Ab-Initio Theory of Superconductivity in a Magnetic Field II: Numerical solution.

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We numerically investigate the Spin Density Functional theory for superconductors (SpinSCDFT) and the approximated exchange-correlation functional, derived and presented in the preceding paper I. As a test system we employ a free electron gas featuring an exchange-splitting, a phononic pairing field and a Coulomb repulsion. SpinSCDFT results are compared with Sarma, the Bardeen Cooper and Schrieffer theory and with an Eliashberg type of approach. We find that the spectrum of the superconducting Kohn-Sham SpinSCDFT system is not in agreement with the true quasi particle structure. Therefore, starting from the Dyson equation, we derive a scheme that allows to compute the many body excitations of the superconductor and represents the extension to superconductivity of the $G_0W_0$ method in band structure theory. This superconducting $G_0W_0$ method vastly improves the predicted spectra.

I. INTRODUCTION

Interaction between the magnetic (M) and superconducting (SC) order leads to complex and fascinating phenomena. Apart from the Meissner effect as the most apparent aspect of this interaction on macroscopic length scales, for singlet superconductors, the ferromagnetic parallel spin alignment competes with spin anti-parallel Cooper pair formation. While for triplet superconductors such as UGe$_2$, a ferromagnetic (F) order is possible even in a bulk geometry, F/SC interfaces or SC surfaces in an external magnetic field allow to study the microscopic competition of a large spin-splitting also for singlet superconductors. This may lead to spatial inhomogeneities of the SC order parameter, such as the phase predicted by Fulde and Ferrell and Larkin and Ovchinnikov. Furthermore, the spin valve behavior of complex F/SC structures may provide opportunities for novel devices making use of the unique electronic configuration that appears due to the vicinity of these two competing phases (see Ref. 7 for a review).

These effects are addressed in the theoretical literature so far mostly within model or semi-empirical calculations due to the lack of a complete and efficient ab-initio theory. This leaves the prediction of essential material dependent properties as critical temperature and excitation gap in the presence of a magnetic field out of reach. The Spin Density Functional theory for superconductors (SpinSCDFT) approach presented by Ref. 8 (hereafter referred to as I) may fill this gap, as the theory has the computational convenience of a Kohn-Sham density functional framework and allows to calculation of material dependent SC parameters from the crystal structure. The SpinSCDFT in principle exact, but relies on the approximation of the exchange-correlation ($xc$) potential. A first approach to derive such an $xc$ potential relies, in turn, on the Sham-Schlüter equation for a SC and is presented in I.

In this work, we present numerical results for SpinSCDFT, aiming to achieve a deeper understanding of this theoretical framework and to characterize and validate the $xc$ potential, as derived in I. In particular we will investigate the properties of the Kohn-Sham pairing function, that is a key object in SCDF$^{11,12}$. The test system we adopt for this analysis is a spin-splitted free electron gas with a phononic and Coulomb coupling. Details of the model will be presented in Sec. II. One advantage of this simplified model with a homogeneous exchange splitting is its similarity to the starting point of Ref. 13 and 14 for their discussion of the Eliashberg equations and BCS theory, respectively. As compared to Ref. 13, we use a different notation (compare I) and take a more general route which reduces to the earlier results in the case that the magnetic field homogeneously splits the electronic states. We will compute the temperature vs exchange splitting diagram of the model using, apart from SpinSCDFT, the BCS theory and the Eliashberg equations. Then, in Sec. V we will compare our SpinSCDFT results with the BCS approach (reviewed in Sec. III) and with the reference Eliashberg method (Sec. IV).

The SpinSCDFT Kohn-Sham system proves to give qualitatively correct results for the $J-T$ diagram. However, we find in Sec. V that it does not show a physical excitation spectrum. A similar problem is very well known in conventional DFT, and is usually called the band gap problem. Since the excitation gap is a very important property of superconductors, it is important to devolve methods to compute it. Therefore, the last part of this work will be devoted to describe an extension of the $G_0W_0$ method to our superconducting system and show that it entirely solves the problem, similar to its normal state counterpart$^{15}$.

II. A TEST SYSTEM

The model system which we will use to investigate the SpinSCDFT formalism is based on a non interacting electron gas under the influence of an homogeneous magnetic field $B_0$. The energy of its electronic states $\varepsilon_{k\sigma}$, relative to the Fermi energy $E_F$ ($k = k, n$ where here $n$ is a band
index and we use the notation \(-k = -\mathbf{k}, n\), reads

\[
\epsilon_{k\sigma} = \frac{1}{2} k^2 \epsilon_f - E_f - \text{sign}(\sigma) \mu_B B_0. \tag{1}
\]

The Fermi energy is defined by integrating the density of states (DOS) up to \(E_f\) to have \(N_e\) electrons in the system. We set the density to \(N_e/\Omega_{uc} = 1 a_0^{-3}\) (\(a_0\) is the Bohr radius and \(\Omega_{uc}\) the unit cell volume) which leads to a relatively large \(E_f\) of 4.78 Ha ignoring the small imbalance in up and down spin occupations. We also define a center of energy between spin splitted states \(\epsilon(k) = \frac{1}{2}(\epsilon_{k\uparrow} + \epsilon_{k\downarrow}) = \frac{1}{2} k^2 \epsilon_f \) and the splitting \(J(k) = \frac{1}{2}(\epsilon_{k\uparrow} - \epsilon_{k\downarrow}) = -\mu_B B_0\). This will prove useful since, as seen in I, many SpinSCDFT entities depend on \(k\) only via these two parameters \(\epsilon\) and \(J\).

Superconductivity is induced in this model by an electron-phonon like attractive interaction, expressed by the Gaussian Eliashberg function\(16\):

\[
a^2F(\omega) = \lambda \frac{\omega}{2 \omega_w \sqrt{\pi}} e^{-\frac{1}{2} \left(\frac{\omega - \omega_w}{\omega_w}\right)^2}. \tag{2}
\]

This model depends on three parameters: \(\lambda\) the electron-phonon coupling constant\(10\); \(\omega_w\) the center of mass of the phonon spectrum, and \(\omega_w\) the width of the optical branch. In the calculations we fix these numbers to \(\omega_w = 2.2\text{mHa}\) \(\omega_w = 0.5\text{mHa}\) and \(\lambda = 0.7\) which lead to coupling properties that are loosely similar to those of MgB\(_2\).\(17\). The resulting spectrum is plotted in Fig. 1 and compared with a recomputed one of MgB\(_2\). In SpinSCDFT one can consider a general Coulomb coupling on the same footing as the phonon interaction. Here, we use a simple Thomas-Fermi based model that was used before in SCDFT\(11,18\). In this model the screened Coulomb matrix elements between a state of energy \(\epsilon\) and one of energy \(\epsilon'\) is given by

\[
C^{\text{stat}}(\epsilon, \epsilon') \approx -\frac{\pi \rho^{\text{EG}}(\epsilon')}{2 \sqrt{\epsilon + E_f} (\epsilon' + E_f)} \times \\
\times \ln \left( \frac{\epsilon + \epsilon' + 2E_f + 2\sqrt{(\epsilon + E_f)(\epsilon' + E_f)} + \frac{1}{2} k_{\tau F}^2}{\epsilon + \epsilon' + 2E_f - 2\sqrt{(\epsilon + E_f)(\epsilon' + E_f)} + \frac{1}{2} k_{\tau F}^2} \right). \tag{3}
\]

The screening parameter is chosen to be \(k_{\tau F}^2 = (0.005)^2\text{Ha}\). With this parameter, the shape of the model \(C^{\text{stat}}(\epsilon, \epsilon')\) is shown in Fig. 2. All properties of the test system depend on the Bloch vector \(\mathbf{k}\) and the band index \(n\) only via the single particle energy \(\epsilon_k\). For brevity we use the notation \(\epsilon = (\epsilon, J)\). With \(\epsilon\) and \(J\) as defined in the previous section, we may cast a Brillouin zone integral into the isotropic formulation with the double DOS

\[
\varrho(\epsilon) = \sum_k \delta(\epsilon - \frac{\epsilon_{k\uparrow} + \epsilon_{k\downarrow}}{2}) \delta(\frac{J - \epsilon_{k\uparrow} - \epsilon_{k\downarrow}}{2}). \tag{4}
\]

This quantities describes the number of states on equal center of energy \(\epsilon\) and splitting \(J\) surfaces. In our model \(\varrho(\epsilon)\) the external field is homogeneous. This means the number of states on equal splitting surfaces has a delta distribution character that peaks at \(J_0 = -\mu_B B_0\). In the remainder of the paper, \(J_0\) replaces the \(J\) integrals almost everywhere so we simplify the notation using \(J_0 \rightarrow J\).

