One-dimensional model for BiS\textsubscript{2} superconductivity: analyzing the pressure effect over T\textsubscript{c}

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Abstract. The recently synthesized compound SrFBiS\textsubscript{2} [Lei H et al. 2013 Inorg. Chem. 52 106851] has been shown to become superconducting [Lin X et al. 2013 Phys. Rev. B 87 020504] through the substitution of Sr\textsuperscript{2+} by La\textsuperscript{3+}. In addition, application of moderate hydrostatic pressure in Sr\textsubscript{0.5}RE\textsubscript{0.5}FBiS\textsubscript{2} (RE=Ce, Nd, Pr, and Sm) [Jha R et al. 2015 J. Appl. Phys. 117 013901] has shown a dramatic increase in the superconducting transition temperature T\textsubscript{c}. In this work, using a recently proposed one-dimensional model for BiS\textsubscript{2}-based superconductors [Griffith M A et al. 2015 submitted to Phys. Rev. B ], the authors analyze the effect of pressure over T\textsubscript{c}.

1. Introduction

After the discovery of the cuprates in 1986 [1], the search for new layered superconducting materials has attracted much attention, with important discoveries occurring in the last 15 years. For example, it was discovered in 2001 that MgB\textsubscript{2} has T\textsubscript{c} = 39 K [2] and in 2008 superconductivity (SC) in the iron pnictides was reported [3]. Both MgB\textsubscript{2} and the iron pnictides have highlighted the importance of multiband SC [4], to the point that the recent literature on cuprates devoted to multiband models has substantially increased [5]. An unrelated development has been the explosion of research in topological superconductors [6], due to proposals to ‘engineer’ Majorana fermion quasiparticles through midgap excitations of a chiral p-wave superconductor. This has led to renewed interest in the Ruthenate compound Sr\textsubscript{2}RuO\textsubscript{4}, discovered in 1994 [7], which is one of the few candidates to realizing p-wave-type SC [8; 9], another candidate being the organic superconductor (TMTSF)\textsubscript{2}PF\textsubscript{6}. It should also be emphasized that, as was the case for intermetallics with A15 structure (like Nb\textsubscript{3}Sn or V\textsubscript{3}Si) [10], the Ruthenates display ‘hidden’ quasi-one-dimensional (quasi-1d) SC [11] (while organic superconductors are explicitly 1d). Finally, we also mention SC in doped semiconductors, studied since before the 60s [12], with the interest greatly increasing after the discovery of SC in Borondoped Diamond with T\textsubscript{c} = 4 K [13].

It is then interesting to notice that one of the latest families of superconductors to be discovered, those containing BiS\textsubscript{2} planes, [14] presents many of the aspects mentioned above:
a layered structure with intercalated charge reservoirs [15], like in the cuprates and in the iron superconductors; a possible double superconducting gap [16], as in MgB$_2$ [2]; its minimal model contains two bands [17], and Fermi surface nesting effects seem to be important [18] (as in the iron pnictides [3]); because it contains a heavy element (Bismuth), spin-orbit effects are enhanced and some proposals linking BiS$_2$ superconductivity to spin-triplet pairing and a weak topological superconducting state have been made [19]; based on first-principles electronic structure calculations, it has been pointed out the ‘subtle’ 1d character of its band structure [17], which has been recently experimentally confirmed through polarization-dependent AngularResolved Photoemission Spectroscopy (ARPES) measurements [20]; finally, a few members of the BiS$_2$ family have semiconducting parent compounds that become metallic/superconducting with electron doping and/or application of moderate hydrostatic pressure, which also can lead to sizable increase in $T_c$ [21].

In this work, to advance the understanding of SC in BiS$_2$, where there is no consensus yet if SC is of the conventional or unconventional type [22], we concentrate in these last two aspects: one-dimensionality of the electronic structure and the pronounced effects pressure has over the superconducting phase. To model that, the authors take the following approach: i) adopt a 1d three-orbital model for BiS$_2$, adding the Cooper-pairing by hand, ii) solve the gap equations at the mean-field level, iii) study the dependence of the superconducting gap with the variation of the hopping terms, whose magnitude one expects to increase under applied pressure iv) decide on the acceptance or not of specific pair-scattering terms based on semi-quantitative agreement with experiments. Regarding this last point, we look specifically in what range of electron-filling the hopping terms, whose magnitude one expects to increase under applied pressure iv) decide on the acceptance or not of specific pair-scattering terms based on semi-quantitative agreement with experiments. To make the connection with BiS$_2$ more explicit, and thus obtain semi-quantitative agreement with experiments, all the parameter values of the single-particle Hamiltonian were obtained through first-principles Density Functional Theory (DFT) calculations for a two-dimensional (2d) five-band model (see Table 1). It should be noted that, although our calculations are done specifically for SrFBiS$_2$, this marked increase of $T_c$ with pressure has been observed in many other members of the BiS$_2$ family of superconductors [23].

