Possible coexistence of charge density wave and superconductivity and enhancement of the transition temperature for the layered quasi-two-dimensional superconductor 2H-NbSe$_2$

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Abstract
Starting with a two-band Hamiltonian with pairing interaction and interband coupling, and a charge density wave (CDW) Hamiltonian using Green’s function formalism, we demonstrate possible coexistence of superconductivity and charge density wave (CDW). The enhancement of the critical temperature with multi-band system is also established. The results are in broad agreement with experimental observations.

1. Introduction

Superconductivity was discovered in 1911 by Kamerlingh Onnes [1]. Today, superconductivity is a phenomenon observed by certain materials with properties of zero electrical resistance and perfect diamagnetism. In 1956, Leon N Cooper explained that a pair of electrons that interact above a Fermi surface can have a net attraction where they form a bound state such that their total energy is greater than zero [2]. He suggested that such bound electron pair can be responsible to produce superconducting state. In 1957, Bardeen, Cooper and Schrieffer jointly investigated BCS theory [3]. BCS theory gave a successful explanation for low $T_c$ superconductors. Superconducting materials can be classified into conventional and unconventional superconductors based on the operating value of the transition temperature. A superconductor is considered as an unconventional superconductor if it cannot be explained by BCS theory. Generally, high temperature superconductors are considered as unconventional superconductors. The practical applications of conventional superconductors are limited due to the very low operating temperatures.

The discovery of high Tc materials came up with many feasible applications in the life of mankind. These applications include high-speed trains, magnetic energy storage, magnetic resonance imaging (MRI) for medical applications, Josephson devices, Superconducting Quantum Interference Devices (SQUID), Magnetoencephalography, microwave devices and resonators to high energy physics experiments, etc [4–6]. Because of the need to increase the value of the critical temperature, many scholars around the world are working day and night. The quest to achieve high temperature superconductivity is the dream of many scientists around the globe. In particular, the mechanism of Room Temperature Superconductivity (RTS) is one of the most challenging unresolved problems in contemporary physics [4–7]. RTS is very active research in condensed matter physics. One of the crucial questions is the elucidation of the mechanism of RTS. Although the mechanism of RTS still remains elusive, a lot of progress has been made resulting in a major reduction in the number of proposed mechanisms under consideration [6, 7]. High temperature superconductors were first discovered in family of cuprates with $T_c \approx 35$ K by Bednorz and Muller in 1986. After this discovery, the value of the transition temperature in cuprate perovskites was found to raise up to 164 K under high pressure [8]. In cuprates, it was known that, the mechanism was by the involvement of multi-electronic species [9]. Next to cuprates, Iron based superconductors were discovered [10]. The discovery of iron-based superconductors...
opened many interesting scientific issues to the scientific community. Some of the issues include: the presence of complex electronic band structure, the coexistence of magnetic and superconducting order parameters, and structural effects [11, 12]. It is known that, iron with a large magnetic moment was widely believed to be harmful to the emergence of superconductivity because of the competition between the static ordering of electron spins and the dynamic formation of electron pairs [10, 13].

Another promising candidate towards RTS are the class of hydrogen containing compounds under high pressure which are called hydrides [14, 15]. The idea for metallization of hydrogen under high pressure was suggested around 1960s [16, 17]. Very recently, superconductivity with a critical temperature 203 K was observed in sulfur hydride under high pressures [18]. Today, the family of hydrides are the best promising candidates for RTS [18, 19]. Hydrides hold a promise to possess very-high-temperature superconductivity due to high vibrational frequencies, strong electron-phonon interaction, and partially covalent bonding [18–21]. Currently, there are some theoretically predicted polyhydrides to become stable at high pressures towards high temperature superconductivity [21–23].

In 1959, multi-band approach was proposed by H Suhl, B T Matthias, and L R Walker [24] to extend BCS theory to include the involvement of two or more bands [25–27]. According to the conventional BCS theory, all the electrons on an isotropic Fermi surface make equal contribution to the superconducting pairing, meaning with constant energy gap. However, when the Fermi surface has multiple bands, with more or less itinerant electrons overlapping on the Fermi surface, BCS theory will not give sufficient information. Hence, the presence of two or more bands will be necessary to consider the involvement of different energy gaps. In this mechanism, it was suggested that, two different energy gaps, \( \Delta_1 \) and \( \Delta_2 \), with corresponding intraband coupling strengths \( \lambda_{11} \) and \( \lambda_{22} \) vanish at the same critical temperature with additional coupled interband terms can enhance the transition temperature [28]. In this case, the presence of interband pair coupling, \( \lambda_{AB} \), enhances the critical temperature. Very recently, a multi-band proposal based on the idea of steep band/flat band model was suggested on the assumption that first electronic component with vanishing Fermi velocity in the intermediate polaronic regime, while the second being in the weak coupling regime with high Fermi velocity to study roadmap to room temperature superconductivity [29–31]. The idea of flat band was discussed in many papers [31–38].

The coexistence of two or more order parameters in materials is one of the most striking property in condensed matter physics [39–53]. Examples of such coexistences are the coexistence between superconductivity and charge density wave (CDW) [39–42], the coexistence of spin density wave (SDW) and superconductivity [43–50], the interplay of magnetic and superconducting order parameters [51–53]. The idea of CDWs was first studied for the case of a one-dimensional solid of lattice constant \( a \) by Peierls [34]. In Peierls theory, CDWs in 1D solid can be formed by electrons and phonons because of the presence of Fermi-surface nesting. Today, different theories and experiments suggested that, CDWs can be formed by Fermi-surface nesting [55], by saddle point singularities [55, 56], or by electron–phonon interactions [57]. CDWs are periodic modulations of conduction electron densities and the associated lattice distortions in solids having a broken symmetry which can be described by a complex order parameter [58, 59]. CDWs occur in many condensed matter systems. One kind of very interesting CDW system is found in transition metal dichalcogenides (TMDs) which show a common coexistence phase diagram with the superconducting state [60].

The coexistence of superconductivity and charge density wave (CDW) order parameters is a fundamental question in the theory of superconductivity [60–62]. Because of such coexistences, the area of high-temperature superconductivity become an active area of research [63]. Low-dimensional materials possess very different properties from their bulk counterparts [64, 65]. One of such well-known low-dimensional materials are two-dimensional transition metal dichalcogenides (TMDs) [64–67]. Since the number of layers can significantly affect the CDW state, 2D layered materials can show interesting phenomena in the coexistence of CDW and superconducting order parameters. To study such phenomena of coexistences for 2D materials, different authors used different theoretical and computational techniques. Using Density Functional Theory (DFT), it was shown that, CDW hampers exciton condensation in the case of \( \text{I}_{\text{T}}\text{TiSe}_{2} \) [68]. With similar DFT approach, the effect of dimensionality on CDW for layered \( 2\text{H-NbSe}_{2} \) was described [69]. Also, in these materials, it was shown that, the CDW can be suppressed by external parameters like pressure, doping, or electrostatic gating eventually leading to the emergence of superconductivity [58, 60, 62–66]. Niobium diselenide (NbSe_{2}) is one of the first discovered TMDs which received much attention in the study of the coexistence of superconductivity and CDW in the layered 2H \([63–67]\). The layered compound 2H \[\text{NiSe}_{2}\] is a two-gap superconductor [64–66] having a transition temperature \( T_{\text{C}} = 7.3 \) K as well as a charge-density wave (CDW) transition of \( T_{\text{CDW}} = 33.5 \) K [70, 71].

Previous studies showed that the combination of weak-coupling with strong coupling strongly enhances superconducting phases [30, 31, 72–74]. The coexistence of steep and flat energy bands in the vicinity of the Fermi surface gives rise to large density of states. In flat bands, the effective mass of the electrons is large, the kinetic energy is quenched, and the Coulomb interaction term is important [72]. Flat bands are frequency-
independent dispersionless bands which play crucial role in ferromagnetism, Wigner crystal, edge states, topological insulators, superconductivity, etc [72–76]. Flat bands are observed in low-dimensional systems, in particular in layered quasi-two-dimensional metal dichalcogenides [77, 78].