III. THE BCS THEORY WITH AN EXCHANGE SPLITTING

The \(J-T\) diagram of a BCS model with a homogeneous exchange splitting parameter \(J\) has been presented by Ref. 14. This approach, that we are going to review here, can only be used to obtain qualitative results. Still, it will be an important guideline in understanding the more involved Eliashberg and SpinSCDFT results of the next sections. In a BCS model\(19\) one replaces the interactions among single electrons with an effective one, keeping only the matrix elements that couple the states \(k, \uparrow\) and \(-k, \downarrow\). The effective interaction is approximated with “a box” centered at the Fermi level (from \(-\Omega_d\) to \(\Omega_d\) which is of the order of the Debye phonon frequency to mimic phononic type of pairing and with height \(-V\)). This leads to a fixed point equation for the mean field gap.
$\Delta^1 \frac{1}{\rho(0)V} = \int_0^{\Omega_d} \frac{d\varepsilon}{\sqrt{\varepsilon^2 + \Delta^2}} (f_\beta(J - \sqrt{\varepsilon^2 + \Delta^2})$ $- f_\beta(J + \sqrt{\varepsilon^2 + \Delta^2})). \tag{5}$

$\rho(0)$ is the DOS at the Fermi level and $J$ is the splitting energy between up and down states. Apart from the solutions $\Delta$ of Eq. (5) there is also the trivial solution $\Delta = 0$. We solve Eq. ((5)) numerically as a function of $T$ and $J$.\textsuperscript{20} The solutions $\Delta(T, J)$ are presented in Fig. 3 a). There, we normalize $\Delta$ to $\Delta_0$, the solution for $T \to 0$ and $J = 0$. Similarly, we normalize the $J$ to $\Delta_0$ and to $T_{\text{c0}}$, the critical temperature for $J = 0$. In this way we remove the explicit dependence on the parameters $\rho(0)V$ and $\Omega_d$.

When one attempts to linearize Eq. (5), a peculiar behavior is found in that the $T_c(J)$ curve bends inwards.\textsuperscript{14} We solve the linearized Eq. (5) and show the resulting $T_c(J)$ as a green line in Fig. 3 a). As pointed out by the Refs. 14 and 23, unlike the original BCS model at $J = 0$, this equation leads to a $J - T$ diagram in which the SC transition can be discontinuous in $\Delta$, i.e. of first order. Below the temperature $T/T_{\text{c0}} \approx 0.6$ at point $A$ and the dashed line in Fig. 3 b) no small $\Delta$ solution to the non-linear equation is found and the initial assumption of the linearization that an arbitrary small solutions exists is not valid.

While we can find a non-vanishing solution $\Delta$ it may not correspond to the stable thermodynamic phase. In Fig. 3 b) we remove the non-vanishing solutions, if the free energy favors the magnetic state. The resulting $T - J$ diagram shows that for $J$ larger than to the Chandrasekhar-Clogston limit at $T = 0$\textsuperscript{21,22} of $J_c = \Delta_0/\sqrt{2}$ no SC solution is stable.

Another interesting approach to describe SC in the presence of a magnetic field is presented by Powell et al.\textsuperscript{23} who use a Hubbard model in connection with a homogeneous exchange splitting. They treat the pairing part of the interactions among electrons in the system in the Hartree-Fock approximation, similar to BCS as described above and consequently arrive at a similar gap equation as compared to Eq. ((5)). The matrix elements of the KS system of SpinSCDFT within the spin decoupling approximation will turn out to have a similar analytic structure.

Also, Ref. 23 discusses why the transition is of first order. They observe that for $J < \Delta$ and $T = 0$ the gap equation (5), and consequently $\Delta$, is independent on $J$. Thus $\Delta(J) = \Delta_0$ for $J < \Delta_0$. At $\varepsilon < \sqrt{J^2 - \Delta^2}$ on the other hand the Fermi functions at $T = 0$ in Eq. (5) are equal and thus cancel. Also for this type of solution $\Delta$ must be larger than $J$ and for $J > \Delta$ only the trivial solution $\Delta = 0$ can be found. At this point follows that $\Delta(T = 0K, J) = \Delta_0 \theta(\Delta_0 - J$) and the transition is discontinuous $T = 0$.

The above analysis will be crucial later, in Sec. IV and V, to guide the discussion of the more sophisticated approaches, that feature a qualitatively similar behavior. In the next section we will discuss results of the Eliashberg method (as derived in I, Sec. IV) when applied to our test system of Sec. II.

IV. SOLUTIONS TO THE PHONON ONLY ELIASHBERG EQUATIONS

We solve the Eliashberg Eqs. (I.130) to (I.132). The approximations used here, for the special case of homogeneous exchange field, lead to equations similar to those derived by Vonsovsky et al.\textsuperscript{13}.

Similar to every equation that describes a spontaneously broken symmetry, in addition to a possible finite solution, the Eliashberg Eqs. (I.130) to (I.132) always have the solution $\Delta_{n}^{\text{g}}(J) = 0$. Usually, this non-SC solution is not stable below $T_c$ in the sense that small symmetry breaking fields (that in the self consistent iteration scheme is equivalent to a small but non-zero starting guess) lead to the finite $\Delta_{n}^{\text{g}}(J)$ solution via iteration of the Eliashberg Eqs. (I.130) to (I.132). Thus, we say that in this case the $\Delta_{n}^{\text{g}}(J) = 0$ solution has a zero basin of attraction; Only the starting value $\Delta_{n}^{\text{int}}(J) = 0$ leads to the final solution $\Delta_{n}^{\text{g}}(J) = 0$. Whenever $J > 0$, the $\Delta_{n}^{\text{g}}(J) = 0$ solution has a zero basin of attraction below $T_c$.

From Eq. (I.113) we know that the complex $\Delta_{n}^{\text{g}}$ changes the poles of the Green function. We assume the term $A_{2}^{\text{g}}(\omega_n)$ to be zero, for simplicity. Then from the analytic continuation to the real axis of Eq. (I.113), we see that the energy $\omega$ of such a pole satisfies the condition $\omega = \text{sign}(\sigma)J_k \pm \sqrt{\varepsilon_k^2 + \Delta(\omega)^2}$ which is analogous to the usual Eliashberg equations (compare also Ref. 24).

At $T = 0$, the analytic continuation of $\Delta_{n}^{\text{g}}$ the real axis is purely real in the range of the Fermi energy and its value there defines the SC excitation gap\textsuperscript{24}. Thus, the Matsubara component $n = 0$ of $\Delta_{n}^{\text{g}}$ is related to the SC excitation gap of the quasi particle system. We choose this as a characteristic property that we investigate as a function of $J$ and $T$. In the following we generate two $J - T$ diagrams shown in Fig. 4. In a) we follow the SC solution, i.e. we take the converged $\Delta_{n}^{\text{g}}(J)$ as input for the calculation at $\Delta_{n}^{\text{g}}(J + \Delta J)$, starting at $J = 0$ with $\Delta J$ positive. This way we compute the diagram "from left to right" and test the stability of the $\Delta_{n}^{\text{g}}(J) \neq 0$ solution. In b), we take the converged $\Delta_{n}^{\text{g}}(J)$ as input for the calculation at $\Delta_{n}^{\text{g}}(J - \Delta J)$, starting at $J = 0.5$mHa. Thus, we generate the diagram "from right to left". Because for large $J$ $\Delta_{n}^{\text{g}}(J)$ is zero, we start from a small, symmetry breaking value at $\Delta_{n}^{\text{g}}(J - \Delta J)$ instead of zero. This way we test the stability of the trivial $\Delta_{n}^{\text{g}}(J) = 0$ solution.