We can summarize our results as follows: Taking into account a three-orbital model, where Sulfur contributes with orbitals $s$ and $p$, and Bismuth with a $p$ orbital (see Fig. 1), we consider all possible pair-scattering terms (intra and interband, restricted to pairs formed by same-band electrons), individually and in conjunction, and solved the resulting gap equations at the mean-field level. We obtain that i) no single-band pair-scattering process, acting isolatedly, can describe the experiments (as specifically defined above), unless an unrealistic pair-coupling is assumed ($g > 0.1$ eV); this seems to indicate that multi-gap SC is a natural consequence of our model ii) two different types of multi-gap SC (see detailed description below) are in semi-quantitative agreement with experiments iii) the gap dependence with hopping (see Fig. 5) indicates a qualitative difference between the two hoppings considered in our model. These important results establish an appropriate effective 1d model to simulate the properties of BiS$_2$. We expect that our work will motivate other groups to investigate other similar purely 1d effective models (an abbreviated version of these results has been submitted elsewhere [24]).

2. Model

We consider a linear chain with a unit cell consisting of two sites denoted $a$ and $b$, see Fig. 1. The $a$ sites (Sulfur) have orbitals $s$ and $p$, while $b$ sites (Bismuth) have just one $p$ orbital. In second quantization notation, the annihilation operator for an $s$ orbital in unit cell $n$ is denoted as $c_{a,n}$, and those for Sulfur and Bismuth $p$ orbitals are denoted $p_{a,n}$ and $p_{b,n}$, respectively. The non-interacting part of the Hamiltonian can then be written as

$$
\mathcal{H} = \sum_n \left[ (\epsilon_{s,n} + \mu)n_{s,n} + \sum_{i=a,b} (\epsilon_{p_i,n} + \mu)n_{p_i,n} + t_{pp}[p_{a,n}^\dagger p_{b,n} + p_{b,n}^\dagger p_{a,n+1} + \text{h.c.}] \right]
$$
Table 1. Partial list of tight-binding parameters (in eV) for the 2d five-orbital model. The same parameters are used for the 1d three-orbital model depicted in Fig. 1. The chemical potential corresponds to 1/8-filling of the $p_b$ orbital in the 1d model.

| $\epsilon_{s,n}$ | $\epsilon_{p_a,n}$ | $\epsilon_{p_b,n}$ | $t_{sp}$ | $t_{pp}$ | $\mu$ |
|------------------|-------------------|-------------------|---------|---------|-------|
| -11.2840         | -1.2691           | 0.1635            | -0.9952 | -0.8155 | 0.5007 |

Figure 1. 1d model for BiS$_2$. $t_{pp}$ and $t_{sp}$ are the hopping terms considered in our model. The dashed box indicates the unit cell with atoms $a$ (Sulfur, with orbitals $s$ and $p$) and $b$ (Bismuth, with just one $p$ orbital). Notice the alternating signs of the $t_{sp}$ hoppings [25].

\[
+ t_{sp}[c_n^\dagger p_{b,n} - p_{b,n}^\dagger c_{n+1} + \text{h.c.}] \] (1)

where $\epsilon_{s,n}$ and $\epsilon_{p_i,n}$ describe the energy levels of orbitals $s$ and $p$ (for site $i = a, b$) at unit cell $n$, respectively; $n_{s,n} = c_n^\dagger c_n$ and $n_{p_i,n} = p_{i,n}^\dagger p_{i,n}$ are the number operators, and $\mu$ is the chemical potential. The hopping parameters are indicated in Fig. 1 and the values used in this work (along with orbital energies and chemical potential) are listed in Table 1 in eV units. Note that these parameter values were obtained through a full DFT calculation. The hoppings kept for the 1d model here studied were all the nearest neighbor hoppings in excess of 0.5 eV.

