, which may be a signature of the existence of ‘frozen-Cooper pair’, i.e. paired fermions which are almost immobile. The incomplete variational calculation was undertaken, which might have led to this kind of results.

The ratio of zero temperature pairing gap to the product of Boltzmann constant and critical temperature, denoted by $\frac{\Delta}{k_B T_c}$, obtained was slightly smaller than that of the original BCS formulation. This may be because of the further limitation in the calculation, viz. states with higher order corrections in $\alpha$ were assumed to be insignificant or might be the restriction on the the filling factors on the momentum space. In the strong correlation regime ($\alpha \approx 1$), $\frac{\Delta}{k_B T_c}$ goes to zero or approaches to zero. Therefore, the $s$-wave pairing is no more feasible in this strongly correlated region, although there may be a possibility of the existence of the anisotropic (d-wave) pairing.

Here, in this paper, we will not elaborate on the first approach (case I), but rather we concentrate on the second formalism and as a future plan, we are willing to treat the first one as a separate problem. In the next section, we give a detailed presentation on the second approach (case II) accompanied with all the calculations and aspects.

### 3 Mathematical formulation and construction of correlated BCS states

Here, we start with the well-known microscopic BCS pairing states and later we introduce the electronic correlation to describe the correlated BCS states. The microscopic BCS pairing state which was modelled to capture the physics of the pairing between a pair of fermions in the presence of whole FS is written as

$$|\Psi\rangle_{BCS} = \prod_k (u_k + v_k c_{k,\uparrow}^+ c_{-k,\downarrow}^+ |FS\rangle), \quad (5)$$

where $u_k$ and $v_k$ are the complex Bogoliubov amplitudes corresponding to the unoccupied paired and occupied paired states, respectively, and they are connected with each other by the normalization condition given by

$$(|u_k|^2 + |v_k|^2) = 1. \quad (6)$$

Here, $|FS\rangle$ is the non-interacting Fermi sea ground state and we will define it later.

Our aim is now to introduce correlation among the pairing fermions, i.e. we would like to switch on the interaction, in the system. This can be done either by (i) defining a variational correlated basis state [15,26] or by (ii) introducing new correlated fermion creation, annihilation operators [27,28]. The operator algebra is not exactly the same as the fermion operators. Hence, creation operator is a definite conjugate of annihilation operator but they do not follow the anti-commutation relation as followed by the fermion operators. Therefore, we are not taking this route of defining new correlated operators, rather we follow the correlated basic state technique.

Our proposed CBCS state, namely the Gutzwiller projected out BCS pairing states, is defined in the following way: (i) at first, we define the FS ground state for the real construction of the well-known microscopic BCS ground state; (ii) the pairing states for the correlated fermions are modelled by introducing the Gutzwiller partial projection operator in k-space which projects out the double occupancy on a lattice site with an amplitude $\alpha$. Here, the CBCS state denoted by $|\Psi\rangle_C$ is defined as

$$|\Psi\rangle_C = \prod_{s,l} (1 - \alpha \sum_{k', m'} c_{k', l, \uparrow}^+ c_{k, m', \downarrow}^+ c_{m', l, \downarrow}^+ c_{k, m, \uparrow}^+ \delta^{(m' - k')\sigma_y}) (u_l + v_l c_{l, \uparrow}^+ c_{-l, \downarrow}^+ |FS\rangle), \quad (7)$$

where $c_{k, \sigma}^+ (c_{k, \sigma})$ is the fermion creation (annihilation) operator in momentum and spin states $k$ and $\sigma (\uparrow, \downarrow)$, respectively.