Comparing a) and b) we see that the borders of stability between the stability of $\Delta_{n}^{\text{g}}(J) = 0$ and $\Delta_{n}^{\text{g}}(J) \neq 0$ do not agree. In fact, we find a region where both, the $\Delta_{n}^{\text{g}}(J) = 0$ and the $\Delta_{n}^{\text{g}}(J) \neq 0$ solution have a finite basin of attraction; here the normal and the SC state are (meta) stable. The shape of the border of the region
where $\Delta_n^s(J) = 0$ is unstable resembles closely to the linear BCS solution which we show in Fig. 4 a) as a green dashed line.

We plot the $\Delta_n^s(J)$ at $T = 10K$ in Fig. 5 a) and 40K in Fig. 5 b) as a function of $J$ on the vertical axis. The corresponding equal temperature lines are blue in Fig. 4. We find that the shape is largely independent on the splitting $J$ and the temperature $T$ except for a scale factor. Thus $\Delta_n^s = 0$ is sufficient to investigate the behavior of the theory. For low temperatures the down-scaling is much less pronounced and it is safe to say that the pairing is almost unaffected by the presence of a splitting up until the point where the SC phase is suppressed. For a high temperature, instead, the down-scaling is more pronounced and the transition becomes continuous above a certain temperature.

V. RESULTS OF SPINSCDFT WITH THE G0-FUNCTIONAL

In this Section we discuss the numerical solution of the SpinSCDFT gap equation (I.95) using the $xc$-potential derived in Sec. I.C. We refer to this functional as the G0-functional.

In Eq. (I.95) of I, we have derived the gap equation of SpinSCDFT using the G0-functional. This equations (I.95), in turn, is derived from the Sham-Schlüter equation for a superconductor, written in I in the form

$$\int d\epsilon\delta S^s_\beta[\Delta^s_\beta](\epsilon, \epsilon')\Delta^s_\beta(\epsilon') = 0.$$  \hspace{1cm} (6)

From the previous discussion in the Secs. III and IV, a continuous transition is to be expected for a small exchange field intensity $J$ as compared to the transition temperature.

For the point of the continuous transition Eq. (6) can be linearized in $\Delta^s_\beta$. Similar to I we use the notation with a breve to indicate linearized entities $\tilde{S}_\beta = S^s_\beta[\Delta^s_\beta = 0]$. Thus, in this case $T_c(J)$ can be computed from the condition that $\tilde{S}_\beta = \tilde{S}^s_\beta + \tilde{S}_\beta^{xc} + \tilde{S}^s_\beta$ has a singular eigenvalue

$$\det \tilde{S}_\beta = 0.$$  \hspace{1cm} (7)

The corresponding shape of the solution $\Delta^s_\beta/||\Delta^s_\beta||$ is the right eigenfunction to such a singular eigenvalue.

$\tilde{S}_\beta(\epsilon, \epsilon')$ is given in Eq. (I.80). To investigate the structure and properties of the SpinSCDFT $xc$-potential is easier within the linearized form, since the matrix $\tilde{S}_\beta(\epsilon, \epsilon') = \tilde{S}^s_\beta(\epsilon, \epsilon') + \tilde{S}_\beta^{xc}(\epsilon, \epsilon') + \tilde{S}^s_\beta(\epsilon, \epsilon')$ is independent of the potential $\Delta^s_\beta$. As discussed in detail in I, $\tilde{S}^s_\beta(\epsilon, \epsilon')$ corresponds to the Nambu (off) diagonal self-energy contribution. $\tilde{S}^s_\beta$ is due to the $ve_{xc}$ part of the Sham-Schlüter equation. In Sec. VA we present and discuss the shape of the contributions $\tilde{S}^s_\beta(\epsilon, \epsilon')$, $\tilde{S}^{xc}_\beta(\epsilon, \epsilon')$, $\tilde{S}^s_\beta(\epsilon, \epsilon')$ and the $T_c(J)$ curve from the linearized $xc$-potential.

Finally, the properties of the general non-linear gap equation, i.e. the $J-T$ diagram of the solutions to Eq. (6) with and without the Coulomb repulsion will be presented in Sec. VB.

A. Linearized Sham-Schlüter Equation

As discussed before, in the part of the $J-T$ diagram for a relatively small applied field (i.e. low splitting $J$ and high $T$) we expect a second order phase transition. This section deals with the corresponding continuous transition. In Sec. V A 1, will show the shape of $\tilde{S}^s_\beta$, $\tilde{S}^{xc}_\beta$, and $\tilde{S}^s_\beta$. To determine the point of the transition according to Eq. (7), in Sec. V A 2 we investigate the spectrum of $\tilde{S}_\beta$ as a function of temperature and splitting and the corresponding solutions $\Delta^s_\beta/||\Delta^s_\beta||$. Then we will discuss
The shape of the $T_c(J)$ curve in Sec. V A 3 from this linear approach.

1. Temperature Dependence of $\tilde{S}_β$

The three contributions to $\tilde{S}_β(\varepsilon, \varepsilon')$ are (see Sec. I.C., Eqs. (1.91), (1.92), (1.93) and (1.94))

$$\tilde{S}_β(\varepsilon, \varepsilon') = (\tilde{S}_β^0(\varepsilon) + \tilde{S}_β^M(\varepsilon)) \delta(\varepsilon - \varepsilon') + \tilde{S}_{\beta p\beta}(\varepsilon, \varepsilon') + \tilde{S}_{C\beta}(\varepsilon, \varepsilon'). \tag{8}$$

In this linear Sham-Schlüter form, $\tilde{S}_β^M(\varepsilon)$ and $\tilde{S}_β^0(\varepsilon)$ multiply $\Delta_0(\varepsilon)$ directly. They are shown for several $T$ for $J = 0.0mHa$ and $J = 0.1mHa$ in Fig. 6 panel a) and b), respectively. Note the logarithmic center of energy scale $\varepsilon$ in all the plots in this section. The color scale (blue to red) indicates increasing temperatures. All terms have features only in the close vicinity to $\varepsilon = 0$ and quickly decay to zero within a characteristic energy width of the phonon coupling. This energy scale is the analog of Debye frequency $\omega_0$ in Eq. (2). However the $\varepsilon$ dependence shown in Fig. 6 in the presence (panel b) and the absence (panel a) of an exchange splitting is very different. In fact, in Fig. 6 a) where $J = 0$ both $\tilde{S}_β^0(\varepsilon)$ and $\tilde{S}_β^0(\varepsilon)$ are positive and monotonically decreasing as a function of $|\varepsilon|$. In presence of a $J \neq 0$ (Fig. 6 b), instead, they have the following complex temperature and energy dependence: For small $T$ in the range $|\varepsilon| < J$, $\tilde{S}_β^0(\varepsilon)$ is negative and, in the limit $T \to 0$, $\tilde{S}_β^0(\varepsilon)$ and $\tilde{S}_β^0(\varepsilon)$ approach zero from opposite sides. At $|\varepsilon| \approx J$ both $\tilde{S}_β^0(\varepsilon)$ and $\tilde{S}_β^0(\varepsilon)$ vary very rapidly. This behavior is smoothed out with increasing $T$ and at temperatures high enough with respect to $J$ the non-splitted behavior is recovered. The temperature and $J = 0mHa$ and $J = 0.1mHa$ dependence of $\tilde{S}_{\beta p\beta}(\varepsilon, \varepsilon')$ is shown in Fig. 6 c) and d), respectively. $\tilde{S}_β^M$ serves as a scale that other kernel contributions have to be compared with, so we choose a color scale that is relative to the maximum of $\tilde{S}_β^M$, indicated on the right of every plot.