Until now, different theoretical studies were carried out to unlock the mystery how CDW state coexists with superconductivity in 2D materials in general and in TMDs in particular. However, there is no clear mathematical relationship which can show how CDW and superconducting order parameters can be related for such 2D materials. The objective of this paper is to present clear mathematical relationship which can show how CDW and superconducting order parameters can be related for such 2D materials. This study can help in understanding of the mechanisms of the coexistence of superconducting and CDW order parameters in 2D systems in particular and superconductivity in general.

This study focuses on the theoretical investigation of the coexistence of superconductivity and CDW order parameters for layered quasi-two-dimensional 2H-NbSe2. We considered based on the idea that, flat (frequency independent dispersionless) band can coexist with a steep band as discussed in [15, 23, 29–33]. We developed a two-band Hamiltonian with temperature dependent double-time Green’s function approach. Temperature dependent double-time Green functions are most convenient methods to study systems of large numbers of particles [79, 80]. Since they can satisfy a set of coupled equations like those of two coupled energy gaps for two-band model [81], one can solve the coupled gap equations by decoupling the higher order Green functions into lower order ones with the help of appropriate decoupling procedures [53, 80–82].

This paper is organized in four sections. In section 2, we developed a system Hamiltonian for a two-band model. From our model Hamiltonian, we obtained analytical expressions relating the transition temperature with the superconducting and CDW order parameters. Furthermore, the superconducting transition temperature in the absence of CDW order parameter (for a pure superconducting region) and in the presence of CDW term will be analyzed. Section 3 presents derivation of mathematical expression for temperature dependent CDW order. Finally, section 4 presents results and discussion for layered quasi-2D superconductor 2H-NbSe2.

2. Model Hamiltonian

In order to derive analytic expressions for the superconducting transition temperature in the presence of CDW term, we consider two-band model in the presence of interband (band-to-band) pair scattering. We consider the following model Hamiltonian for a two-band system having two different electronic systems:

\[ \hat{H} = \hat{H}_I + \hat{H}_S + \hat{H}_{12} + \hat{H}_C \]  

(1.1)

where, the terms \( \hat{H}_I \) and \( \hat{H}_S \) denote the intraband Hamiltonians for band 1 and band 2 respectively, and the terms \( \hat{H}_{12} \) and \( \hat{H}_C \) stand for the interband and CDW Hamiltonians respectively. The intraband Hamiltonians are given by:

\[ \hat{H}_I = \sum_{k,\sigma} \epsilon_I(k) a_{k,\sigma}^{\dagger} a_{k,\sigma} - \sum_{k,\sigma} U_I(k) a_{k,\sigma}^{\dagger} a_{-k,\sigma}^{\dagger} a_{-k,\sigma} a_{k,\sigma}; \]  

(1.2)

\[ \hat{H}_S = \sum_{k,\sigma} \epsilon_S(k) b_{k,\sigma}^{\dagger} b_{k,\sigma} - \sum_{k,\sigma} U_S(k) b_{k,\sigma}^{\dagger} b_{-k,\sigma}^{\dagger} b_{-k,\sigma} b_{k,\sigma}; \]  

(1.3)

The interband Hamiltonian term is given by:

\[ \hat{H}_{12} = -\sum_{k,\sigma} U_{12} \{ a_{k,\sigma}^{\dagger} a_{-k,\sigma}^{\dagger} b_{k,\sigma} b_{-k,\sigma} + b_{k,\sigma}^{\dagger} b_{-k,\sigma}^{\dagger} a_{-k,\sigma} a_{k,\sigma}\}. \]  

(1.4)

In equations (1.2), (1.3), the symbols \( a^{\dagger}(a) \) and \( b^{\dagger}(b) \) denote the usual raising and lowering quantum mechanical operators with spin (\( \sigma \)) up or down (\( \uparrow \) or \( \downarrow \)), and \( U_I \) and \( U_S \) are the intraband potentials for band 1 and band 2 respectively. The subscript \( k \) stands for the wave vectors of the particles. For the sake of simplicity, let us use the mean-field (MF) approximation for the above Hamiltonians. In our MF approximation, the intraband terms can be defined by:

\[ \Delta_I^+ \equiv \sum_k U_I(k) \langle \{ a_{k,\sigma}^{\dagger}, a_{-k,\sigma} \} \rangle, \quad \Delta_I \equiv \sum_k U_I(k) \langle \{ a_{-k,\sigma}^{\dagger}, a_{k,\sigma} \} \rangle, \]  

(1.5)

\[ \Delta_S^+ \equiv \sum_k U_S(k) \langle \{ b_{k,\sigma}^{\dagger}, b_{-k,\sigma} \} \rangle, \quad \Delta_S \equiv \sum_k U_S(k) \langle \{ b_{-k,\sigma}^{\dagger}, b_{k,\sigma} \} \rangle. \]  

(1.6)
Also, the CDW Hamiltonian term in the MF approximation can be defined as:
\[ \hat{H}_C \equiv -\Delta_C \sum_k (a_{k+Q}^+ b_k + b_{k+Q}^+ a_k). \] (1.7)

If we consider \( \Delta \) as a real quantity, the magnitudes of \( \Delta_1 \) and \( \Delta_2 \) are equal and the same is true for \( \Delta_1^\dagger \) and \( \Delta_2^\dagger \). With this assumption, the intraband Hamiltonians under the MF consideration become:
\[ H_1^{\text{MF}} \equiv \sum_{k,\sigma} \varepsilon(k) a_{k,\sigma}^+ a_{k,\sigma} - \Delta_1 \sum_k (a_{k+Q}^+ a_{k-1} + a_{k+1} a_k), \] (1.8a)
\[ H_2^{\text{MF}} \equiv \sum_{k,\sigma} \varepsilon(k) b_{k,\sigma}^+ b_{k,\sigma} - \Delta_2 \sum_k (b_{k+Q}^+ b_{k-1} + b_{k+1} b_k). \] (1.8b)

The interband terms under the MF approximation are defined by:
\[ \Delta_1^\dagger \equiv \sum_k U_{11}(k) \langle \langle b_k^+, b_{k+1}^+ \rangle \rangle, \quad \Delta_2 \equiv \sum_k U_{12}(k) \langle \langle a_{k+1}, a_k \rangle \rangle. \] (1.9)
\[ \Delta_1^\dagger \equiv \sum_k U_{11}(k) \langle \langle a_k^+, a_{k-1}^+ \rangle \rangle, \quad \Delta_2 \equiv \sum_k U_{12}(k) \langle \langle a_{k+1}, a_k \rangle \rangle. \] (1.10)

Again, considering \( \Delta \) as a real quantity the interband terms can be presented in the form:
\[ H_{1,2}^{\text{MF}} \equiv -\Delta_1 \sum_k (a_{k+Q}^+ a_{k-1} + b_{k+1}^+ b_k) - \Delta_2 \sum_k (b_{k+Q}^+ b_{k-1} + a_{k+1} a_k). \] (1.11)

Substituting equations (1.7), (1.8) and (1.11) in equation (1.1), we get:
\[ H_{\text{MF}} \equiv \sum_{k,\sigma} \varepsilon(k) a_{k,\sigma}^+ a_{k,\sigma} + \sum_{k,\sigma} \varepsilon(k) b_{k,\sigma}^+ b_{k,\sigma} - \Delta_1 \sum_k (a_{k+Q}^+ a_{k-1} + a_{k+1} a_k) - \Delta_2 \sum_k (b_{k+Q}^+ b_{k-1} + b_{k+1} b_k) - \Delta_1 \sum_k (a_{k+Q}^+ a_{k-1} + b_{k+1} b_k) - \Delta_2 \sum_k (b_{k+Q}^+ b_{k-1} + a_{k+1} a_k) - \Delta_1 \sum_k (b_{k+Q}^+ b_{k-1} + b_{k+1} b_k) - \Delta_2 \sum_k (a_{k+Q}^+ a_{k-1} + a_{k+1} a_k). \] (1.12)