An early 2d minimal model for BiS$_2$ contains two orbitals: Bismuth $p_x$ and $p_y$ orbitals [17]. Therefore, before deriving the self-consistent gap equations, the inclusion of the Sulfur $p$ and $s$ orbitals should be justified, mainly the latter one, which lies deep below the Fermi energy (see DFT parameter values in Table 1). Figure 2 shows the density of states (DOS) obtained for a 2d model of BiS$_2$ involving five orbitals: two Bismuth $p$ orbitals ($p_x$ and $p_y$), two Sulfur $p$ orbitals ($p_x$ and $p_y$), and one Sulfur $s$ orbital. From the examination of the DOS one can conclude that, at the Fermi energy $E_F = 0$ (which, in this plot, is between 1/8- and 1/4-filling, for the 2d model), the participation of the Sulfur $s$ orbital [dot-dashed (green) curve], is quite relevant, even more than that of the Sulfur $p$ orbitals [dashed (blue) curve]. In addition, it is easy to recognize the characteristic 1d DOS profile for the Sulfur $p$ orbital at the top of the valence band and for the Bismuth $p$ and Sulfur $s$ orbitals at the bottom of the conduction band (compare with the DOS for the actual 1d model, shown in Fig. 3). This, coupled to the above mentioned polarized ARPES results indicating the one-dimensionality of the electronic structure of BiS$_2$, justifies our model. We now proceed to the derivation of the self-consistent gap equations.

3. Self-consistent gap equations at zero temperature

After taking a Fourier transform of the non-interacting part, and introducing pair-scattering terms between the electrons, the total Hamiltonian can be written as

\[
\mathcal{H}(k) = \sum_k \{ (\epsilon_{as} + \mu) c_k^\dagger c_k + \sum_{i=a,b} (\epsilon_{p_i} + \mu) p_{i,k}^\dagger p_{i,k} + 2t_{pp} \cos(k) [p_{ak}^\dagger p_{bk} + \text{h.c.}] \}
\]
\[ + 2it_{sp} \sin(k)[c_{pk}^\dagger p - \text{h.c.}] - \sum_{i,j,k,k'} g_{ij} \{ \gamma_{i,k,k'}^\dagger \gamma_{j,k,k'} - \gamma_{i,k,k'} \gamma_{j,k,k'} + \text{h.c.} \} \]  

where, in the last line, \( \gamma_{i,j,k\sigma} (\sigma = \pm \text{ and } \tilde{k} \text{ indicates } -k) \) stands for either one of \( c_{k\sigma}, p_{a,\bar{k}\sigma}, \) or \( p_{b,k\sigma} \). Note that it is implicit in the form of the expression for the pair-scattering term that we are only considering singlet Cooper pairs composed of electrons from the same band, as pairing of different-band electrons tends to promote pair-density-wave (inhomogeneous) superconducting ground states [26]. Already anticipating results that will be discussed below (see Fig. 3), we describe how to obtain the gap equations when an specific set of pair-scattering processes are taken in account. Considering terms involving \textit{intragroup} scattering in the \( s \) and \( p_b \) bands and \textit{interband} scattering between the \( s \) and \( p_b \) bands, the last term of eq. (2) (which we denote as \( \mathcal{H}^{SC} \)) can be written as

\[
\mathcal{H}^{SC} = -\sum_{k,k'} \{ g_{ss}[c_{k+}^\dagger c_{k+}^\dagger c_{k-} - c_{k-}] + g_{p_b p_b}[P_{b,k+}P_{b,k+} + P_{b,k+}^\dagger P_{b,k+}^\dagger] \\
+ g_{sp}[c_{k+}^\dagger c_{k+}^\dagger P_{b,k+} - P_{b,k+} + P_{b,k+}^\dagger P_{b,k+}^\dagger - c_{k-}c_{k-}] \}. 
\]

Note that, based on experimental evidence [23], we consider the pairing couplings \( g_{ij} \) as being \( \bar{k} \)-independent, \textit{i.e.}, we assume \( s \)-wave pairing functions. Applying a mean-field decoupling eq. (3) becomes

\[
\mathcal{H}^{SC} = -\sum_{k} \{ \Delta_{ss}(c_{k+}^\dagger c_{k+} + c_{k+}^\dagger c_{k-}) + \Delta_{p_b p_b}(P_{b,k+}P_{b,k+} + P_{b,k+}^\dagger P_{b,k+}^\dagger) \\
+ \Delta'_{ss}(P_{b,k+}P_{b,k+} + P_{b,k+}^\dagger P_{b,k+}^\dagger) + \Delta'_{p_b p_b}(c_{k+}^\dagger c_{k+}^\dagger + c_{k-}c_{k-}) \},
\]