For $J = 0mHa$ we note that the size of $\tilde{S}_{\beta p\beta}(\varepsilon, \varepsilon')$ (Fig. 6 c) decays faster with temperature the one of the diagonal $\tilde{S}_β^0$ and $\tilde{S}_β^0$ (the the position of "white" in the color scale of Fig. 6 c) moves to the left with increasing temperatures). Furthermore, being both positive and diagonal, $\tilde{S}_β^M$ and $\tilde{S}_β^0$ have to be compared with the eigenvalues of $\tilde{S}_{\beta p\beta}^M$. $\tilde{S}_β^0$ and $\tilde{S}_β^0$ alone would result in a positive definite Sham-Schlüter matrix for $J = 0mHa$ (compare Fig. 6 a) at all temperatures so there is not non-trivial solution to Eq. (6). Thus, technically, the phase transition from the SC to the non SC regime with the singular eigenvalue is induced by this relative reduction of $\tilde{S}_β^0$ as compared to $\tilde{S}_β^0$ plus $\tilde{S}_β^0$. We will turn to a systematic analysis of the eigenvalues of the linearized Sham-Schlüter matrix $\tilde{S}_β$ in Sec. V A 2.

The relative scale reduction is also found for the splitted $\tilde{S}_{\beta p\beta}$. At $\varepsilon \approx 0$, however, we stay much below the
Moreover, the sign change of \( J \) shows that for very low temperature and \( \beta \), the diagonal repulsion.

Figure 6. (color online) Contributions to the linearized Sham-Schlüter Eq. (6). In the top row we show the diagonal contributions that originate from the Nambu off phonon (Coulomb) self-energy. The color scale of \( \tilde{S}^M \) for negative values (decreasing: blue to white to green) is relative to \( \max(\tilde{S}^M) \) (white). Red to yellow to white indicates increasingly positive values. Note that \( \tilde{S}^M \) and \( \tilde{S}^{ph} \) switch sign at \( \epsilon \approx 0 \) for \( J = 0.1 \text{mHa} \) at low \( T \) as compared to \( J = 0 \text{mHa} \).

The scale of \( \tilde{S}^M \) and exceed it only for higher temperatures. Moreover, the sign change of \( \tilde{S}^M \) is effectively reducing the diagonal repulsion.

A purple line in Fig. 6 d) indicates the zero contour and shows that for very low \( T \), \( \tilde{S}^{ph}\) is positive for approximately the region where \( |\epsilon| < J \) or \( |\epsilon'| < J' \) and has a sharp negative spike at \( \epsilon = \epsilon' \approx J \). Thus, as a curious fact, the phonon interaction is not "attractive" everywhere in this case. We show the shape of the static Coulomb part \( \tilde{S}^{ec} \) in Fig. 6 row e) and f) for \( J = 0 \text{mHa} \) and \( J = 0.05 \text{mHa} \), respectively. Apart from the differences in sign, the overall behavior of the Coulomb term and phonon terms is roughly similar with significant deviations in the fact that it does not change sign for a low temperature and exchange splitting, compare Fig. 6 d) with f).

In summary we can say that we see relevant changes in the shape of the contributions to \( \tilde{S}^{ph}\) for a finite exchange splitting for the low temperature limits in the region \( |\epsilon| < |J| \) as compared to the spin degenerate case. At higher temperatures the splitting becomes less important. We point out that we know from the earlier discussion that this is the region, where we expect the linearization to be unjustified. From the form of the Bogoliubov eigenvalues \( \xi^{\pm}_\gamma = \text{sign}(\gamma)J + \text{sign}(\alpha)\sqrt{\epsilon^2 + |\Delta^s|^2} \) we expect that, whenever \( \Delta^s \) is larger than \( J \), will see a behavior more similar to the case \( J = 0 \). The reason is that, then, only the \( \alpha = + \) branch has positive excitation energies \( \xi^+_\gamma \geq 0 \), meaning that the ground state does not correspond to some of the excitations \( \tilde{\gamma}_k \) being occupied (see the discussion in I. III. A. 2.d and by Ref. 14).

2. Critical Temperatures and the Shape of \( \Delta^s \)

Since we compute the critical temperature from Eq. 7, i.e. the occurrence of a singular eigenvalue of \( \tilde{S}_\beta \), in this section, we will investigate the full spectrum as a function of \( T \) and \( J \). The KS potential \( \Delta^s_k \) is proportional to the right eigenvector of \( \tilde{S}_\beta \) that is associated to a singular eigenvalue. Thus, all eigenfunctions \( \Delta^s_k \) we show are normalized to a common arbitrary value. In this Subsection, we are not considering the Coulomb contribution when we calculate the spectrum of \( \tilde{S}_\beta \) as a function of temperature in Fig. 7. In the spin-degenerate case (\( J = 0 \text{mHa} \)) we see that the eigenvalues decrease in mag-
temperatures. There is a temperature regime \( T \) zero and become positive. Beyond small splitting \( T \), the negative eigenvalue crosses zero, at the temperature all eigenvalues but one are positive valued; magnitude with temperature in a monotonous way. At low temperature the discontinuous type. We investigate this issue in the next Subsection VA3.

Increasing the number of sampling points increased the relative value at the discontinuity so this lead us to the conclusion that we are numerically sampling an unbound function. It has to be understood that an unbound function cannot be the linearized solution to an originally non-linear fixed-point problem. This because at the pole the function is not small and a linearization cannot be justified. We expect that in the non-linear equation these type of solutions will be suppressed. We therefore ignore these other solutions in the following discussion and always refer to the continuous, bound, high temperature solution.

As a side remark we point out that comparing \( T^{\text{SCDFT}}_c(J=0) \approx 30 \text{K} \) with the solution the Eliashberg equations, the latter predicts a much higher \( T^{\text{Eliash}}_c(J=0) \approx 50 \text{K} \). For a detailed comparison, see Fig. 4 b) where we show the linearized \( T^{\text{SCDFT}}_c(J) \) in the phase diagram of the Eliashberg equations. We also observe via the black curve of Fig. 4 b), that the Eliashberg solutions predict a SC phase that is less susceptible against a splitting. The reason for the lower \( T_c \) prediction is that within the xc-potential construction \( G \) was replaced with \( G^{\text{KS}} \) which violates Migdal’s theorem\(^{11} \). The solution has recently presented by Sanna et al.\(^{25} \) using a corrected self-energy in the functional construction. We will come back to this point and elaborate on the distinction in the Appendix A. As a curious result, the linearized \( T^{\text{SCDFT}}_c(J) \) curve bends upwards and starts an almost linear increase at the point where the transition is expected to become of discontinuous type. We investigate this issue in the next Subsection VA3.

3. Analysis of the \( B_0 \) dependence of \( T_c \)

Using the condition of \( \tilde{S}_\beta \) to be positive definite we compute the \( T_c(J) \) curve of the model (see Fig. 11). At a low field the \( T_c(J) \) curve behaves as expected; the critical temperature is slowly reducing with increasing \( J \). Similar to the Eliashberg results in Sec. IV, the SpinSCDFT pair potential seems to be more resistant against a splitting than the BCS approach predicts.

In the regime of a first order phase transition, where the conditions for a linearization are not met, SpinSCDFT behaves differently as compared to the linear BCS solution of Fig. 3. While in neither case, BCS nor SpinSCDFT, a linearization can be expected to yield sensible results for a discontinuous first order transition, the behavior of the \( T_c(J) \) curve from SpinSCDFT is certainly more unphysical. At high field, past \( J \approx 0.15 \text{mHa} \) the \( T_c(J) \) curve bends outwards and starts an almost linear increase with \( J \).