Let us study the Hamiltonian given in equation (1.12) by the method of Green functions. In our case we use the equation of motion method. The equation of motion for the Green’s function \( \langle \langle a_{k,1}^+, a_{k,1}^- \rangle \rangle \) in band 1 is given by:
\[ \omega \langle \langle a_{k,1}^+, a_{k,1}^- \rangle \rangle \omega = [a_{k,1}^+, a_{k,1}^-] + \langle \langle [a_{k,1}^+ - \hat{H}_1 + \hat{H}_2 + \hat{H}_{12} + \hat{H}_C], a_{k,1}^- \rangle \rangle \omega. \] (1.13)

Each of the commutation relations in equation (1.13) are given by:
\[ [a_{k,1}^+, \hat{H}_1^{\text{MF}}] = \left[ a_{k,1}^+, \left( \sum_{k,\sigma} \varepsilon(k) a_{k,\sigma}^+ a_{k,\sigma}^\dagger - \Delta_1 \sum_k (a_{k+Q}^+ a_{k-1} + a_{k+1} a_k) \right) \right] \]
\[ = \sum_{k,\sigma} \varepsilon(k) [a_{k,1}^+, a_{k,\sigma} a_{k,\sigma}^\dagger] - \Delta_1 \sum_k [a_{k+Q}^+ a_{k-1} + a_{k+1} a_k] \]
\[ = -\varepsilon(k) k_{1,1}^+ + \Delta_1 a_{k,1}. \] (a)

Similarly, the remaining three terms are given by:
\[ [a_{k,1}^+, \hat{H}_2] = 0 \] (b)
\[ [a_{k,1}^+, \hat{H}_{12}] = \Delta_{12}(k) a_{k,1} \] (c)
\[ [a_{k,1}^+, \hat{H}_C] = \Delta_C(k) a_{k,1}. \] (d)

Plugging equations (a) to (d) in equation (1.13) and rearranging, we get:
\[ \langle \langle a_{k,1}^+, a_{k,1}^- \rangle \rangle \omega = \frac{\Delta_{12}(k)}{(\omega + \varepsilon - \Delta_C)} \langle \langle a_{k,1}, a_{k,1}^- \rangle \rangle \omega + \frac{\Delta_1(k)}{(\omega + \varepsilon - \Delta_C)} \langle \langle a_{k,1}, a_{k,1}^- \rangle \rangle \omega. \] (1.14)

According to equation (1.14), we see that, the correlation function \( \langle \langle a_{k,1}^+, a_{k,1}^- \rangle \rangle \omega \) in relation to band 1 contains two coupled order parameters, namely, \( \Delta_1 \) and \( \Delta_2 \). Now, let us identify the cutoff frequencies by labeling \( \omega_1 \) and \( \omega_2 \), such that the interband cutoff frequency mixing from band 1 to band 2 by \( \omega_{12} \). With this labeling, equation (1.14) reads:
When each of the commutation relations in equation (1.15) are evaluated, we get:

\[
\langle [a_{-k1}, A_{+k1}] \rangle_\omega = \frac{\Delta_1(k)}{(\omega_1 + \epsilon_1 - \Delta_C)} \langle \{a_{-k1}, a_{+k1}\} \rangle_\omega + \frac{\Delta_2(k)}{(\omega_2 + \epsilon_2 - \Delta_C)} \langle \{a_{-k1}, a_{+k1}\} \rangle_\omega.
\]  

(1.15)

In equation (1.15), we find the equation of motion for the Green’s function \(\langle [a_{-k1}, a_{+k1}] \rangle_\omega\) with the help of double time temperature-dependent Green’s function formalism as we did above. So, we have:

\[
\omega \langle [a_{-k1}, a_{+k1}] \rangle_\omega = [\{a_{-k1}, a_{+k1}\}]_\omega + \langle \{\hat{H}_1, a_{+k1}\} \rangle_\omega = 1 + \langle \{\hat{H}_{11}, \hat{H}_{12} + \hat{H}_{1b}, a_{+k1}\} \rangle_\omega.
\]

(1.16)

The commutation relations given in equation (1.16) are given by:

\[
[a_{-k1}, \hat{H}_1] = \epsilon_1(k) a_{-k1} + \Delta_1(k) a_{+k1}^{+} \\
[a_{-k1}, \hat{H}_2] = 0 \\
[a_{-k1}, \hat{H}_{12}] = \Delta_2(k) a_{+k1}^{+} \\
[a_{-k1}, \hat{H}_{1b}] = -\Delta_C(k) a_{-k1}.
\]

(1.17)

Upon substituting equations (1.17) in (1.16) in each of the corresponding terms, we obtain:

\[
\langle [a_{-k1}, a_{+k1}] \rangle_\omega = \frac{\Delta_1}{(\omega_1 + \epsilon_1 - \Delta_C)(\omega_1 - \epsilon_1 + \Delta_C) - \Delta_1^2} + \frac{\Delta_2}{(\omega_1 + \epsilon_1 - \Delta_C)(\omega_2 + \epsilon_2 - \Delta_C) - \Delta_2^2}.
\]

(1.18)

Using equations (1.17) in (1.16) in each of the corresponding terms, we obtain:

\[
\langle [b_{+k1}, b_{-k1}] \rangle_\omega = \frac{\Delta_1}{(\omega_1 + \epsilon_1 - \Delta_C)(\omega_1 - \epsilon_1 + \Delta_C) - \Delta_1^2} + \frac{\Delta_2}{(\omega_1 + \epsilon_1 - \Delta_C)(\omega_2 + \epsilon_2 - \Delta_C) - \Delta_2^2}.
\]

(1.19)

Each of the commutators in equation (1.19) are given by:

\[
[b_{+k1}, \hat{H}_1] = -\epsilon_2(k) b_{+k1}^{+} + \Delta_2 b_{-k1} \\
[b_{+k1}, \hat{H}_2] = \Delta_2(k) b_{-k1} \\
[b_{-k1}, \hat{H}_{12}] = \Delta_2(k) a_{-k1} \\
[b_{-k1}, \hat{H}_{1b}] = \Delta_C(k) b_{+k1}^{+}.
\]

(1.20)

Putting equations (1.17) in (1.16) and simplifying the result, we get the following equation:

\[
\langle [b_{+k1}, b_{-k1}] \rangle_\omega = \frac{\Delta_1}{(\omega_2 + \epsilon_2 - \Delta_C)(\omega_2 + \epsilon_2 - \Delta_C) - \Delta_1^2} + \frac{\Delta_2}{(\omega_1 + \epsilon_1 - \Delta_C)(\omega_1 - \epsilon_1 + \Delta_C) - \Delta_2^2}.
\]

(1.21)

In equation (1.21), the equation of motion for the Green’s function \(\langle [b_{-k1}, b_{+k1}] \rangle_\omega\) is:

\[
\omega \langle [b_{-k1}, b_{+k1}] \rangle_\omega = 1 + \langle \{\hat{H}_{11}, \hat{H}_{12} + \hat{H}_{1b}, b_{+k1}^{+}\} \rangle_\omega.
\]

(1.22)