which can be rewritten as

\[
\mathcal{H}^{SC} = -\sum_{k} \{ \Delta_{1}(c_{k+}^\dagger c_{k+} + c_{k+}^\dagger c_{k-}) + \Delta_{2}(P_{b,k+}P_{b,k+} + P_{b,k+}^\dagger P_{b,k+}^\dagger) \},
\]

with the following definitions

\[
\Delta_{1} = \Delta_{ss} + \Delta'_{p_b p_b} = g_{ss} \sum_{k} \langle c_{k+}^\dagger c_{k+} \rangle + g_{p_b p_b} \sum_{k} \langle P_{b,k+}P_{b,k+} \rangle
\]

and

\[
\Delta_{2} = \Delta'_{ss} + \Delta_{p_b p_b} = g_{p_b p_b} \sum_{k} \langle c_{k+}^\dagger c_{k+} \rangle + g_{p_b p_b} \sum_{k} \langle P_{b,k+}P_{b,k+} \rangle
\]

where \( \langle \rangle \) indicates an average over the ground state. If we consider the following relation, \( g_{ss} = g_{p_b p_b} = g_{p_p} = g \), then it follows that \( \Delta_{ss} = \Delta_{ss}' \) and \( \Delta_{p_p p_p} = \Delta'_{p_p p_p} \) (therefore \( \Delta_{1} = \Delta_{2} = \Delta \)), and we obtain the gap equation as

\[
\Delta = g \sum_{k} \{ \langle c_{k+}^\dagger c_{k+} \rangle + \langle P_{b,k+}P_{b,k+} \rangle \}.
\]

We want to derive a self-consistent equation for \( \Delta \) and then analyze the effect of variations in the hopping parameters over it. In order to determine the correlations \( \langle c_{k+}^\dagger c_{k+} \rangle \) and \( \langle P_{b,k+}P_{b,k+} \rangle \) in the gap equation, we need to calculate the anomalous Green’s functions \( \langle c_{k+}^\dagger c_{k-} \rangle \) and \( \langle P_{b,k+}P_{b,k+} \rangle \). These calculations are long and tedious, and thus are presented in the appendix. After writing the equation of motion for the propagators \( \langle p_{b,k+}p_{b,k+} \rangle \) and \langle c_{k+}^\dagger c_{k+} \rangle \), and through lengthy algebraic manipulations, we arrive at expressions for \( \Delta_{1} \) and \( \Delta_{2} \)

\[
\Delta_{1,2} = -g_{ss;sp_b} kF \int_{-1}^{1} dk \sum_{j=1}^{3} \frac{|D_{ss}(-\omega_{k,j})|}{\omega_{k,j}r_j} - g_{sp_b;sp_b} kF \int_{-1}^{1} dk \sum_{j=1}^{3} \frac{|D_{p_p p_p}(-\omega_{k,j})|}{\omega_{k,j}r_j}
\]

which, after the simplifying step mentioned above, results in \( \Delta_{1} = \Delta_{2} = \Delta \) (the terms under the two integrals are fully developed in the appendix).
Figure 2. Density of states obtained through DFT for the five-orbital model of the SrFBlS$_2$ compound. Note the importance of the Sulfur $s$-orbitals [dot-dashed (green) line] at the Fermi energy ($E_F = 0$).

Figure 3. DOS for the 1d model using the same parameters as for the 2d DOS calculation. Note that, as in the case of the 2d DOS, the strong hybridization between the $s$ and $p_b$ orbitals brings a considerable amount of the $s$-orbital spectral weight to the Fermi energy, which for 1/8-filling ($\mu = 0.5007$) is indicated by the vertical dotted line.

4. Results

As mentioned in the Introduction, our strategy was to solve the gap equations at the mean-field level (hopping amplitudes fixed at the values obtained by DFT), and look for solutions at least qualitatively compatible with experiments, i.e., for chemical potential values around 1/8-filling and for coupling strengths $g$ that are not unrealistically large. Taking into account the pair-scattering terms in eq. (4) and following the derivations up to eq. (9), we obtain the gap function $\Delta$, which has a dependence with $\mu$ as shown in Fig. 4, for three different values of coupling $g$. It is interesting to note that the value of $\mu$ around which the three domes are centered corresponds to an electron filling close to that where SC has been found for most members of the BiS$_2$ family, i.e., 1/8-filling [27]. This is an important result, as $\mu$ was not fixed from the start. It is taken as a free parameter, whose value, obtained self-consistently, was used to determine which gap equations (for specific pair-scattering terms) produced acceptable results. Indeed, if the value of $\mu$ for which SC was found is too far removed from 1/8-filling, that gap equation (and the pair-scattering term generating it) is rejected.