In figure 11 b), the eigenfunctions to the singular eigenvalues of \( \tilde{S}_\beta \) for increasing \( J \) are plotted. We can clearly observe that the upturn the \( T_c(J) \) curve is accompanied by an increasing localization of \( \Delta_\beta \) at the Fermi level. The usual high energy tail gets more and more suppressed. For very large splittings, \( \Delta_\beta \) becomes numerically noisy.
Reintroducing the Coulomb coupling to \( \hat{S}_\beta \) we observe a similar behavior. In this case \( \Delta_s \) shows a characteristic negative tail induced by the Coulomb renormalization mechanism\(^{26,27} \) as it occurs within SCDF\(^{11,12,28} \). From the comparison between \( T_{c;\text{spinSCDFT}}(J) \) with the green dashed BCS curve in Fig. 11, we note that in the second order regime \( T_{c;\text{BCS}}(J) \) scales down with \( J \) faster. In order to make the strong coupling SpinSCDFT theory more similar to the weak coupling BCS approach we disregard \( S_\beta^S \) in Fig. 11 e) and f). In this case we are only considering the effectively attractive coupling among electrons via phonons, similar to Fröhlich\(^{29} \) and BCS. The effective Fröhlich interaction requires the coupling to be small, and moreover we neglect the phonon influence on the normal state (Nambu diagonal) part of the self-energy entirely. Thus this approximation is called the weak coupling limit. As expected, the resulting \( T_{c;\text{spinSCDFT}}(J)/T_{c;\text{spinSCDFT}}(0) \) and \( T_{c;\text{BCS}}(J)/T_{c;\text{BCS}}(0) \) behave very similarly. Here the \( T_c(J) \) curves shown in Fig. 11 e) also feature the linear increase for high splitting. Moreover we observe a discontinuous jump of the critical temperature at a certain splitting \( J_c \) which is accompanied by the eigenfunction dramatically changing shape. After the jump, the solution does not have a common sign convention but shows positive and negative parts. Also here we find numerically noisy solutions.

The BCS \( T_c(J) \) curve, fitted to the same \( T_c(0\text{mHa}) \), matches the weak coupling SpinSCDFT \( T_c(J) \) curve Fig. 11 e), not the strong coupling curve of Fig. 11 a). This points out that the strong coupling \( S_\beta^S \) term does not simply scale \( T_c(J) \) down equally on both, \( T \) and \( J \) axis. Instead, \( S_\beta^S \) leads to a larger \( T_c(J) \) reduction of the temperature axis. Thus we conclude that strong coupling systems are less affected by an exchange splitting relative to their \( T_c(0\text{mHa}) \).

B. Non-Linear Sham-Schlüter Equation

The previous section has shown the importance to consider the fully nonlinear Sham-Schlüter equation \( S_\beta[J]\Delta_s^0 \). \( \Delta_s^0 = 0 \) of Eq. (6) when working in the limit of strong external field/large exchange splitting \( J \). We solve the
To the common notation for SC in the Appendix A. This approach is similar in time we introduce the one-cycle Dyson equation iteration to the quasi-particle structure at the same computationally convenient DFT scheme and a good approximation to the KS excitations as quasi-particles. In order to have the obtaining \( \chi \) low temperatures (the purple to blue lines in Fig. 14).

To complete the discussion of the \( J \) and \( T \) dependence of SpinSCDFT, we need a characteristic number of a given \( \Delta_s^\varepsilon(J) \) solution. As mentioned, \( \Delta_s^\varepsilon(\varepsilon = 0, J) \) is not a sensible choice, because it neither corresponds to an excitation gap nor is it a measure for the size of the potential \( \Delta_s^\varepsilon(\varepsilon) \).

Instead, we chose \( \int \Delta_s^\varepsilon(\varepsilon)d\varepsilon \) and the resulting SpinSCDFT \( J-T \) diagram of Fig. 12 shows a transition at a point where, from the shape of the non-linear BCS and Eliashberg diagram the first order phase transition is to be expected. However, following this discontinuous transition, the solutions \( \Delta_s^\varepsilon(\varepsilon) \) do not vanish but have a different shape. In Fig. 16, we show the \( \Delta_s^\varepsilon(\varepsilon) \) with increasing splitting on the equal-temperature line at \( T = 10K \) and the transition is clearly seen. In general, while before a critical splitting \( J_c(T) \) the potential is little effected by the splitting, past \( J_c(T) \) the solutions \( \Delta_s^\varepsilon(\varepsilon) \) localize at the \( \Delta_s^\varepsilon(\varepsilon) \) Fermi level and show positive as well as negative regions. This behavior is similar to the shape of the potential from the linearized \( S \) as given in Fig. 11 b). We show the \( T_c(J) \) curve from the linear equation as a dashed blue line in Fig. 12 and see that it marks the border of the appearance of the curious solutions in the non-linear equation past the range in \( J \) of the second order phase transition.

Due to the Coulomb renormalization, including the Coulomb repulsion, \( \int \Delta_s^\varepsilon(\varepsilon)d\varepsilon \) is predominantly negative. Thus, as a physical property, we compute the number of condensed electrons \( N_{SC} = \int \int |\chi(r,r')|^2 \) instead. We show the SpinSCDFT \( J-T \) diagram including the
C. Numerical calculation of the DOS from the G₀W₀ GF

We compute the GF according to the SC G₀W₀ scheme derived in the Appendix A. In detail, we solve the Eq. (A38) using the Eqs. (A23) to (A26) together with the Eqs. (A2) to (A5) for the model and couplings described in Section II. We exclude the Coulomb potential at this point for a better comparison with Eliashberg theory although there is no difficulty to include it.

In Fig. 13 we compute the G₀W₀ corrected DOS at every point in J and T and extract the SC excitation gap. We find that the curious solutions past the transition Jₓ(T) lead to almost no excitation gap. The reason is that for the self-energy in the calculation of the SC DOS in the Appendix A ∆ₚₑ(ε) is integrated in ε. If the high ε region, away from the Fermi level, is strongly suppressed, as in the KS potential past the Jₓ(T), the effect on the excitation gap is negligible.

Comparing with SpinSCDFT G₀W₀ gap of Fig. 13 with the BCS (Fig. 3) and the Eliashberg J − T diagram (4) we conclude that the point of the transition can be clearly identified. Moreover this one-cycle correction sheds light onto the appearance of the Fermi-level localized solutions past the critical field Jₓ(T). We have seen that for small T and J = 0 the non-linear ∆ₚₑ(ε) go to zero at the Fermi level (compare Fig. 14) while the analogue of G₀W₀ GF, the excitation gap of Fig. 13, takes its largest value at T = 0 and shows the expected monotonous decay with temperature to Tₓ.

This implies a significant difference in the quasi parti-
cle states if a splitting occurs with such a $\Delta_\sigma^e(J)$. While the KS particle with the dispersion $E^s_\sigma = \text{sign}(\sigma)J + \alpha \sqrt{\varepsilon^2 + \Delta_\sigma^e(J)^2}$ is strongly altered by the splitting because the Bogoliubov branches change their order (compare the earlier discussion in the conclusion of Sec. V A 1 and in I) this is not the case in the true quasi particle structure. In fact, from Fig. 15, we see that the SC solutions $\Delta_\sigma^e(J)$ if $J > 0$ do not go to zero and, instead, rise with $J$ to prevent this situation. On the other hand, after the discontinuous transition we find $\Delta_\sigma^e(0, J) < J$.

In the functional construction, the replacement $G \rightarrow G^{KS}$ is thus a strong suspect for the occurrence of this curious solutions past the SC transition. This is because $G$ and $G^{KS}$ deviate in that the latter can be non-gapped while still corresponding to a SC solution.