When each of the commutation relations in equation (1.22) are evaluated, we get:

\[
[b_{-k1}, \hat{H}_1] = \epsilon_2(k) b_{+k1}^{+} + \Delta_2 b_{+k1}^{+} \\
[b_{-k1}, \hat{H}_2] = \Delta_2(k) b_{-k1} \\
[b_{-k1}, \hat{H}_{12}] = \Delta_C(k) a_{-k1}.
\]
Using expressions (m)–(p) in equation (1.21), we get the following equation:

\[
\langle b_{k+1}^+ b_{k+1}^- \rangle = \frac{1}{\omega_2 + \varepsilon_2 - \Delta_C} + \frac{\Delta_2}{\omega_2 + \varepsilon_2 - \Delta_C} \langle b_{k+1}^+ b_{k+1}^- \rangle_{\omega_2} + \frac{\Delta_1}{\omega_2 + \varepsilon_1 - \Delta_C} \langle b_{k+1}^+ b_{k+1}^- \rangle_{\omega_1}. \tag{1.22}
\]

Solving for \(\langle b_{k+1}^+ b_{k+1}^- \rangle\) from (1.20) and (1.22), we have:

\[
\langle b_{k+1}^+ b_{k+1}^- \rangle = \frac{\Delta_2}{\omega_2 + \varepsilon_2 - \Delta_C} (\omega_2 - \varepsilon_2 + \Delta_C - \Delta_2^2) + \frac{\Delta_1}{\omega_2 + \varepsilon_1 - \Delta_C} (\omega_2 + \varepsilon_1 - \Delta_C - \Delta_2^2). \tag{1.23}
\]

With the help of partial fraction decomposition equations (1.18) and (1.23) can be re-written in the following form:

\[
\langle a_{\eta+1}^+ a_{\eta+1}^- \rangle = -\frac{1}{2} \left( \frac{\Delta_1 + \Delta_C}{\omega_1^2 - \varepsilon_1^2(k) - (\Delta_1 + \Delta_C)^2} + \frac{\Delta_1 - \Delta_C}{\omega_1^2 - \varepsilon_1^2(k) - (\Delta_1 - \Delta_C)^2} \right) \tag{1.24a}
\]

\[
\langle b_{k+1}^+ b_{k+1}^- \rangle = -\frac{1}{2} \left( \frac{\Delta_2 + \Delta_C}{\omega_2^2 - \varepsilon_2^2(k) - (\Delta_2 + \Delta_C)^2} + \frac{\Delta_2 - \Delta_C}{\omega_2^2 - \varepsilon_2^2(k) - (\Delta_2 - \Delta_C)^2} \right). \tag{1.24b}
\]

The coupled superconducting order parameters \(\Delta_1\) and \(\Delta_2\) with respect to band 1 and band 2 respectively are related to the Green’s functions \(\langle a_{\eta+1}^+ a_{\eta+1}^- \rangle\) and \(\langle b_{k+1}^+ b_{k+1}^- \rangle\) by the following relations:

\[
\Delta_1 = -\frac{U_1}{\beta} \sum_k \langle a_{\eta+1}^+ a_{\eta+1}^- \rangle_k - \frac{U_2}{\beta} \sum_k \langle b_{k+1}^+ b_{k+1}^- + a_{-k} a_{-k} \rangle_k, \tag{1.25a}
\]

\[
\Delta_2 = -\frac{U_2}{\beta} \sum_k \langle b_{k+1}^+ b_{k+1}^- \rangle_k - \frac{U_1}{\beta} \sum_k \langle b_{k+1}^+ b_{k+1}^- + a_{-k} a_{-k} \rangle_k. \tag{1.25b}
\]

Substituting equation (1.25a) into equations (1.24a) and (1.25b) into (1.24b), we get the following equations:

\[
\Delta_1 = -\frac{U_1}{2\beta} \sum_{k,n} \left( \frac{\Delta_1 + \Delta_C}{\omega_{1,n}^2 - \varepsilon_1^2(k) - (\Delta_1 + \Delta_C)^2} + \frac{\Delta_1 - \Delta_C}{\omega_{1,n}^2 - \varepsilon_1^2(k) - (\Delta_1 - \Delta_C)^2} \right) \tag{1.26a}
\]

\[
\Delta_2 = -\frac{U_2}{2\beta} \sum_{k,n} \left( \frac{\Delta_2 + \Delta_C}{\omega_{2,n}^2 - \varepsilon_2^2(k) - (\Delta_2 + \Delta_C)^2} + \frac{\Delta_2 - \Delta_C}{\omega_{2,n}^2 - \varepsilon_2^2(k) - (\Delta_2 - \Delta_C)^2} \right) \tag{1.26b}
\]

Introducing the imaginary Matsubara frequency [66] of the form:

\[
i\omega_p = \frac{i(2p + 1)\pi}{\beta} \tag{1.27}
\]

and, using the following tangent hyperbolic identity:

\[
\sum_p \left( \frac{1}{(2p + 1)^2 + y^2} \right) = \frac{1}{2y} \tanh \left( \frac{1}{2} y \right), \tag{1.28}
\]

where, \(p\) is an integer, into equations (1.26), we arrive at the following expressions for the relationship between the superconducting and charge density wave (CDW) order parameters for a multi-band superconductor:
\[ \Delta_1 = \frac{U_1}{2} \left[ \sum_k \left( \frac{(\Delta_1 + \Delta_C)}{2\epsilon_1(k)} \right) \tanh \left( \frac{1}{2} \beta \epsilon_1(k) \right) + \sum_k \left( \frac{(\Delta_1 - \Delta_C)}{2\epsilon'_1(k)} \right) \tanh \left( \frac{1}{2} \beta \epsilon'_1(k) \right) \right] \\
+ \frac{U_2}{2} \left[ \sum_k \left( \frac{(\Delta_2 + \Delta_C)}{2\epsilon_2(k)} \right) \tanh \left( \frac{1}{2} \beta \epsilon_2(k) \right) + \sum_k \left( \frac{(\Delta_2 - \Delta_C)}{2\epsilon'_2(k)} \right) \tanh \left( \frac{1}{2} \beta \epsilon'_2(k) \right) \right]. \quad (1.29a) \]

\[ \Delta_2 = \frac{U_1}{2} \left[ \sum_k \left( \frac{(\Delta_2 + \Delta_C)}{2\epsilon_2(k)} \right) \tanh \left( \frac{1}{2} \beta \epsilon_2(k) \right) + \sum_k \left( \frac{(\Delta_2 - \Delta_C)}{2\epsilon'_2(k)} \right) \tanh \left( \frac{1}{2} \beta \epsilon'_2(k) \right) \right] \\
+ \frac{U_2}{2} \left[ \sum_k \left( \frac{(\Delta_1 + \Delta_C)}{2\epsilon_1(k)} \right) \tanh \left( \frac{1}{2} \beta \epsilon_1(k) \right) + \sum_k \left( \frac{(\Delta_1 - \Delta_C)}{2\epsilon'_1(k)} \right) \tanh \left( \frac{1}{2} \beta \epsilon'_1(k) \right) \right]. \quad (1.29b) \]

Where, we have used the definitions:
\[ \epsilon_1(k) = \sqrt{\epsilon_1^2(k) + (\Delta_1 + \Delta_C)^2}, \quad \epsilon'_1(k) = \sqrt{\epsilon_1^2(k) + (\Delta_1 - \Delta_C)^2}, \quad (1.30a) \]
\[ \epsilon_2(k) = \sqrt{\epsilon_2^2(k) + (\Delta_2 + \Delta_C)^2}, \quad \epsilon'_2(k) = \sqrt{\epsilon_2^2(k) + (\Delta_2 - \Delta_C)^2}. \quad (1.30b) \]