In the above equation, Gutzwiller projection operator has been defined in the k-space which takes care of the effect of exclusion of double occupancy on a single site in real space. The variational parameter $\alpha$ can be determined by minimizing the total energy expression.
For the time being, the normalization factor is not being included in defining the CBCS state. We will consider this factor indeed in the subsequent sections and we add an appendix (Appendix 1) with some relevant steps for the calculation of normalization factor. Generally, the Gutzwiller projected out state is defined in terms of the partial projection operator in real space as given below:

\[ |\Psi_G\rangle = \prod_i (1 - \alpha \hat{n}_{i}\hat{n}_{i}) |FS\rangle, \quad (8) \]

where \( \hat{n}_{i,\sigma} \) is the fermionic occupation number operator at site \( i \) with spin \( \sigma \) and \( \alpha \) is a variational parameter in Gutzwiller’s original formulation, which decides the amplitude for double occupancy of a site \( (0 \leq \alpha \leq 1) \); \( |FS\rangle \) is the Fermi sea (FS) ground state and it can be written in terms of the fermion creation operators as

\[ |FS\rangle = \prod_{k,\sigma} e^{+}_{i,\sigma} c^{+}_{j,-\sigma} e^{i(\epsilon_{r_i}-\epsilon_{r_j})} k |\text{vac}\rangle, \quad (9) \]

where \( i \) and \( j \) are the site indices in real space and \( k \) represents the fermion wave vectors which has the upper bound of Fermi momentum \( (k_F) \). \( |\text{vac}\rangle \) represents the vacuum state that stands for the state with zero occupation on every site in real space and for \( k \)-space, all the momentum states being empty.

For the evaluation of the ground state energy \( W \), we combine Eqs. (1) and (7). By definition,

\[ W = \frac{C\langle \Psi |H|\Psi \rangle_C}{C\langle \Psi |\Psi \rangle_C}. \quad (10) \]

Here, the first term in Eq. (10) corresponds to the kinetic energy operator expectation value \( (T) \) and is given by

\[ T = \frac{C\langle \Psi |\sum_k 2\epsilon_{k} b^{+}_{k} b_{k} |\Psi \rangle_C}{C\langle \Psi |\Psi \rangle_C}. \quad (11) \]

This term is evaluated using the orthogonality of the independent states and it comes out as (some significant steps are put in Appendix 1)

\[ T = 2 \sum_k \frac{\epsilon_{k} |v_{k}|^2 (1 - \alpha)^2}{1 + |v_{k}|^2 \alpha (\alpha - 2)}. \quad (12) \]

The two-body attractive interaction potential contribution \( (V) \) to the ground state energy is given by

\[ V = \frac{C\langle \Psi |\sum_{k,l} V_{k,l} b^{+}_{k} b_{l} |\Psi \rangle_C}{C\langle \Psi |\Psi \rangle_C}, \quad (13) \]

where any two states specified with the index \( k \) and \( l \) are connected by a matrix element \( V_{k,l} \).

Simplifying, we get

\[ V = \sum_{k,l} \frac{V_{k,l} u_{k} v_{l}^* v_{l} (1 - \alpha)^2}{1 + |v_{k}|^2 \alpha (\alpha - 2))}. \quad (14) \]

[Recalling that, \( 0 \leq \alpha \leq 1 \).]

Thus, the expression for the total ground state energy \( (W) \) becomes

\[ W = 2 \sum_k \frac{\epsilon_{k} |v_{k}|^2 (1 - \alpha)^2}{1 + |v_{k}|^2 \alpha (\alpha - 2)} + \sum_{k,l} \frac{V_{k,l} u_{k} v_{l}^* v_{l} (1 - \alpha)^2}{1 + |v_{k}|^2 \alpha (\alpha - 2))}. \quad (15) \]

The ‘superconducting pairing gap’ \( (\Delta_k) \) in this Coulomb correlated phase is defined as

\[ \Delta_k = - \sum_{l} V_{k,l} (b_{k}^{+}). \quad (16) \]

Incorporating the expectation value of the pair operator in the CBCS state, Eq. (16) becomes

\[ \Delta_k = - \sum_{l} V_{k,l} b_{l}^{+}. \quad (17) \]

The total energy \( W \) and the pairing-gap \( \Delta_k \) are both functions of the pairing amplitudes, \( u_k \) and \( v_k \). The function \( W \) can now be minimized with respect to all three variables, viz. \( u, v \) and \( \alpha \) to obtain the characteristics of the pairing correlation in the presence of the Coulomb correlation.