If one takes the maximum value obtained for $\Delta$ in Fig. 4 for $g = 25$ meV [(red) circles], $\Delta \approx 4$ meV, and uses the BCS relation $2\Delta/k_BT_c = 3.52$, one obtains $T_c \approx 26$ K. A maximum $T_c \approx 11$ K has been measured for LaO$_{1-x}$F$_x$BiS$_2$ at 1/8-filling ($x = 0.5$) [23], indicating that our results, for a realistic value of $g$, produce a $T_c$ qualitatively similar to experiments. A comment should be made on the horizontal width of the dome for the (red) solid circles curve in Fig. 4. At the base of the dome, the electron filling varies roughly from 0.25 to 0.26 electrons per $p_b$-orbital (Bismuth). Although there is still some controversy about the actual filling around which SC occurs [27], a few of the published $T_c$ vs. doping results indicate a broader dome. We believe that the narrower dome we obtain is an artifact of the 1d model. Indeed, the DOS close to 1/8-filling for our 1d model (see Fig. 3) has a very pronounced van Hove singularity, therefore a very strong variation of DOS with the chemical potential. This strong dependence, for smaller values of $g$ (as the ones plotted in the main panel in Fig. 4), seems to result in a superconducting phase that is very sensitive to the chemical potential, leading to a narrow dome. In the inset to
Figure 4. Pairing interaction $\Delta$ as a function of the chemical potential $\mu$ for different values of the coupling constant $g$.

Figure 5. Left panel: Results showing the dependence of $\Delta$ with $t_{sp}$ for a few values of the chemical potential $\mu$ in the dome region in Fig. 4 for $g = 40.5$ meV and $t_{pp} = -0.8155$ eV. Right panel: Same as left panel, but now varying $t_{pp}$ and keeping $t_{sp}$ fixed.

Fig. 4, we show results for a larger $g = 140$ meV value. In it, we see a much broader variation in electron filling, from 0.2 to 0.31 [(black) open diamonds curve]. The actual system is quasi-1d, implying that once a three-dimensional superconducting state stabilizes, it will be less sensitive to variations in the chemical potential. To have the same effect in a purely 1d model we have to increase the pairing coupling, as shown in the inset to Fig. 4.

It is reasonable to expect that applying hydrostatic pressure in a crystal lattice will enhance the overlap between the orbitals and therefore increase the magnitude of the hopping terms. Making the assumption that this increase is similar to the change in lattice parameter, which for an applied pressure of 2 GPa will amount to a change of $\approx 1\%$ [28], we solve the gap equations for increasing values (in magnitude) of $t_{sp}$ and plot the results in the left panel in Fig. 5 for some $\mu$ values in the dome region in Fig. 4 (for $g = 40.5$ meV). For a variation of $|t_{sp}| \approx 0.5\%$ the value of $\Delta$ roughly doubles, which is in semi-quantitative agreement with experimental results for $T_c$ obtained for LaO$_{0.5}$F$_{0.5}$BiS$_2$ and CeO$_{0.5}$F$_{0.5}$BiS$_2$ [29]. A similar calculation for the variation in $t_{pp}$, shown in the right panel in Fig. 5, shows no changes in $\Delta$, up to the same percent variation as for $t_{sp}$. This seems to be consistent with previous results [25] showing that antisymmetric hybridization is very effective in increasing the SC gap amplitude. To test this hypothesis, extensive calculations are underway where the condition $g_{ss} = g_{pp} = g_{sp} = g$ is relaxed [30].

There is another choice of pair-scattering terms in eq. (4) which produces results (not shown) very similar to the ones just described. One just needs to replace $s$ by $p_a$ in eq. (4). As already mentioned, these two were the only situations where the results obtained were compatible with the criteria described above for acceptance of the gap equation results. For all the other possibilities, either the coupling parameter $g$ was unrealistically large or the electron-filling was too far removed from 1/8-filling.