In order to study the CDW order parameter, \( \Delta_C \), with its corresponding transition temperature, \( T_{CDW} \), and to analyze its coexistence with the superconducting order parameter, it will be important to find the equation of motion for the CDW Hamiltonian with the help of the double time temperature dependent Green’s function formalism. Let us consider the Green’s function \( \langle [a_{\uparrow k+Q}^+, b_{\downarrow k}^+]_\omega \rangle \). Following the same procedure as above, the equation of motion for the CDW Hamiltonian can be presented in the form:
\[ \omega \langle [a_{\uparrow k+Q}^+, b_{\downarrow k}^+]_\omega \rangle = \langle \left[ [a_{\uparrow k+Q}^+, \hat{H}_{MF}], b_{\downarrow k}^+ \right] + \langle \left[ [a_{\uparrow k+Q}^+, \hat{H}_{MF}], b_{\downarrow k}^+ \right] + \langle [a_{\uparrow k+Q}^+, \hat{H}_{MF}], b_{\downarrow k}^+ \rangle \rangle. \quad (1.31) \]

When each of the commutation relations in (1.31) are evaluated, we get the following:
\[ [a_{\uparrow k+Q}^+, \hat{H}_{MF}] = -\epsilon_1(k)a_{\uparrow k+Q}^+ + \Delta_1 a_{\downarrow -k+Q}^+ \quad (q) \]
\[ [a_{\uparrow k+Q}^+, \hat{H}_{MF}] = 0 \quad (r) \]
\[ [a_{\uparrow k+Q}^+, \hat{H}_{MF}] = \Delta_2 a_{\downarrow -k+Q}^+ \quad (s) \]
\[ [a_{\uparrow k+Q}^+, \hat{H}_{MF}] = \Delta_C a_{\uparrow k+Q}^+ \quad (t) \]

Plugging equations (q)–(t) into equation (1.31) and simplifying the result, we get the following expression:
\[ \omega \langle [a_{\uparrow k+Q}^+, b_{\downarrow k}^+]_\omega \rangle = \frac{\Delta_1}{(\omega_1 + \epsilon_1(k) - \Delta_C)} \langle [a_{\downarrow -k+Q}^+, b_{\downarrow k}^+]_\omega \rangle \\
+ \frac{\Delta_2}{(\omega_2 + \epsilon_2(k) - \Delta_C)} \langle [a_{\downarrow -k+Q}^+, b_{\downarrow k}^+]_\omega \rangle. \quad (1.32) \]

Again, in equation (1.32), let us find the equation of motion for the Green’s function \( \langle [a_{\downarrow -k+Q}^+, b_{\downarrow k}^+]_\omega \rangle \). As we did above, the equation of motion for the correlation function \( \langle [a_{\downarrow -k+Q}^+, b_{\downarrow k}^+]_\omega \rangle \) is expressed as:
\[ \omega \langle [a_{\downarrow -k+Q}^+, b_{\downarrow k}^+]_\omega \rangle = 1 + \langle \left[ [a_{\downarrow -k+Q}^+, \hat{H}_{MF}], a_{\uparrow k+Q}^+ \right] + \langle \left[ [a_{\downarrow -k+Q}^+, \hat{H}_{MF}], a_{\uparrow k+Q}^+ \right] + \langle [a_{\downarrow -k+Q}^+, \hat{H}_{MF}], b_{\downarrow k}^+ \rangle \rangle. \quad (1.33) \]

Each of the commutators given in (1.33) are given by:
\[ [a_{\downarrow -k+Q}^+, \hat{H}_{MF}] = \epsilon_1(k + Q)a_{\downarrow k+Q}^+ + \Delta_1 a_{\uparrow k+Q}^+ \quad (u) \]
\[ [a_{\downarrow -k+Q}^+, \hat{H}_{MF}] = 0 \quad (v) \]
\[ [a_{\downarrow -k+Q}^+, \hat{H}_{MF}] = \Delta_2 a_{\uparrow k+Q}^+ \quad (w) \]
\[ [a_{\downarrow -k+Q}^+, \hat{H}_{MF}] = -\Delta_C a_{\downarrow -k+Q}^+. \quad (x) \]

Putting equations (u)–(x) into equation (1.33), and rearranging, we obtain the following result for the CDW Green’s function:
Putting (1.33) into (1.34), and using partial fraction decomposition, we obtain the following Green function for the CDW Hamiltonian:

\[ \langle \langle a_{-(k Q)}^+, b_{-k}^+ \rangle \rangle_{\omega} = -\frac{1}{2} \left( \frac{(\Delta_1 + \Delta_C)}{\omega_1^2 - \epsilon_1^2(k) - (\Delta_1 + \Delta_C)^2} + \frac{(\Delta_1 - \Delta_C)}{\omega_1^2 - \epsilon_1^2(k) - (\Delta_1 - \Delta_C)^2} \right) \]

(1.35)

Now, the CDW order parameter, \( \Delta_C \), can be related to the correlation function \( \langle \langle a_{-(k Q)}^+, b_{-k}^+ \rangle \rangle \) via the relation:

\[ \Delta_C = \frac{U_c}{\beta} \sum_k \langle \langle a_{-(k Q)}^+, b_{-k}^+ \rangle \rangle. \]

(1.36)

Following the same procedure as above with the same lines of reasonings, we show that, the CDW order parameter is given by:

\[ \Delta_C = \frac{U_c}{\beta} \sum_k \left( \frac{\Delta_C + \Delta_i}{2E} \right) \tanh \left( \frac{1}{2} \beta E(k) \right) + \frac{U_c}{\beta} \sum_k \left( \frac{\Delta_C - \Delta_i}{2E'} \right) \tanh \left( \frac{1}{2} \beta E'(k) \right). \]

(1.37)

Where, \( U_c \) stands for coulomb interaction parameter for the CDW, and \( \Delta_i \) is the superconducting order parameter which represents either \( \Delta_1 \) or \( \Delta_2 \) depending on the band under consideration, and the energy excitations \( E \) and \( E' \) are defined by:

\[ E = \sqrt{\epsilon_1^2 + (\Delta_C + \Delta_i)^2}, \quad E' = \sqrt{\epsilon_1^2 + (\Delta_C - \Delta_i)^2}. \]

(1.38)

Equations (1.37) and (1.29) will determine the coexistence of CDW and superconducting order parameters for the layered 2H-NbSe\(_2\) superconductor. From (1.29) and (1.37), we see that: if \( \Delta_i = 0 \) and \( \Delta_C = 0 \) the system represents a pure superconducting region, if \( \Delta_i = 0 \) and \( \Delta_C \neq 0 \) the system represents a pure CDW region, and if \( \Delta_i \neq 0 \) and \( \Delta_C \neq 0 \) our system represents coexistence region.

In the absence of CDW term, replacing the summations by integrals and introducing a constant density of states, \( N_s(0) \) at the Fermi level by the definitions: \( \lambda_1 \equiv N_s(0) U_1 \), \( \lambda_2 \equiv N_s(0) \lambda_1 \), \( \lambda_2 \equiv U_2 \sqrt{N_s(0) N_s(0)} \), the pairs of equations in (1.29) can be rearranged to obtain the following result for a two-band superconductor:

\[ \frac{\lambda_2}{1 - \lambda_2} F_2(T, \Delta_2) = \frac{\lambda_1}{1 - \lambda_1} F_1(T, \Delta_1) \]

(1.39)

Where, the functions, \( F(T, \Delta_i) \), are given by:

\[ F(T, \Delta_i) \equiv \int_0^{\lambda_{\text{coh}}} \frac{1}{\sqrt{\epsilon_i^2 + \Delta_i^2(T)}} \tanh \left( \frac{\sqrt{\epsilon_i^2 + \Delta_i^2(T)}}{2k_B T} \right) d\epsilon_i. \]

(1.40)

For the coexistence of dispersionless (flat) band with a steep band, we consider \( \epsilon_i \) as independent of momentum \( k \), constant, say, \( \epsilon_i \sim z \), while \( \epsilon_i \) in the usual BCS approximation, the transition temperature to obtain from (1.39) reduces to the expression obtained in [29–31]:

\[ 1 = \lambda_{11} \frac{\lambda_{\text{coh}}}{z} \tanh \left( \frac{z}{2k_B T_C} \right) + \lambda_{12} \ln \left( \frac{1.14 \lambda_{\text{coh}}}{k_B T_C} \right), \]