D. Triplet components

The present implementation of SpinSCDFT assumes the spin decoupling approximation, i.e. assumes the pairing to be of spin singlet type (compare Sec. I III A 2.c). However, it was also shown in I that a magnetic splitting creates triplet components in the pairing potential, even for a purely singlet order parameter density. Triplet components appear as an intermediate step, in the self-energy that leads to the G0-functional in I since the Nambu off diagonal upspin and downspin components are in general not equal and of opposite sign. They can be intermediate since such triplet self-energy contributions lead to triplet as well as singlet order parameter contributions. The intermediate triplet self-energy that leads to singlet order parameter contributions can be included in the spin decoupling approximation functional without difficulties. From the theoretical side, this is an unpleasant signature of formal inconsistency. We have, in fact, computed the critical temperature and KS gaps with and without these intermediate triplet self-energy terms. In Fig. V A 2 and Fig. 11, we observe that their effect is negligibly small. The possibility of a triplet condensation, i.e. non-vanishing triplet order parameter contributions, in not investigated further in this work.

E. Extension to real materials

In this work, properties of the free electron gas with a phonon and Coulomb coupling subject to an homogeneous exchange splitting have been calculated. To compute real materials without the use of adjustable parameters, the electron-phonon coupling and the Coulomb potential has to be calculated from first principles. Then, according to the equations (I.122),(I.123) and (I.124) these couplings, as well as the computed single particle states $\varepsilon_{k\sigma}$ may well have a distribution in $J$ different from the homogeneous $J_b = -\mu_0 B_0$ that we are considering here. Also, sometimes, several regions in the Brillouin zone (or: in $k$) have different couplings and a different SC pairing as in the well known case of MgB$_2$.

The isotropic formulation does not have to be given up, often it is enough to group this regions which we refer to as multi-band SC. We extend notation $\varepsilon = (\varepsilon, J, b)$ \[ \int d\varepsilon = \int d\varepsilon \int dJ \sum b \] where $b$ labels the groups of quantum numbers $\{k\}$ sharing similar pairing.

VI. SUMMARY AND CONCLUSION

In this work, we have presented parameter free ab-initio calculations of a superconductor in presence of an homogeneous exchange splitting as for example the result of an external magnetic field. We have used two approaches: A generalization of the Eliashberg approach and SpinSCDFT. SCDFT allows the direct inclusion of Coulomb interactions in a straightforward way, while its direct inclusion remains to be problematic within Eliashberg where one has to rely on the $\mu^*$ approach. The Eliashberg equations, on the other hand, provide the reference for the phononic self-energy, allowing to understand and develop functionals for SpinSCDFT.
We have implemented a code that solves the SpinSCDFT equations with a linear and non-linear xc-potential and the non-linear Eliashberg equations derived in I. The xc functional is derived in I from the Sham-Schlüter equation based on the replacement of the interacting with the SC KS GF. We have investigated the behavior of the xc-potential on a model of a free electron gas with a tunable, homogeneous exchange splitting $J$, a phonon coupling that resembles to the one of MgB$_2$ and, optional, a static Coulomb interaction in the Thomas-Fermi approximation. We compute the SC properties of this system and find that in the regime of a second order phase transition in the $T$ vs $J$ diagram. SpinSCDFT results in a curve that compares similar in shape to the Eliashberg solutions. Removing the contributions in the functional that arise from the normal state (Nambu diagonal) part of the self-energy we arrive at a shape that is very similar to the BCS behavior. Including the Coulomb interaction reduces the critical temperature but otherwise does not largely effect the shape of the $J$ -- $T$ diagram.

In agreement with BCS and Eliashberg, SpinSCDFT predicts a discontinuous transition in $\Delta_s(\varepsilon)$ for large $J$ except that the $\Delta_s(\varepsilon)$ past the transition are not zero but have a curious shape that has positive and negative values. Furthermore, the solutions $\Delta_s(\varepsilon)$ increasingly adopt non-vanishing values more or less only directly at the Fermi level $\varepsilon \approx 0$. In addition, we find that the non-linear SpinSCDFT solutions go to zero at $\varepsilon \approx 0$ for $T \rightarrow 0$ and thus the SC KS GF is not gapped while the interacting and $G_0W_0$ GF is. Since we have noted in I that the low center of energy range is where $\Delta_s(\varepsilon)$ compared with $J$ because the Bogoliubov eigenvalues at $\varepsilon = 0$ read $E_s^\sigma(0,J) = \text{sign}(\sigma)J + \alpha|\Delta_s(0,J)|$ we believe that this range is crucial. In contrast to the ones before the transition, the curious $\Delta_s(\varepsilon)$ past $J$, have $|J| > |\Delta_s(0,J)|$.

We perform a $G_0W_0$ like correction to the GF where we solve the Dyson equation with the same self-energy that we used originally for the $xc$-potential construction. The resulting excitation spectrum (here in the isotropic case the DOS) is gapped and behaves as one would expect for a SC. From this result we conclude that a fitting technique similar to A. Sanna et al.$^{25}$ will allow us to reproduce the $J$ -- $T$ diagram of Eliashber while keeping the possibility to include the Coulomb potential in addition to a numerically simple form where the Matzubara summations can be computed analytically.

The theoretical definition of SC is the existence of a non vanishing order parameter $\chi$ (Eq. I.4), while experimentally SC are usually characterized by the properties of their excitation spectrum, namely the single particle gap at the Fermi level$^{11}$. This can be rather directly extracted from the solution to the Eliashberg equations on the imaginary axis since $\Delta_{s=0}^s(J)$ is closely related this excitation gap itself$^{24}$ and we use it in Fig. 5 for the $J$ -- $T$ diagram.

The SC KS system of SpinSCDFT is designed to reproduce the densities of the interacting system not the quasi particle spectrum. On the other hand, for a normal metal the KS particles are often in good agreement with experiment so that the resulting KS excitation spectrum is used as an approximation to the interacting quasi particle spectrum. With the potential $\Delta_s(\varepsilon)$ of Fig. 14 it turns out in SCDFT, also for the zero field case$^{25}$, this is not always the case, since e.g. for $T \rightarrow 0$ the SC KS system is not gapped.

To predict a proper excitation spectrum without having to solve the Many-Body problem self-consistently we introduce the $G_0W_0$ approximation in the context of SC. This means to solve the Dyson equation once while replacing the interacting GF with the SC KS GF in the self-energy. Here we use the same approximations for the self energy made to arrive at the functional in I which means we use $\Sigma^{KS} = \Sigma[G^{KS}]$ instead of the true self-energy $\Sigma[G]$.

In this Section we work in the isotropic formulation but note that the approach is easily generalized to the anisotropic case. We use the notation $\varepsilon = \varepsilon, J, b$ and the isotropic Dyson equation

$$ G_n(\varepsilon) = \left((G_n^{KS}(\varepsilon))^{-1} + \Sigma_n^{KS}(\varepsilon)\right)^{-1}, \quad (A1) $$

that follows form the assumption that the couplings depend on $k$ via the center of energy $\frac{\varepsilon k - \varepsilon_{k\pm}-\varepsilon}{2} \rightarrow \varepsilon$ and the splitting $\frac{\varepsilon k_{\pm}-\varepsilon_{k\pm}}{2} \rightarrow J$ and the isotropic bands $b$ (that is a set of quantum numbers $\{\vec{k}\}$). We introduce the notation $G_{n\sigma'\sigma}(\varepsilon)\rightarrow I_{\sigma\sigma}(\varepsilon)G_{k\sigma'\pm\pm\pm\pm}(\omega_n)$. The averaging procedure $I_{\sigma\sigma}(\varepsilon)$ on equal splitting and equal center of energy surfaces is defined in Eq. I.120. We refer to the non-vanishing matrix elements with a spin label that refers to the first index of $G_{k\sigma'\pm\pm\pm\pm}(\omega_n)$ and similar for the self-energy.