5. Conclusions
Motivated by recent experiments in superconducting members of the BiS$_2$ family of compounds showing its ‘hidden’ 1d electronic structure and the strong effect that pressure has over its superconducting state, we propose an effective 1d model where the kinetic energy part of the
Hamiltonian is obtained through DFT calculations for the 2d model for BiS$_2$. Supported by the DOS results shown in Fig. 2, we add the Sulfur p- and s-orbital to the p-orbital of Bismuth. Despite being several eV below the other two orbitals, the s-orbital undergoes strong hybridization with the Bismuth p-orbital and has a sizable contribution to the DOS at the Fermi energy, justifying its inclusion in the model (see Figs. 1 and 2). Pair scattering terms are then added and treated at the mean-field level. We solve the gap equations and systematically probe what combination of pair-scattering terms produce results in qualitative agreement with the experiments, i.e., approximate location of the superconducting phase in a $T$ vs. doping phase diagram, realistic coupling constant values, and dependence with hopping parameters (simulating application of hydrostatic pressure). We find that single-gap SC does not produce acceptable results. This is quite relevant, as there is experimental evidence that BiS$_2$ presents two gaps [23]. We find that if we consider s- and $p_b$-type pairs, and allow for intra and interband scattering we obtain results in semi-quantitative agreement with experiments. The same is true if we choose $p_a$- and $p_b$-type pairs, and also allow for intra and interband scattering. The interesting point here is that the $t_{sp}$ hopping is the one that, in both cases, enhances SC when its magnitude increases, whereas the effect on $\Delta$ of increasing $t_{sp}$ is marginal. This last point reinforces the need for considering the Sulfur $s$ orbital explicitly. We argue that the anti-symmetric character of the $t_{sp}$ hopping (as stressed in previous work by one of the authors [25]) may explain its enhanced effect in the superconducting state.

**Appendix**

In the gap equations for $\Delta_1$ and $\Delta_2$ (eqs. (6) and (7) in the main text), the correlation functions are related to the Green’s functions (propagators, from now on) $\langle\langle c_{k+};c_{k-}\rangle\rangle$ and $\langle\langle p_{bk+};p_{bk-}\rangle\rangle$ through the equation

$$\langle\langle \gamma_k;\gamma_{k'}\rangle = i \int_{-\infty}^{+\infty} d\omega f(\omega)\left[\langle\langle \gamma_{k+};\gamma_{k'}\rangle\rangle_{\omega+i\eta} - \langle\langle \gamma_{k+};\gamma_{k'}\rangle\rangle_{\omega-i\eta}\right],$$

(A.1)

where $\gamma$ stands for the annihilation operators $c$ or $p_b$, and $\eta \rightarrow 0$. In order to calculate the propagators we will write their equations of motion (taking from now on $\hbar = 1$)

$$\omega\langle\langle c_{k+};c_{k-}\rangle\rangle = \frac{1}{2\pi}\langle\langle c_{k+},c_{k-}\rangle\rangle + \langle\langle [c_{k+},H];c_{k-}\rangle\rangle$$

(A.2)

and

$$\omega\langle\langle p_{bk+};p_{bk-}\rangle\rangle = \frac{1}{2\pi}\langle\langle p_{bk+},p_{bk-}\rangle\rangle + \langle\langle [p_{bk+},H];p_{bk-}\rangle\rangle,$$

(A.3)

where $\mathcal{H}(k)$ is the Hamiltonian for the system (eq. (2) in the main text) and $\{,\}$ and $[,]$ indicate an anticommutator and a commutator, respectively.

Let us develop further the equation of motion for the first propagator $\langle\langle c_{k+};c_{k-}\rangle\rangle$. Making use of standard relations for fermion creation and annihilation operators, we obtain

$$\omega_s^{(-)}\langle\langle c_{k+};c_{k-}\rangle\rangle - 2it_{sp}\sin(k)\langle\langle p_{bk+};c_{k-}\rangle\rangle + \Delta_1\langle\langle c_{k+};c_{k-}\rangle\rangle = 0,$$

(A.4)

where $\omega_s^{(-)}$ stands for $\omega - \epsilon_s + \mu$.

In the process above, two new propagators were created, viz., $\langle\langle p_{bk+};c_{k-}\rangle\rangle$ and $\langle\langle c_{k+};c_{k-}\rangle\rangle$. Therefore, in order to close the system of equations for the propagators, we also need the equation of motion for $\langle\langle c_{k+};c_{k-}\rangle\rangle$, $\langle\langle p_{bk+};c_{k-}\rangle\rangle$, $\langle\langle p_{bk+};c_{k-}\rangle\rangle$, $\langle\langle p_{bk+};c_{k-}\rangle\rangle$, and $\langle\langle p_{bk+};c_{k-}\rangle\rangle$. 