(i) Coulomb correlation as a tuning parameter: As a first step, for simplicity, we consider the variation with respect to \( u \) and \( v \) only, treating \( \alpha \) simply as free parameter. The variables \( u_k \) and \( v_k \) are taken here as a parametric transformation of the kind

\[ u_k = \sin \theta_k; v_k = \cos \theta_k. \quad (18) \]

Making use of this, Eqs. (15) and (17) become

\[ W = 2 \sum_k \frac{\epsilon_{k} (1 - \alpha)^2 \cos^2 \theta_k}{1 + \alpha (\alpha - 2) \cos^2 \theta_k} + \frac{1}{4} \sum_{k,l} \frac{V_{k,l}(1 - \alpha)^2 \sin 2\theta_k \sin 2\theta_l}{1 + \alpha (\alpha - 2) \cos^2 \theta_k \cos^2 \theta_l} \]

and

\[ \Delta_k = - \sum_{l} \frac{1}{2} V_{k,l} (1 - \alpha)^2 \sin 2\theta_k \frac{1}{1 + \alpha (\alpha - 2) \cos^2 \theta_l}. \quad (19) \]

These two fundamental equations now contain the parameters \( \theta \) and \( \alpha \).
Minimization with respect to the Bogoliubov amplitudes:
We minimize the total energy $W$ with respect to the variable $\theta_k$ by taking

$$\frac{\partial W}{\partial \theta_k} = 0. \quad (21)$$

This minimization procedure leads to an effective gap equation as given below:

$$\varepsilon_k(1 - \alpha)^2 \frac{\sin 2\theta_k}{\cos^2 \theta_k(\alpha^2 - 2\alpha + 2) - 1} = \Delta_k \quad (22)$$

[making use of Eq. (20)]

Now combining Eqs. (20) and (22), we obtain

$$\Delta_k = \frac{(1 - \alpha)^2 \sin 2\theta_k}{\varepsilon_k(1 - \alpha)^2 \cos^2 \theta_k - \sin^2 \theta_k}. \quad (23)$$

Let us rewrite the tuning parameter $\alpha$ as

$$\alpha = (1 - g) \quad (24)$$

with the allowed regime for the new parameter $g$ being also the same as that of $\alpha$, viz. $0 \leq g \leq 1$. Now under this transformation, the gap equation (Eq. 20) becomes

$$\Delta_k = -\frac{1}{2} \sum_i V_{k,i} \frac{g^2 \sin 2\theta_i}{\sin^2 \theta_i + g^2 \cos^2 \theta_i} \quad (25)$$

with

$$\frac{\Delta_k}{\varepsilon_k} = \frac{g^2 \sin 2\theta_k}{g^2 \cos^2 \theta_k - \sin^2 \theta_k}. \quad (26)$$

Combining Eqs. (25) and (26), we obtain the following equation:

$$\sum_{k,l} V_{kl} \frac{\sin 2\theta_l}{\sin^2 \theta_l + g^2 \cos^2 \theta_l} \times [(1 - g)(\sin^2 \theta_k \sin^2 \theta_l - g^4 \cos^2 \theta_k \cos^2 \theta_l)] = 0. \quad (27)$$

The above equation obtained by extremization condition gives two possible solutions for $g$, among which $g = 1$ is a natural root of this equation. Root $g = 1$ sets the ideal or the zero correlation regime for the system and indeed for this solution the ground state energy as well as the pairing gap will have the maximum magnitude. The other roots can be evaluated by solving Eq. (27) in a detailed manner.

We have eliminated $\sin \theta_k$ and $\cos \theta_k$ in terms of $\Delta_k, \varepsilon_k, g$ using Eqs. (26) and (27). Then making use of Eq. (25), we obtain the following self-consistent equation for $\Delta_k$:

$$\Delta_k = -\frac{1}{2} \sum_i V_{k,i} \frac{1}{g^2 \Delta_i(1 + g^2)^2 + 4g^2 \varepsilon_i^2)^2} \frac{1}{\left[1 + \frac{\Delta_i^2}{g^2 \varepsilon_i^2}\right]^2}. \quad (28)$$

The superconducting gap functions occurring in the above equation correspond to the Coulomb correlated fermion pair and these results are valid in both strong and weak correlation regimes. In the absence of induced Coulomb correlation, i.e. $g = 1 \text{ or } \alpha = 0$, this gap is identical to the non-interacting fermion pairing gap, as defined in the conventional BCS formalism.