1. Imaginary Axis Formulation

The inversion of the Dyson Eq. (A1) to compute the GF explicitly is very analogous to the derivation of the Eliashberg equations in I, Sec. I.4.A.1. We compute $G_n(\varepsilon)$ via Eq. (A1) and the non-vanishing components are found to be (suppressing the arguments of $\Delta_{s=0}^s(J)$, $\Sigma_n^{KS}(\varepsilon)$, $\Sigma_f^{KS}(\varepsilon)$, $A_n^{KS}(\varepsilon)$, $\Sigma_n^{KS}(\varepsilon)$, $\Sigma_n^{KS}(\varepsilon)$)
and $\Sigma^{\pm}_n(\epsilon)$

\[
\tilde{G}_{n\sigma}^{i,-1} = \frac{1}{2\tilde{\Sigma}_{n\sigma}} \sum_{\alpha} \frac{\tilde{\Sigma}_{n\sigma} + \alpha (\tilde{\Sigma}_{n\sigma} + \text{sign}(\sigma) \Delta^{\pm}_n)}{\tilde{\omega}_n - \Sigma_n^{\pm} + \text{sign}(\sigma) (J + \Sigma'_n) + \alpha \tilde{\Sigma}_{n\sigma}}
\]

(A2)

\[\tilde{G}_{n\sigma}^{i,-1} = \frac{1}{2\tilde{\Sigma}_{n\sigma}} \sum_{\alpha} \frac{\tilde{\Sigma}_{n\sigma} + \alpha (\tilde{\Sigma}_{n\sigma} - \text{sign}(\sigma) \Delta^{\pm}_n)}{\tilde{\omega}_n - \Sigma_n^{\pm} + \text{sign}(\sigma) (J + \Sigma'_n) + \alpha \tilde{\Sigma}_{n\sigma}}
\]

\[\tilde{G}_{n\sigma}^{i,-1} = \frac{\text{sign}(\sigma)}{2\tilde{\Sigma}_{n\sigma}} \sum_{\alpha} \frac{\alpha \left( \tilde{\Sigma}_{n\sigma} + \i\sigma \Sigma_n^{\alpha} + \text{sign}(\sigma) \left( \Sigma_n^{\alpha} - \i\sigma \Sigma_n^{\alpha} \right) \right)}{\tilde{\omega}_n - \Sigma_n^{\alpha} + \text{sign}(\sigma) (J + \Sigma'_n) + \alpha \tilde{\Sigma}_{n\sigma}}
\]

(A4)

\[\tilde{G}_{n\sigma}^{i,-1} = \frac{\text{sign}(\sigma)}{2\tilde{\Sigma}_{n\sigma}} \sum_{\alpha} \frac{\alpha \left( \tilde{\Sigma}_{n\sigma} - \i\sigma \Sigma_n^{\alpha} + \text{sign}(\sigma) \left( \Sigma_n^{\alpha} + \i\sigma \Sigma_n^{\alpha} \right) \right)}{\tilde{\omega}_n - \Sigma_n^{\alpha} + \text{sign}(\sigma) (J + \Sigma'_n) + \alpha \tilde{\Sigma}_{n\sigma}}
\]

(A5)

with

\[
\tilde{\Sigma}_{n\sigma}(\epsilon) = \left( \epsilon + \Sigma_n^{\pm} + \text{sign}(\sigma) \Delta^{\pm}_n \right)^2 + \left( \Sigma_n^{\alpha} + \i\sigma \Sigma_n^{\alpha} + \text{sign}(\sigma) \left( \Sigma_n^{\alpha} - \i\sigma \Sigma_n^{\alpha} \right) \right) \times \left( \Sigma_n^{\alpha} - \i\sigma \Sigma_n^{\alpha} + \text{sign}(\sigma) \left( \Sigma_n^{\alpha} + \i\sigma \Sigma_n^{\alpha} \right) \right) \frac{1}{2}
\]

(A6)

where the self-energy parts are constructed similar to the Eliashberg theory with the result

\[
\Sigma_n^{\omega} = \frac{1}{4} \sum_{\sigma} \left( \tilde{\Sigma}_{n\sigma}^{KS,1,1} + \tilde{\Sigma}_{n\sigma}^{KS,-1,-1} \right)
\]

(A7)

\[
\Delta_n^{\omega} = \frac{1}{4} \sum_{\sigma} \text{sign}(\sigma) \left( \tilde{\Sigma}_{n\sigma}^{KS,1,1} + \tilde{\Sigma}_{n\sigma}^{KS,-1,-1} \right)
\]

(A8)

\[
\Sigma_n^{J} = \frac{1}{4} \sum_{\sigma} \left( \tilde{\Sigma}_{n\sigma}^{KS,1,-1} + \tilde{\Sigma}_{n\sigma}^{KS,-1,1} \right)
\]

(A9)

\[
\Sigma_n^{J} = \frac{1}{4} \sum_{\sigma} \text{sign}(\sigma) \left( \tilde{\Sigma}_{n\sigma}^{KS,1,1} - \tilde{\Sigma}_{n\sigma}^{KS,-1,-1} \right)
\]

(A10)

\[
\Sigma_n^{J} = \frac{1}{4} \sum_{\sigma} \left( \tilde{\Sigma}_{n\sigma}^{KS,1,-1} + \tilde{\Sigma}_{n\sigma}^{KS,-1,1} \right)
\]

(A11)

\[
\Sigma_n^{J} = \frac{1}{4} \sum_{\sigma} \text{sign}(\sigma) \left( \tilde{\Sigma}_{n\sigma}^{KS,1,-1} - \tilde{\Sigma}_{n\sigma}^{KS,-1,1} \right)
\]

(A12)

\[
\Sigma_n^{\alpha\Delta} = \frac{-1}{4} \sum_{\sigma} \text{sign}(\sigma) \left( \tilde{\Sigma}_{n\sigma}^{KS,1,-1} + \tilde{\Sigma}_{n\sigma}^{KS,-1,1} \right)
\]

(A13)

\[
\Sigma_n^{\alpha\Delta} = \frac{1}{4} \sum_{\sigma} \text{sign}(\sigma) \left( \tilde{\Sigma}_{n\sigma}^{KS,1,-1} - \tilde{\Sigma}_{n\sigma}^{KS,-1,1} \right).
\]

(A14)

Note, however, that $\tilde{\Sigma}_{n\sigma}^{KS,1,-1}$ contains a triplet contribution that is generated by the coupling imbalance of the spin channels. The isotropic variants of the Eqs. (I.66) to (I.69) are given by

\[
\Sigma_{n\sigma}^{KS,1,1} = \int d\Omega \int d\epsilon' \alpha^{2} F_\sigma(\epsilon, \epsilon', \Omega) \times \sum_{\sigma} \frac{\alpha \epsilon' + F'}{2F'} M_{ph}(\Omega, E_{\sigma'} \i\sigma, \omega_n)
\]

(A15)

\[
\Sigma_{n\sigma}^{KS,-1,-1} = \int d\Omega \int d\epsilon' \alpha^{2} F_\sigma(\epsilon, \epsilon', \Omega) \times \sum_{\sigma} \frac{\alpha \epsilon' + F'}{2F'} M_{ph}(\Omega, -E_{\sigma'} \i\sigma, \omega_n)
\]

(A16)

\[
\Sigma_{n\sigma}^{KS,1,-1} = -\text{sign}(\sigma) \int d\Omega \int d\epsilon' \alpha^{2} F_\sigma(\epsilon, \epsilon', \Omega) \times \sum_{\sigma} \frac{\alpha \Delta^{\sigma}_{\epsilon'}}{2F'} M_{ph}(\Omega, E_{\sigma'} \i\sigma, \omega_n)
\]

(A17)

\[
\Sigma_{n\sigma}^{KS,-1,1} = -\text{sign}(\sigma) \int d\Omega \int d\epsilon' \alpha^{2} F_\sigma(\epsilon, \epsilon', \Omega) \times \sum_{\sigma} \frac{\alpha \Delta^{\sigma}_{\epsilon'}}{2F'} M_{ph}(\Omega, -E_{\sigma'} \i\sigma, \omega_n)
\]

(A18)

with $\Delta^{\sigma}_{\epsilon'}$ short hand for $\Delta^{\sigma}_{\epsilon'}(\epsilon')$, the averaged $\Delta^{\sigma}_{\epsilon'}$ and $F' = \sqrt{\epsilon^2 + \Delta^2}$. Furthermore $E_{\sigma'} = \text{sign}(\sigma)J + \text{sign}(\alpha)F'$ and similarly the Eqs. (I.75) and (I.76) become

\[
\Sigma_{c\sigma}^{KS,1,1} = -\text{sign}(\sigma) \sum_{\alpha} \int d\epsilon' \frac{\alpha \Delta^{\sigma}_{\epsilon'}}{2F'} C_{\alpha\sigma}^{stat}(\epsilon, \epsilon') f_\beta(E_{\sigma'})
\]

(A19)

\[
\Sigma_{c\sigma}^{KS,-1,1} = -\text{sign}(\sigma) \sum_{\alpha} \int d\epsilon' \frac{\alpha \Delta^{\sigma}_{\epsilon'}}{2F'} C_{\alpha\sigma}^{stat}(\epsilon, \epsilon') f_\beta(-E_{\sigma'})
\]

(A20)

With these equations we can compute the $G_0W_0$ GF from the results of a converged SpinSCDF calculation.