This procedure generates a system of equations given by

\[
D \cdot \begin{pmatrix}
\langle \langle c_{k-}^1 ; c_{k-} \rangle \rangle \\
\langle \langle p_{ak+} ; c_{k-} \rangle \rangle \\
\langle \langle p_{ak-} ; c_{k-} \rangle \rangle \\
\langle \langle c_{k+} ; c_{k-} \rangle \rangle \\
\langle \langle p_{bk+} ; c_{k-} \rangle \rangle \\
\langle \langle p_{bk-} ; c_{k-} \rangle \rangle \\
\end{pmatrix} = \begin{pmatrix}
\frac{1}{2\pi} \\
0 \\
0 \\
0 \\
0 \\
0 \\
0 \\
\end{pmatrix}, \tag{A.5}
\]

where

\[
D = \begin{bmatrix}
\omega_s^{(-)} & 0 & 0 & \Delta_1 & -\bar{t}_{spb} & 0 \\
0 & \omega_p^{(+)} & 0 & 0 & 0 & \bar{t}_{pbp} \\
0 & 0 & \omega_p^{(-)} & 0 & -\bar{t}_{papb} & 0 \\
\Delta_1 & 0 & 0 & \omega_s^{(+)} & 0 & \bar{t}_{spb} \\
\bar{t}_{spb} & 0 & -\bar{t}_{papb} & 0 & \omega_p^{(+)} & \Delta_2 \\
0 & -\bar{t}_{papb} & 0 & -\bar{t}_{spb} & \omega_p^{(-)} & \Delta_2 \\
\end{bmatrix}. \tag{A.6}
\]

and we defined \(\omega_q^{(\pm)} = \omega \pm \epsilon_q \mp \mu,\) for \(q = s, p_a,\) or \(p_b;\) \(\bar{t}_{spb} = 2it_{spb}\sin(k);\) and \(\bar{t}_{papb} = 2t_{papb}\cos(k).\)

Using Cramer’s method to solve the system of equations in (5), we have that

\[
\langle \langle c_{k+} ; c_{k-} \rangle \rangle = \frac{|D_{ss}|}{|D|}, \tag{A.7}
\]

where the matrix \(D_{ss}\) is obtained by replacing the 4th column in matrix \(D\) by the column-matrix defined in the right side of eq. (5) (note that \(|D|\) means the determinant of matrix \(D\)). Repeating the same procedure for \(\langle \langle p_{bk+} ; p_{bk-} \rangle \rangle\) we obtain

\[
D \cdot \begin{pmatrix}
\langle \langle c_{k-}^1 ; p_{bk-} \rangle \rangle \\
\langle \langle p_{ak+} ; p_{bk-} \rangle \rangle \\
\langle \langle p_{ak-} ; p_{bk-} \rangle \rangle \\
\langle \langle c_{k+} ; p_{bk-} \rangle \rangle \\
\langle \langle p_{bk+} ; p_{bk-} \rangle \rangle \\
\langle \langle p_{bk-} ; p_{bk-} \rangle \rangle \\
\end{pmatrix} = \begin{pmatrix}
0 \\
0 \\
0 \\
0 \\
0 \\
\frac{1}{2\pi} \\
\end{pmatrix}, \tag{A.8}
\]

obtaining, as above,

\[
\langle \langle p_{bk+} ; p_{bk-} \rangle \rangle = \frac{|D_{papb}|}{|D|}, \tag{A.9}
\]

where \(D_{papb}\) is obtained, as above, by replacing the 5th column in matrix \(D\) by the column-matrix defined in the right side of eq. (8). In eqs. (7) and (9), \(|D|\) is a sixth degree biquadratic polynomial that can be written as

\[
|D| = \sum_{n=0}^{3} B_{2n} \omega^{2n} = \prod_{n=1}^{6} (\omega - \omega_n) = \prod_{n=1}^{3} (\omega^2 - \omega_n^2) \tag{A.10}
\]

where the last equation is obtained by noting that \(\omega_1 = -\omega_4, \omega_2 = -\omega_5,\) and \(\omega_3 = -\omega_6.\) The coefficients \(B_{2n}\) are functions of the parameters of the Hamiltonian. The \(\omega_n\) are the zeros of \(|D|\) and represent the energy excitations of the system.
To finally determine the gap equations, it is appropriate to make use of the following identity

$$\left|D\right|^{-1} = \sum_{n=0}^{\infty} \frac{1}{r_n} \left[ \frac{1}{2\omega_n} \left( \frac{1}{\omega - \omega_n} - \frac{1}{\omega + \omega_n} \right) \right],$$

(A.11)

where

$$r_1 = (\omega_1^2 - \omega_2^2)(\omega_1^2 - \omega_3^2); \quad r_2 = (\omega_2^2 - \omega_1^2)(\omega_2^2 - \omega_3^2); \quad r_3 = (\omega_3^2 - \omega_1^2)(\omega_3^2 - \omega_2^2).$$