The pairing potential $V_{k,i}$ is playing the crucial role here in pair formation and depending on the nature of the bosonic mediator, we can set the interaction frequency regime in the one-well model. Let it be done first for the phonon-mediated pairing and we set the upper cut-off frequency as $\omega_c$, where $\omega_c \gtrsim \omega_D; \omega_D$ is the Debye frequency in the normal metallic phase.

We first take the phonon-mediated pairing case. This potential well is defined as following the BCS prescription:

$$V_{k,i} = -V \text{ for } -\hbar \omega_c \leq \varepsilon_k, \varepsilon_l \leq +\hbar \omega_c \quad (29)$$

Assuming isotropic (s-wave) pairing for gap function on the Fermi surface, we take $\Delta_k = \Delta_1$. Then performing the summation over all possible momentum states in the right-hand side of Eq. (28), we obtain the following equation:

$$1 = \int_{-\hbar \omega_c}^{\hbar \omega_c} VN(\varepsilon) d\varepsilon,$$

where $N(\varepsilon)$ is the single spin electronic density of states per unit volume, which is nearly constant around the Fermi level and is approximated by $N_0$. The product of $N_0$ and $V$ is defined as the dimensionless attractive coupling constant $\lambda$ as usual, i.e. $N_0 V = \lambda$.

The integral on the right-hand side of Eq. (30) is evaluated. In this context, we take an approximation, viz. for $\frac{\Delta}{\varepsilon} \ll 1$. Thereafter, using this approximation and rearranging the integrand, Eq. (30) becomes

$$1 = 2g \lambda \int_0^{\hbar \omega_c} \frac{[\Delta^2 + \varepsilon^2]^{2}}{B^2 + \varepsilon^2} d\varepsilon, \quad (31)$$

where $B$ is the effective energy cut-off frequency.
where
\[
A^2 = \frac{\Delta^2(1 + g^2)^2}{4g^2},
\]
and,
\[
B^2 = \frac{\Delta^2(3 + g^2)}{4g^2}.
\]

Here, \(A\) and \(B\) are real quantities since \(g^2\) and \(\Delta^2\) are both real for \(g\) values being within the range \(0 \leq g \leq 1\).

Now, integrating the right-hand side of Eq. (31) numerically, we obtain
\[
2g\lambda\sqrt{A^2 - B^2}\tan^{-1}\left[\frac{\hbar\omega_c \sqrt{A^2 - B^2}}{B\sqrt{\hbar^2\omega_c^2 + A^2}}\right] - \frac{1}{2}\log A^2
+ \log\left[\hbar\omega_c + \sqrt{\hbar^2\omega_c^2 + A^2}\right] = 1.
\]

The first term within the above simplified result cannot contribute for the parameter regime of \(g\). This is because the argument of \(\arctan\) function becomes imaginary for the allowed ranges of \(g\) between 0 and 1 which is not physically acceptable. The factor \(A^2 - B^2\) is greater than zero only for \(g > 1\), which is again unphysical. Therefore, from Eq. (34), we get the solution for the superconducting gap \((\Delta_P)\) function as
\[
\Delta_P = \frac{4\hbar\omega_c g \exp\left(-\frac{1}{\lambda g}\right)}{1 + g^2}.
\]

Thus, the superconducting gap arising from Coulomb correlated fermion pairs (with free Coulomb correlation parameter) is given by the above equation. It must be kept in mind, however, that the Coulomb correlation is treated here simply as a tunable or free parameter by choosing from the physically allowed range of \(g\) values.