(1.41a)

\[ 1 = \lambda_{22} \ln \left( \frac{1.14 \lambda_{\text{coh}}}{k_B T_C} \right) + \frac{\lambda_{12}}{z} \tanh \left( \frac{z}{2k_B T_C} \right). \]

(1.42b)

Now, if \( \left( \frac{z}{2k_B T_C} \right) \gg 1 \), \( \tanh \left( \frac{z}{2k_B T_C} \right) \to 1 \), in which the transition temperature can be evaluated, and if \( \left( \frac{z}{2k_B T_C} \right) \ll 1 \), \( \tanh \left( \frac{z}{2k_B T_C} \right) \to 1 \), we get the following result:

\[ k_B T_C = \frac{\lambda_{11} \lambda_{\text{coh}}}{\lambda_{12} - \lambda_{11}} + \frac{1.14 \lambda_{\text{coh}}}{\lambda_{22} - \lambda_{11}} e^{\frac{\lambda_{12} - \lambda_{11}}{\lambda_{22} - \lambda_{11}}} \cdot \]

(1.43)

This was obtained in [29–31], the distinction between our treatment and [29–31] is that, our two-band Hamiltonian includes the CDW term that will be analyzed in the following sub-section, and, the methodology employed here to derive the two-band Hamiltonian is with a different approach, with the use of Green functions and equation of motion methods.
2.1. In the presence of charge density wave order ($\Delta_C$) parameters

Let us consider the Hamiltonian in (1.29), for the case where $\Delta_C \neq 0$. To simplify the analysis of the problem, we will treat the intraband and interband terms separately. If only the intraband term is treated, the expression in (1.29a) reads:

$$\Delta_i = \frac{U_i}{2} \left[ \sum_k \left( \frac{\Delta_i + \Delta_C}{2\varepsilon_i(k)} \right) \tanh \left( \frac{1}{2} \beta \varepsilon_i(k) \right) + \sum_k \left( \frac{\Delta_i - \Delta_C}{2\varepsilon_i(k)} \right) \tanh \left( \frac{1}{2} \beta \varepsilon_i(k) \right) \right].$$  

(1.44)

Changing the summation into integration by introducing a constant density of states at the Fermi surface and defining a dimensionless electron-phonon coupling constant $\lambda_1 \equiv N_i U_i$, the transition temperature for the intraband term is obtained from the condition $\Delta_i \to 0$ and, we get the following:

$$\frac{1}{\lambda_1} = \int_0^{\hbar \omega_i} \frac{1}{\sqrt{\varepsilon_i^2 + \Delta_C^2}} \tanh \left( \frac{\sqrt{\varepsilon_i^2 + \Delta_C^2}}{2k_B T_C} \right) d\varepsilon_i + \int_0^{\hbar \omega_i} \frac{\Delta_C^2}{2k_B T_C (\varepsilon_i^2 + \Delta_C^2)} d\varepsilon_i$$

(1.45)

To simplify the analysis, let us define the integrals of (1.45) separately as:

$$\frac{1}{\lambda_1} \equiv I_1 + I_2 + I_3. $$

(1.46)

Where, the integrals $I_1$, $I_2$, and $I_3$ denote for the first, second, and third integrals in (1.45) respectively. The first integral, $I_1$, can be solved by converting it back to the Matsubara summation and employing the properties of the Zeta function. In this case, we have:

$$I_1 = \int_0^{\hbar \omega_i} \frac{1}{\sqrt{\varepsilon_i^2 + \Delta_C^2}} \tanh \left( \frac{\sqrt{\varepsilon_i^2 + \Delta_C^2}}{2k_B T} \right) d\varepsilon_i = \int_0^{\hbar \omega_i} \frac{1}{\varepsilon_i} \tanh \left( \frac{\varepsilon_i}{2k_B T} \right) d\varepsilon_i$$

$$- \int_0^{\hbar \omega_i} d\varepsilon_i \sum_n \frac{4\beta \Delta_C^2}{(2n + 1)^2 \pi^2 + \beta^2 \varepsilon_i^2} + ...$$

$$\Rightarrow I_1 \approx \ln \left( \frac{1.34 \beta \hbar \omega_i}{2} \right) - \frac{4 \beta \Delta_C^2}{\pi^2} \int_0^{\infty} \frac{dy}{(1 + y)^2} \sum_n \frac{1}{(2n + 1)^2}. $$

(1.47)

Where, $\beta = \frac{1}{k_B T}$, and we have used the substitution: $y = \frac{\beta \varepsilon_i}{2}$. Using the properties of Integral Laplace transforms, the value of the integral is:

$$\int_0^{\infty} \frac{dy}{(1 + y)^2} = \frac{\pi}{4}. $$

(1.48)

And, the value of the series under the summation is obtained from the properties of the Zeta function:

$$\sum_n \frac{1}{(2n + 1)^2} = \frac{7\zeta(3)}{8} = 1.0518. $$

(1.49)

Where, $\zeta(3) = 1.20206$. The second integral, $I_2$, is evaluated by substitution method of integration. Now, subsisting $\varepsilon_i = \Delta_C \tan(\alpha)$, the integral, $I_2$, becomes:

$$I_2 = \frac{\Delta_C^2}{2k_B T_C} \int_0^{\hbar \omega_i} \frac{1}{(\Delta_C^2 + \Delta_C^2)} d\varepsilon_i = \frac{\Delta_C}{2k_B T_C} \tan^{-1} \left( \frac{\hbar \omega_i}{k_B T_C \Delta_C} \right). $$

(1.50)

Now, collecting the values of the three integrals and neglecting $\Delta_C^2$ terms for large values of $\Delta_C$ as in [73], the intraband contribution in (1.45) becomes:

$$\frac{1}{\lambda_1} \approx \ln \left( \frac{1.34 \hbar \omega_i}{k_B T_C} \right) + \frac{\Delta_C}{2k_B T_C} \tan^{-1} \left( \frac{\hbar \omega_i}{\Delta_C} \right). $$

(1.51)

From this, the dependency of the CDW order parameter on the superconducting intraband term becomes:

$$k_B T_C = 1.134 \hbar \omega_i e^{-\frac{1}{\alpha \tan^{-1}(\Delta_C / \Delta_C)}}. $$

(1.52)

Where, we have introduced:

$$\alpha \equiv \frac{1}{2k_B T_C} \tan^{-1} \left( \frac{\hbar \omega_i}{\Delta_C} \right). $$

(1.53)
Similarly, the dependency of the CDW order parameter on the interband term is written as:

\[ k_b T_C = 1.134 \hbar \omega_{12} e^{-\frac{1}{2k_b T_C} \gamma} \Delta_C. \]  

(1.54)

where, we have used:

\[ \gamma \equiv \frac{1}{2k_b T_C} \tan^{-1} \left( \frac{\hbar \omega_{12}}{\Delta_C} \right). \]  

(1.55)

Also, with the same lines of reasoning, one can write similar expressions for band 2. The expressions given in (1.52) and (1.54) are applicable for the special case of weak-coupling BCS approximation. Our next task is to consider the combination of flat band with steep band model in the presence of CDW term, and to obtain analytical relationship for the coexistence of superconducting and CDW order parameters for the layered quasi-two-dimensional 2H-NbSe₂ superconductor. Now, returning back to equation (1.29), after changing the summation into integration, and making simple algebraic rearrangement, we obtain the following form:

\[ \frac{\lambda_{12} F_{12}(T, \Delta_2, \Delta_C)}{[2 - \lambda_1 F_1(T, \Delta_1, \Delta_C)]} \times \frac{\lambda_{21} F_{21}(T, \Delta_1, \Delta_C)}{[2 - \lambda_2 F_2(T, \Delta_2, \Delta_C)]} = 1. \]  