Substituting eq. (11) into eqs. (7) and (9), and after using eq. (1), we have

$$\langle \gamma_k^- \gamma_{k+} \rangle = i \sum_{j=1}^{3} \int_{-\infty}^{+\infty} d\omega f(\omega) \frac{D_{\gamma\gamma}(\omega)}{2\omega_j r_j} \times \left( C_+(\omega) - C_-(\omega) \right),$$

(A.12)

where we have defined the following quantities

$$C_{\pm}(\omega) = \lim_{\eta \to 0^\pm} \left( \frac{1}{\omega \pm \omega_j - i\eta} - \frac{1}{\omega \pm \omega_j + i\eta} \right).$$

(A.13)

Now, using the fact that

$$\delta(x) = \frac{1}{2\pi i} \lim_{\eta \to 0^+} \left( \frac{1}{x - i\eta} - \frac{1}{x + i\eta} \right),$$

(A.14)

we finally get

$$\langle \gamma_k^- \gamma_{k+} \rangle = i \sum_{j=1}^{3} \int_{-\infty}^{+\infty} d\omega f(\omega) \frac{D_{\gamma\gamma}(\omega)}{\omega_j r_j} \times \left( \frac{1}{\omega \pm \omega_j - i\eta} - \frac{1}{\omega \pm \omega_j + i\eta} \right) \times \left( C_+(\omega) - C_-(\omega) \right),$$

(A.15)

where $f_{FD}(\omega_j) = 1/[\exp(\omega_j/k_BT) + 1].$

Substituting eq. (15) into the equations for $\Delta_1$ and $\Delta_2$ in the previous page, and taking the limit $T \to 0$, we can write the following self-consistent equations

$$\Delta_1 = \Delta_{ss} + \Delta'_{p\bar{p}_h} = -g_{ss} \sum_{k} \pi \sum_{j=1}^{3} \frac{|D_{ss}(\omega_j)|}{\omega_j r_j} - g_{sp_h} \sum_{k} \pi \sum_{j=1}^{3} \frac{|D_{p\bar{p}_h}(\omega_j)|}{\omega_j r_j},$$

(A.16)

and

$$\Delta_2 = \Delta'_{ss} + \Delta_{p\bar{p}_h} = -g_{sp_h} \sum_{k} \pi \sum_{j=1}^{3} \frac{|D_{ss}(\omega_j)|}{\omega_j r_j} - g_{p\bar{p}_h} \sum_{k} \pi \sum_{j=1}^{3} \frac{|D_{p\bar{p}_h}(\omega_j)|}{\omega_j r_j}. $$

(A.17)

In the thermodynamic limit ($L \to \infty$), we can replace the sum by an integral [in the interval $-k_F \leq k \leq k_F$] by using the standard relation

$$\frac{2\pi}{L} \sum_{k} \Delta_k = \frac{1}{2\pi} \int_{-k_F}^{k_F} dk,$$

(A.18)

where, $k_F$ is the Fermi wave vector and $L$ is the length of the one-dimensional system. For practical purposes, we change the integration variable ($\hat{k} = k/k_F$), and finally obtain

$$\Delta_1 = -g_{ss} \frac{k_F}{2} \int_{-1}^{1} dk \sum_{j=1}^{3} \frac{|D_{ss}(\omega_{k,j})|}{\omega_{k,j} r_j} - g_{sp_h} \frac{k_F}{2} \int_{-1}^{1} dk \sum_{j=1}^{3} \frac{|D_{p\bar{p}_h}(\omega_{k,j})|}{\omega_{k,j} r_j},$$

(A.19)
and
\[
\Delta_2 = -g_{spb} \frac{k_F}{2\pi} \int_{-1}^{1} \frac{3}{d\tilde{k}} \sum_{j=1}^{3} |D_{ss}(\omega_{k,j})| - g_{pnp} \frac{k_F}{2\pi} \int_{-1}^{1} \frac{3}{d\tilde{k}} \sum_{j=1}^{3} |D_{pnp}(\omega_{k,j})| \quad \omega_{k,j} r_j.
\]

(A.20)

In a one-dimensional system, the Fermi wave vector \( k_F = \frac{\rho \pi}{2} \), where \( \rho = \frac{N}{V} \) is the density of electrons in the material and \( N \) is the total number of electrons. Note that, when \( g_{ss} = g_{pnp} = g_{spb} \), we have \( \Delta_1 = \Delta_2 \).

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