(ii) Inclusion of Coulomb correlation as a variational parameter: So far, the variational nature of the Gutzwiller parameter \(\alpha\) has not been taken into account. Now, we treat \(\alpha\) as a variational parameter too. This is done by minimizing the total energy with respect to \(g\) (which is again equivalent to the minimization with respect to \(\alpha\)). This is expressed as
\[
\frac{\partial W}{\partial g} = 0.
\]

The extremization procedure now leads to the following equation:
\[
\sum_k \varepsilon_k g^2 \sin 2\theta_k + \frac{1}{2} \sum_{k,l} V_{k,l} g \sin 2\theta_l (\sin^2 \theta_k \sin^2 \theta_l - g^4 \cos^2 \theta_k \cos^2 \theta_l) - \frac{\Delta^2}{\hbar^2} (\sin^2 \theta_l + g^2 \cos^2 \theta_l)^2 = 0.
\]

After simplification and making use of Eq. (25), the above equation leads to the following equation:
\[
g^2 = \frac{\Delta_k \tan^2 \theta_k}{\Delta_k - 2\varepsilon_k \tan \theta_k}.
\]

The above equations (Eqs. 38) and (26) are now two independent simultaneous equations involving the variable \(\theta_k\) and \(g\), in which the interplaying character of the pairing correlation and the Coulomb correlation is manifestly present. Analytically, it is somewhat complicated to determine the solution. Therefore, we handled it numerically and after combining it with \(\Delta\) Eq. (25) to obtain the self-consistent gap equation. The self-consistent ‘pairing-gap’ equation is now solved for the attractive potential well as previously defined in Eq. (29).

The boson exchange pairing is taking place within the defined range of the attractive potential and the ‘superconducting pairing-gap’ \((\Delta_{C-P})\) in the presence of Coulomb correlation is given by
\[
\Delta_{C-P} = 2\hbar\omega_c g \exp\left(-\frac{1}{\lambda g}\right).
\]

This time, the pairing gap is specifically denoted as \(\Delta_{C-P}\) to indicate that both the correlations are considered actively in the pair formation.

4 Results and discussion

In the last section, all the mathematical calculations are included where the bosonic mediator for the fermion pairing is phonon. The mediating phonon energy spectrum is considered to be lower than the Fermi energy and here the Fermi energy is assumed to be of the order of 1 eV, while the pair-bound state energy is only few meV. We set the range of potential well depending on the Debye temperature \((\theta_D)\). A table for a series of materials (some of them hold superconducting property), with their Debye temperature around 400 K, can be seen [29,30].

4.1 Case I: Pairing correlation in the presence of passive Coulomb correlation:

At first, the well range is taken as 0.05 eV for the phonon-mediated correlated pairing and the result is plotted here. The plotted result for \(\Delta_P\) against the parameter \(g\) for different coupling constants \(\lambda\) (see Fig. 1).

The result is also plotted for \(\Delta_P\) against coupling constant \(\lambda\) for different \(g\) values (see Fig. 2). The pairing gap opens up, for very small but finite positive values of coupling, even for \(\alpha = 0\) (or \(g = 1\)). Thus, pairing for the uncorrelated fermions in the presence of passive FS also requires finite coupling. The colored lines are for the different coupling values \(\lambda\) and the
Fig. 1 $\Delta P$ vs $g$ for different magnitudes of coupling constant $\lambda$

Fig. 2 $\Delta P$ vs $\lambda$ for different $g$ values

violet line is corresponding to $\lambda = 0.30$. This curve, depicting relatively high coupling, provides the comparatively large pairing gap $\Delta P$, in the intermediate coupling regime ($\lambda \geq 0.30$). In the strong correlation limits, the on-site Coulomb interaction dominates and confines the electrons to their real site positions. The repulsive on-site Coulomb potential dominates over the phonon-mediated attractive electron–electron interaction and that significantly affects the pairing. On other hand, the weak on-site correlation allows the pair formation and the gap is effectively very small for weak coupling even with weak correlation.