(1.56a)

Or, if we express the bands explicitly, after a simple algebraic rearrangement, we get:

\[ \lambda_1 F_1(T, \Delta_1, \Delta_C) + \lambda_2 F_2(T, \Delta_2, \Delta_C) = 2, \]  

(1.56b)

\[ \lambda_1 F_1(T, \Delta_1, \Delta_C) + \lambda_2 F_2(T, \Delta_1, \Delta_C) = 2. \]  

(1.56c)

The functions \( F(T, \Delta_1, \Delta_C) \) are now given by:

\[
2F(T, \Delta_1, \Delta_C) = \int_0^{\hbar \omega_{12}} \left[ \frac{1}{\sqrt{\varepsilon_T^2 + (\Delta_1 + \Delta_C)^2}} \tan \left( \frac{\varepsilon_T^2 + (\Delta_1 + \Delta_C)^2}{2k_b T_C} \right) \right. \\
+ \left. \frac{1}{\sqrt{\varepsilon_T^2 + (\Delta_1 - \Delta_C)^2}} \tan \left( \frac{\varepsilon_T^2 + (\Delta_1 - \Delta_C)^2}{2k_b T_C} \right) \right] d\varepsilon_T. 
\]  

(1.57)

The transition temperature for the intraband term in band 1 is obtained by taking the limit \( \Delta_1 \to 0 \) for the function \( F_1(T, \Delta_1, \Delta_C) \) from equation (1.60). This gives:

\[
F_1(T_C, \Delta_C) = \int_0^{\hbar \omega_{12}} \left[ \frac{1}{\sqrt{\varepsilon_T^2 + \Delta_C^2}} \tan \left( \frac{\varepsilon_T^2 + \Delta_C^2}{2k_b T_C} \right) + \frac{\Delta_C^2}{2k_b T_C (\varepsilon_T^2 + \Delta_C^2)} \sec h^2 \left( \frac{\sqrt{\varepsilon_T^2 + \Delta_C^2}}{2k_b T_C} \right) \right] d\varepsilon_T. 
\]  

(1.58)

Assuming \( \varepsilon_1 \equiv \text{const.} \), say \( z \) for the flat (dispersionless) like band, this integral gives:

\[
F_1(T_C, \Delta_C) = \frac{\hbar \omega_{12}}{\sqrt{z^2 + \Delta_C^2}} \tan \left( \frac{\sqrt{z^2 + \Delta_C^2}}{2k_b T_C} \right) + \frac{\Delta_C^2}{k_b T_C (z^2 + \Delta_C^2)} \sec h^2 \left( \frac{\sqrt{z^2 + \Delta_C^2}}{2k_b T_C} \right). 
\]  

(1.59)

Furthermore, the transition temperature for the interband term in band 1 becomes:

\[
F_{12}(T_C, \Delta_C) = \int_0^{\hbar \omega_{12}} \left[ \frac{1}{\sqrt{\varepsilon_T^2 + \Delta_C^2}} \tan \left( \frac{\varepsilon_T^2 + \Delta_C^2}{2k_b T_C} \right) + \frac{\Delta_C^2}{2k_b T_C (\varepsilon_T^2 + \Delta_C^2)} \sec h^2 \left( \frac{\sqrt{\varepsilon_T^2 + \Delta_C^2}}{2k_b T_C} \right) \right] d\varepsilon_T. 
\]  

(1.60)

Applying Laplace transform and Matsubara frequency, the First integral in (1.60) is given by:

\[
\int_0^{\hbar \omega_{12}} \frac{1}{\sqrt{\varepsilon_T^2 + \Delta_C^2}} \tan \left( \frac{\varepsilon_T^2 + \Delta_C^2}{2k_b T_C} \right) d\varepsilon_T = \ln(1.134/\beta \hbar \omega_{12}) \\
+ 4\beta^3 \Delta_C^2 \sum_{n=0}^{\infty} \frac{1}{(2\pi n + 1)^2 \pi^2 + \beta^2 (\varepsilon_T^2 + \Delta_C^2)} \\
= \ln(1.134/\beta \hbar \omega_{12}) - \frac{7\zeta(3) - (\beta \Delta_C)^2}{8\pi^2}. 
\]  

(1.61)
Again, the second integral in (1.60) is given by:

$$\frac{\Delta_2^2}{2k_B T_c (\epsilon^2 + \Delta^2_c)} \frac{h\omega_{12}}{2} \sec h \left( \frac{\sqrt{\epsilon^2 + \Delta^2_c}}{k_B T_c} \right) $$

$$\left[ 1 \right]_0^{\pi} = \frac{\Delta_2^2}{2k_B T_c} \frac{1}{\epsilon + \Delta_c^2} \sec h \left( \frac{\sqrt{\epsilon^2 + \Delta^2_c}}{k_B T_c} \right)$$

Using equations (1.59)–(1.62) into equation (1.56) and neglect \( \Delta_2^2 \) terms for large values of the CDW order parameter, we get the following result for band 1:

$$1 = \frac{\lambda_{11}}{\lambda_{12}} \tan h \left( \frac{\epsilon}{2k_B T_c} \right) + \frac{\lambda_{12}}{\lambda_{11}} \ln \left( \frac{1.14 h\omega_{12}}{k_B T_c} \right) - \frac{\lambda_{13}}{\lambda_{11}} \left[ \frac{\lambda_{12}^2}{\lambda_{11}} \tan h \left( \frac{h\omega_{12}}{\Delta_c} \right) \right]$$

(1.63a)

Following the same procedure, similar equation for band 2 is:

$$1 = \frac{\lambda_{21}}{\lambda_{22}} \tan h \left( \frac{\epsilon}{2k_B T_c} \right) + \frac{\lambda_{22}}{\lambda_{21}} \ln \left( \frac{1.14 h\omega_{12}}{k_B T_c} \right) - \frac{\lambda_{23}}{\lambda_{21}} \left[ \frac{\lambda_{22}^2}{\lambda_{21}} \tan h \left( \frac{h\omega_{12}}{\Delta_c} \right) \right]$$

(1.63b)

Equations (1.63a) and (1.63b) can be solved analytically for some special cases. For the special case of \( \tan h (\gamma) \ll 1 \), \( \tan h (\gamma) \approx \gamma \), the relationship between the superconducting transition temperature \( T_c \) and CDW order parameter yields the following analytic form:

$$k_B T_c = (1.14 h\omega_{12} e^{-\lambda_{11}^2 / \lambda_{12}} + 1.14 h\omega_{12} e^{-\lambda_{12}^2 / \lambda_{11}}) e^{\frac{\lambda_{11} h\omega_{12} - \lambda_{12} h\omega_{12}}{2(\lambda_{11} - \lambda_{12})}}$$

(1.64)

For the case of \( \tan h (\gamma) \gg 1 \), \( \tan h (\gamma) \approx 1 \), the dependency of CDW order parameter on superconducting transition temperature takes the following analytic form:

$$k_B T_c = [1.14 h\omega_{12} e^{-\lambda_{11}^2 / \lambda_{12}} + 1.14 h\omega_{12} e^{-\lambda_{12}^2 / \lambda_{11}}] e^{\frac{\lambda_{11} h\omega_{12} - \lambda_{12} h\omega_{12}}{2(\lambda_{11} - \lambda_{12})}}$$

(1.65)

where, we have introduced the definitions:

$$\alpha \equiv \frac{1}{k_B T_c} \left[ \frac{h\omega}{\lambda_{11}^2} \right] \gamma \equiv \frac{1}{k_B T_c} \left[ \frac{h\omega}{\Delta_c} \right]$$

(1.66)

The coexistence of superconductivity and CDW order parameter can be studied with the help of equation (1.65). This is discussed in section 4 of the paper.