For the weak-to-intermediate coupling regime, viz. $0.3 \leq \lambda \leq 0.5$, the pairing gap is non-zero for relatively large correlation limit but not for very strong correlation, i.e. $g = 0$. In that scenario, again the $\Delta P$ drops down to zero for the very strong correlation and this also happens for the very strong coupling ($\lambda \rightarrow 1$).

We have seen from Fig. 2 that $\Delta P$ increases with $\lambda$ for a fixed $g$ value, as expected. In other words, it implies that, with increase in the strength of coupling, pair formation is enhanced for the allowed electron states, specified by the $g$ values. For the very low $g$ value (close to zero), where most of the doubly occupied states are eliminated, $\Delta P$ tends to zero. In this regime, there are no available states to form pairs. However, pairing states will be available as $g$ becomes more than zero. The magnitude of $\Delta P$ will increase with ‘$g$’ value and it will be maximum for $g = 1$, corresponding to a specific $\lambda$ value.

4.2 Case II: Pairing correlation in the presence of active Coulomb correlation

The gap function $\Delta_{C-P}$ is first plotted against $g$ for different $\lambda$ values (see Fig. 3) as well as it is also plotted against $\lambda$ for different $g$ values (see Fig. 4). The calculational results are presented here only in the weak to intermediate coupling regime.

Both $\Delta P$ and $\Delta_{C-P}$ are plotted against $g$ (see Figs. 1, 3), and these two follow the similar exponential nature; but the variation of $\Delta_{C-P}$ with $g$ is a little sharper for a specified $\lambda$ value. The pairing correlation is dominating over the on-site repulsion. In other words, it can be said that the electrons are not forced to stiff to their positions; rather they are relatively free to form pair.

In Fig. 4 above, where $\Delta_{C-P}$ is plotted against coupling constant for different Coulomb correlation strengths and it is observed that there exists a minimum value of $g$ to open up the pairing gap. The minimum cutoff values of $g$ (denoted by $g_{\text{min}}$) corresponding to for the different $\lambda$ obtained from our calculations are tabulated below:

These values of $g_{\text{min}}$ give an indication of the available states for pairing in the presence of Coulomb corre-
Values of $g_{\text{min}}$ for different magnitudes of $\lambda$

| $\lambda$ | $g_{\text{min}}$ |
|---------|-------------|
| 0.15    | 0.665       |
| 0.20    | 0.454       |
| 0.25    | 0.357       |
| 0.30    | 0.331       |

Fig. 4 $\Delta_{C-P}$ vs $\lambda$ for different $g$ values

Fig. 5 $\Delta_P$ and $\Delta_{C-P}$ vs $g$ for coupling value $\lambda = 0.30$

5 Conclusions

In this paper, we have presented the results of our investigation of the effect of the Coulomb correlation on the superconducting pairing of fermions, where the pairing mediator is a boson and the repulsive correlation is introduced through Gutzwiller projection operator acting on an ideal BCS ground state. Our aim was to determine the upper bound of Coulomb correlation strength for which the pairing correlation can survive. We had adopted two distinct approaches involving both the (i) passive and (ii) 'active' roles of Coulomb correlation parameter. The main highlights of our calculational results are given below:

(a) The physical characteristics of $\Delta_{C-P}$ is quite similar to that of $\Delta_P$ for the same range of the attractive potential well.

(b) The inter-playing properties of pairing correlation and Coulomb correlation in these two superconducting gaps for a specified range of attractive potential were presented earlier graphically in Figs. 1, 2, 3 and 4. We now directly compare the dependence of these two types of gaps on '$g$' for a fixed $\lambda$ in the same plot [see fig:5]. The red and black lines are for $\Delta_P$ and $\Delta_{C-P}$, respectively. Here, both the pairing gaps are calculated for a particular coupling strength of $\lambda$ (0.30). The inter-playing nature of the two correlations is most prominent in the intermediate regime of $g$, whereas both the pairing gaps exactly match at the two extremities besides their general overlap regions. Also, at the zero correlation, i.e., $g = 1$, both the pairing gaps ($\Delta_P$ and $\Delta_{C-P}$) are identical to the BCS pairing gap. It is interesting to note that $\Delta_P \geq \Delta_{C-P}$ in the entire regime of $g$ values for a fixed $\lambda$.

(c) The pairing phenomena is studied in the weak coupling regime and we exclude the intermediate coupling ($0.3 \leq \lambda \leq 1$) and strong coupling ($\lambda \geq 1$) regime. In the strong coupling regime, there is a possibility of the formation of a composite electron–phonon quasiparticle and the calculation of $\lambda$ itself is quite non-trivial [2, 4, 32].

(d) The approach denoted by us as a case I in the section: 'Model system', where the superconducting pairing itself originates from a Coulomb correlated Fermi sea would be taken up in details soon and reported in a future publication.

(e) The hydrogen saturated systems (general stoichiometry: $XH_n$) generate high phonon frequency spectrum under huge external pressure [7, 9]. This leads to a high phonon driven electron–electron pairing for a high-temperature conventional superconductor. The external pressure-driven metalization increases the bandwidth for the respective superconducting system. Therefore, the role of the external pressure can have similarities in controlling the Coulomb correlation in the pairing mechanism.

(f) In the very recent past, a correlation control phase transition from superconducting state to a correlated normal state has been experimentally reported in NbSe$_2$ [33]. This experiment demonstrates how the system size-dependent Coulomb correlation is competing with the attractive phonon driven electron–electron
interaction, which is independent of system size. In case, the NbSe$_2$ system size is made of the order of a few times of the coherence length, the attractive phonon-mediated electron–electron interaction, competes with the repulsive Coulomb interaction. This competition between these two type correlations leads to a phase transition from the superconducting state to a correlated insulating state. Therefore, in terms of handling correlations, we have found a theoretical approach which is similar to our approach.

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**Author contributions**

KM and RC defined this problem. KM did calculations. KM and RC wrote the manuscript together.

**Data Availability Statement** This manuscript has no associated data or the data will not be deposited. [Authors' comment: Based on our analytical results, we added all the data to this manuscript and there are no more data to deposit.]

**Appendix A**

**Normalization of the Coulomb correlated state:**

\[
\langle \Psi | \Psi \rangle_C = \left\langle 0 \right| \prod_u \left( \prod_m \left( u_{m}^* + v_{m}^* e^{-i \sum_{k'} c_{m',1}^+ c_{k',1}^-} e^{i \sum_{k'} c_{m',1}^+ c_{k',1}^-} \right) - \alpha \sum_{k' \neq k''} \left( c_{k',1}^+ c_{k''}^+ e^{i \sum_{k'} c_{m',1}^+ c_{k',1}^-} e^{i \sum_{k'} c_{m',1}^+ c_{k',1}^-} \right) \right) \left| 0 \right\rangle
\]

\[
\langle \Psi | \Psi \rangle_C = \left\langle 0 \right| \prod_{u,m} \left( u_{m}^* + v_{m}^* c_{m,1}^+ c_{-m,1}^- \right) \prod_{k',m''} \left( 1 - \alpha \sum_{k'' \neq k'''} \left( c_{k'',1}^+ c_{k'''}^+ e^{i \sum_{k''} c_{m',1}^+ c_{k',1}^-} e^{i \sum_{k''} c_{m',1}^+ c_{k',1}^-} \right) \right) \left| 0 \right\rangle
\]

\[
\langle \Psi | \Psi \rangle_C = \left\langle 0 \right| \prod_{u,m} \left( u_{m}^* + v_{m}^* c_{m,1}^+ c_{-m,1}^- \right) \prod_{k',m''} \left( 1 - \alpha \sum_{k'' \neq k'''} \left( c_{k'',1}^+ c_{k'''}^+ e^{i \sum_{k''} c_{m',1}^+ c_{k',1}^-} e^{i \sum_{k''} c_{m',1}^+ c_{k',1}^-} \right) \right) \left| 0 \right\rangle
\]