3. CDW order parameter, \( \Delta_c(T) \), at a temperature (T)

Using equation (1.37) and applying the same procedures as before, the transition temperature for the charge density wave, \( T_{CDW} \), is given by:

$$k_B T_{CDW} = 1.14 h\omega \left( \frac{1}{\lambda_{11}^2 + \eta \Delta_c (\gamma)} \right)$$

(1.67)

where, \( \lambda_1 \) stands for the coupling parameter for CDW, and:

$$\eta \equiv \frac{1}{k_B T_{CDW}} \tan h \left( \frac{h\omega}{\Delta_c} \right)$$

(1.68)

In the usual BCS approximation, the temperature dependent CDW order parameter is given by the following expression:

$$\Delta_c(T) \approx 3.06 k_B T_{CDW} \left[ 1 - \frac{T}{T_{CDW}} \right]^{1/2}$$

(1.69)

Using (1.67) and (1.69), the temperature dependent CDW order parameter is given by:

$$\Delta_c(T) \approx 3.5 h\omega \left[ 1 - \frac{T}{T_{CDW}} \right]^{1/2} e^{-\frac{1}{\lambda_{11}^2 + \eta \Delta_c (\gamma)}}$$

(1.70)

Equation (1.70) is used to determine the temperature dependent CDW gap parameter for the layered quasi-2D superconductor 2H-NbSe$_2$. 

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4. Results and discussion

In this section, we present the results obtained for the coexistence of superconducting and CDW order parameters for the layered quasi two-dimensional superconductor 2H-NbSe$_2$. With the help of Green’s function and equation of motion methods, analytical expressions connecting the superconducting transition temperature ($T_C$) and charge density wave transition temperature ($T_{CDW}$) were obtained with the CDW order parameter ($D$) for the layered superconductor 2H-NbSe$_2$. Using equation (1.51) and a two-gap BCS fit in the absence of CDW term, and using the parameters: $\hbar \omega_1 = \hbar \omega_2 = 8.5$ meV, $\lambda_1 = 0.3$ and $\lambda_2 = 0.4$, we obtained $\Delta_1 = 1.255$ meV and $\Delta_2 = 0.725$ meV. The corresponding phase diagram for this case is shown in figure 1. As reported in experimental work in [64], the layered superconductor 2H-NbSe$_2$ has two gap values $\Delta_1 = 0.73$ meV and $\Delta_2 = 1.26$ meV. Similarly, in [65], the two distinct gaps for this material are $\Delta_1 = 1.25$ meV and $\Delta_2 = 0.55$ meV. Therefore, our calculated values in the absence of CDW term are in broad agreement with previous works the values reported in [64, 65]. Furthermore, in the absence of CDW term, we plotted the corresponding phase diagram as shown in figure 1. From figure 1, we see that the both the larger gap and smaller gap values are in the range of the values reported in [64, 65].

The layered superconductor 2H-NbSe$_2$ has CDW gap values about $\Delta_C \cong (4 - 6)$ meV, and electron-phonon coupling constant $\lambda_C \cong 0.81$ as reported in [64]. Using $\hbar \omega = 8.5$ meV and $\lambda_C = 0.81$ for the electron-phonon coupling constant for the CDW, and with the help of equations (1.67) and (1.70), the phase diagram for the superconductor 2H-NbSe$_2$ is shown in figure 2. According to figure 2, the gap value for the CDW is around 4.3 meV, and it is in the range as reported in [64].
In the presence of charge density wave (CDW) and with the use of equation (1.55), we plotted superconducting transition temperature ($T_C$) versus CDW order parameter as shown in figure 3. As shown in figure 3, the transition temperature decreases with the gap value.

We next plot, graph of CDW transition temperature ($T_{CDW}$) versus CDW order parameter as shown in figure 4.

As we can see from the graphs (1.3) and (1.4), in the presence of CDW ordering, the transition temperature is suppressed by the CDW order parameter. Next, by merging graphs (1.3) and (1.4), we show the coexistence region for superconducting and CDW order parameters as shown in figure 5 for the gap value $\Delta_2 = 1.26$ meV.

For the smaller gap value $\Delta_2 = 0.73$ meV, the variation of CDW order parameter as a function of the superconducting transition temperature ($T_C$) is plotted in figure 6. Furthermore, the behavior of CDW order parameter versus $T_{CDW}$ is shown in figure 7.

As we can see from the figures 6 and 7 in the presence of CDW ordering, the transition temperature is suppressed by the CDW order parameter.

Similarly, to find the region for the coexistence between the lower gap $\Delta_2 = 0.73$ meV and the CDW order parameter, we merge figures 6 and 7 shown in figure 8.
Flat bands are frequency independent (dispersionless) bands which give different exotic behaviors in magnetism and superconductivity [30, 72–74]. In superconductivity, the presence of flat bands will have different thermodynamic and electronic behaviors that is different from the usual BCS theory, for example, see [29–33]. In the presence of dispersionless (flat) bands, electrons are highly confined in a certain electronic band direction and the electronic density of states (DOS) near the Fermi level is high [30]. In particular, in the combination of flat band with a steep band condition, the superconducting transition temperature can be enhanced, for example, see [29]. In our two-band model Hamiltonian, we apply the combination of weak coupling with a strong coupling for the quasi-2D superconductor 2H-NbSe2. In the combination of weak-coupling and strong-coupling flat band model, let us keep the interband coupling term at very small (weak) value and the intraband coupling term somewhat larger than the interband (band to band) value. In the absence of the CDW term, by adjusting the interband coupling constant at a very small value, using equation (1.43) and considering the combination of flat band with a steep band, and using the parameters: \( \hbar \omega_1 = \hbar \omega_2 = 8.5 \text{ meV}, \lambda_{12} = 0.04, \lambda_{12} = 0.01, \lambda_{12} = 0.05, \lambda_{12} = 0.01, \lambda_{12} = 0.06, \lambda_{12} = 0.02, \) we see that the superconducting transition temperature (Tc) for 2H-NbSe2 is greatly enhanced by the intraband contribution as shown in figure 9.

As shown in figure 9, the value of the superconducting transition temperature is greatly enhanced by the intraband contribution in the steep band/flat band combination. As before, in the presence of CDW terms, we studied the coexistence of the flat band/steep band superconductivity with CDW gaps. For the parameters
Figure 7. CDW transition temperature ($T_{CDW}$) versus CDW order parameter for the superconductor 2H-NbSe$_2$.

Figure 8. Coexistence of CDW and superconductivity in NbSe$_2$ for the gap $\Delta_2 = 0.73$ meV.

Figure 9. Enhancement of the transition temperature by the intraband term in the absence of CDW.
\( \lambda_1 = 0.01, \lambda_1 = 0.06, \lambda_2 = 0.3 \), and the other parameters as before, the variation of the superconducting transition temperature with CDW gap parameter in the flat band/steep band case is shown in figure 10.

5. Conclusion

In this paper, we established a detailed theoretical study of the possible coexistence of CDW and superconductivity for the quasi-two-dimensional layered superconductor 2H-NbSe\(_2\). Starting with a two-band Hamiltonian, with fully quantum mechanical many body theory, and using double-time temperature dependent Green's function formalism, we obtained analytical expressions for the dependency of the superconducting transition temperature \((T_C)\) on the CDW order parameters for the intraband and interband contributions. In the absence of CDW terms, for a pure superconducting system, the values of the obtained superconducting order parameters are in broad agreement with the results obtained in \([64, 65]\). In addition, for the combination of dispersionless (flat) and steep bands, the possibility to coexist the CDW with superconducting state is demonstrated. Furthermore, the enhancement of the transition temperatures for the layered 2H-NbSe\(_2\) superconductor was established.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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