(40)
Here, the orthogonality of the states set a condition, for which only the terms with equal number of fermion Creation and annihilation operators will contribute with a non-zero value to that normalization. Therefore,

\[
\mathcal{C}(\langle \Psi | \Psi \rangle)_C = \langle 0 \rangle \prod_{s,m \neq l,j} \left[ u_m v_l + v_m v_l c_{m,l} c_{l,m} + v_m v_l c_{m,l} c_{l,m}^+ \right]
\]

\[
- \alpha v^*_m v_l \sum_{k', m''} c^{-1}_{-m', k''} c^{+1}_{m', k''} \epsilon_{k''} \epsilon_{k'} \epsilon_{m''} \epsilon_{k'} \epsilon_{m''} \epsilon_{m''} \epsilon_{l'', m''} e^{i(k'' - m'') r_{x', k'}},
\]

\[
+ \alpha^2 v^*_m v_l \sum_{k', m''} c^{-1}_{-m', k''} c^{+1}_{m', k''} \epsilon_{k''} \epsilon_{m''} \epsilon_{k'} \epsilon_{m''} \epsilon_{m''} \epsilon_{l'', m''} e^{i(k'' - m'') r_{x', k'}},
\]

\[
e^{i(k'' - m'') r_{x', k'}} e^{i(k'' - m'') r_{x'', l''}} e^{i(k'' - m'') r_{x', k'}}
\]

\[
- \alpha v^*_m v_l \sum_{k', m''} c^{-1}_{-m', k''} c^{+1}_{m', k''} \epsilon_{k''} \epsilon_{m''} \epsilon_{k'} \epsilon_{m''} \epsilon_{m''} \epsilon_{l'', m''} e^{i(k'' - m'') r_{x', k'}},
\]

\[
= \prod_{s,m \neq l,j} \left[ u_m v_l + v_m v_l c_{m,l} c_{l,m} + v_m v_l c_{m,l} c_{l,m}^+ \right]
\]

The contribution of potential energy expectation value is deduced in a similar manner and these are added in this section.

\[
c\langle \Psi | \Psi \rangle_C = \prod_l \left[ |u_l|^2 + |v_l|^2 - 2\alpha |v_l|^2 + \alpha^2 |v_l|^2 \right]
\]

\[
c\langle \Psi | \Psi \rangle_C = \prod_l \left[ 1 + (\alpha^2 - 2\alpha) |v_l|^2 \right]
\]

(Appendix B)

**Total energy expectation W:**

\[
W = \frac{1}{\langle \langle \Psi | \rangle \rangle} \left[ c\langle \langle \Psi | \rangle \rangle \sum_k 2 \varepsilon_k b_k^\dagger b_k + \sum_{k,l} V_{k,l} b_k^\dagger b_l \right]
\]

Kinetische energy operator expectation value:

\[
T = \prod_k \left[ 1 + (\alpha^2 - 2\alpha) |v_k|^2 \right] \sum_{k,s} \varepsilon_k \langle 0 \rangle \left[ \prod_m \left( u_m^* + v_m c_{m,l} c_{l,m} \right) \right] \prod_\sigma \left[ 1 - \alpha \sum_{k', m'} c^{+1}_{m', k'} c^{+1}_{m', k'} c^{+1}_{m', l'} c^{+1}_{m', l'} e^{i(k'' - m'') r_{x', k'}} \right] \prod_l \left( u_l + v_l c_{l,m} c_{m,l}^+ \right) \langle 0 \rangle.
\]

This calculation is done by classifying the contribution coming out from the states which are specified with the power of \(\alpha\), and they are listed as below:

\[
\alpha^0 : 2 \sum_k \frac{\varepsilon_k |v_k|^2}{1 + \alpha(\alpha - 2) |v_k|^2}.
\]

\[
\alpha^1 : 2 \sum_k \frac{-2\varepsilon_k |v_k|^2}{1 + \alpha(\alpha - 2) |v_k|^2}.
\]

\[
\alpha^2 : 2 \sum_k \frac{\alpha^2 \varepsilon_k |v_k|^2}{1 + \alpha(\alpha - 2) |v_k|^2}.
\]

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