2. Real Axis Formulation

To obtain the (L)DOS from the temperature GF we substitute

\[
i\omega_n \rightarrow \omega + i\eta
\]

(A21)

where $\eta$ is a real positive infinitesimal$^{35}$. The expression Eqs. (A2) to (A5) remain essentially unchanged on the real axis, except that we have to insert the SE parts Eq. (A7) to (A14) on the real axis and write $i\eta + \omega$ instead of the Matsubara frequency. Here we have two options, first we may compute the SE parts on the imaginary axis and use a numerical analytic continuation to the real axis, or we can compute analytic formulas for the real axis and use them. We choose the latter because this avoids the sometimes unstable analytic continuation.

We will see that the SE parts, e.g. $\Sigma_{n\sigma}^{\alpha\Delta}(\epsilon)$, on the real axis have to be computed via independent calculations.
of imaginary and real part. The dependence on the Matsubara index of the SE is only via the function \( M_{\text{ph}} \) of Eq. (1.73), i.e. the results of the first Matsubara summation in the SE. Thus on the real axis

\[
M_{\text{ph}}(\Omega, E, \omega) = \frac{\hat{P} n_\beta(\Omega) + f_\beta(E)}{\Omega - E + \omega} - \frac{\hat{P} n_\beta(\Omega) + f_\beta(-E)}{\Omega + E - \omega} - i\pi \left( \left( n_\beta(\Omega) + f_\beta(E) \right) \delta(\Omega - E + \omega) \right. \\
\left. + \left( n_\beta(\Omega) + f_\beta(-E) \right) \delta(\Omega + E - \omega) \right). \tag{A22}
\]

Here \( \hat{P} \) is the principle value operator. Because of the very different nature of the imaginary and real part of the SE we compute both parts independently. Then we obtain

\[
\Im \Sigma^\omega(\epsilon, \omega) = -\pi \int d\epsilon' \sum_{\mu \alpha} \frac{\alpha \epsilon' + F'}{8F'} \left( (n_\beta(E_{\mu} - \epsilon' - \omega) + f_\beta(E_{\mu}')) \left( \alpha^2 \delta_{\mu}^\omega(\epsilon', \epsilon + E_{\mu}') - \alpha^2 \delta_{\mu}^\omega(\epsilon, \epsilon' - E_{\mu}') + \right. \right. \\
\left. \left. \left( n_\beta(E_{\mu} + \epsilon' + \omega) + f_\beta(-E_{\mu}') \right) \left( \alpha^2 \delta_{\mu}^\omega(\epsilon, \epsilon' + E_{\mu}') - \alpha^2 \delta_{\mu}^\omega(\epsilon, \epsilon' - E_{\mu}') \right) \right) \right)
\]

\[
\Re \Sigma^\omega(\epsilon, \omega) = \frac{1}{4\pi} \int d\Omega \int d\epsilon' \sum_{\mu \alpha} \frac{\alpha \epsilon' + F'}{8F'} \frac{\alpha^2 \delta_{\mu}^\omega(\epsilon', \epsilon + \Omega)}{\Omega - E_{\mu}' - \omega} \left( \hat{P} n_\beta(\Omega) + f_\beta(E_{\mu}') \right) \left( \hat{P} n_\beta(\Omega) + f_\beta(-E_{\mu}') \right) \\
+ \frac{1}{4\pi} \int d\Omega \int d\epsilon' \sum_{\mu \alpha} \frac{\alpha \epsilon' + F'}{8F'} \frac{\alpha^2 \delta_{\mu}^\omega(\epsilon, \epsilon' + \Omega)}{\Omega + E_{\mu}' + \omega} \left( \hat{P} n_\beta(\Omega) + f_\beta(E_{\mu}') \right) \left( \hat{P} n_\beta(\Omega) + f_\beta(-E_{\mu}') \right)
\]

and very similar for \( A^{\omega,\epsilon}(\epsilon, \omega) \) that only differs from \( \Sigma^\omega \) by putting a sign(\( \mu \)) into the spin sum. We also obtain \( \Sigma^{\epsilon}(\epsilon, \omega) \) from the relation for \( \Sigma^{\epsilon}(\epsilon, \omega) \) in the same way, i.e. we put a sign(\( \mu \)) into the spin sum. The above equation again points out the problem in the \( \epsilon' \) integral if the energy dependence of \( \alpha^2 \delta_{\mu}^\omega(\epsilon, \epsilon' + \Omega) \) is neglected. Here \( E_{\mu}' \to \alpha|\epsilon'| \) for large \( |\epsilon'| \) so there are parts in the integral that behave as \( \frac{1}{\epsilon'} \) leading to logarithmic divergence. Thus we see explicitly that we cannot compute the energy renormalization without considering the influence of the interaction on the full energy spectrum and quasi-particle occupations as was already discussed in I and Ref. 11.

We define the integrand

\[
\Im B_{\pm}(\epsilon, \epsilon', \omega) = \pi \sum_{\mu \alpha} \text{sign}(\mu) \frac{\alpha \epsilon' + F'}{2F'} \left( n_\beta(E_{\mu} - \epsilon' - \omega) + f_\beta(E_{\mu}') \right) \times \left( \alpha^2 \delta_{\mu}^\omega(\epsilon, \epsilon' + \Omega) - \alpha^2 \delta_{\mu}^\omega(\epsilon, \epsilon' - \Omega) \right)
\]

\[
\Re B_{\pm}(\epsilon, \epsilon', \omega) = -\sum_{\mu \alpha} \text{sign}(\mu) \frac{\alpha \epsilon' + F'}{4F'} \left( \int d\Omega \alpha^2 \delta_{\mu}^\omega(\epsilon, \epsilon' + \Omega) \times \left( \hat{P} n_\beta(\Omega) + f_\beta(E_{\mu}') \right) \times \left( \hat{P} n_\beta(\Omega) + f_\beta(-E_{\mu}') \right) \right)
\]

\[
+ f_\beta(E_{\mu}') \delta(\epsilon, \epsilon') \right) \right)
\]
and further introducing

\[ B_{n}^{\alpha}(\epsilon) \equiv \Sigma_{n}^{\alpha}(\epsilon) + i\Sigma_{n}^{\alpha}(\epsilon) \quad (A29) \]
\[ B_{n}^{\alpha*}(\epsilon) \equiv \Sigma_{n}^{\alpha}(\epsilon) - i\Sigma_{n}^{\alpha}(\epsilon) \quad (A30) \]
\[ B_{n}^{\alpha+}(\epsilon) \equiv \Sigma_{n}^{\alpha+}(\epsilon) + \Sigma_{n}^{\alpha-}(\epsilon) \quad (A31) \]
\[ B_{n}^{\alpha*+}(\epsilon) \equiv \Sigma_{n}^{\alpha+}(\epsilon) - \Sigma_{n}^{\alpha-}(\epsilon) \quad (A32) \]

we obtain the following equations on the real axis

\[ B^{s}(\epsilon, \omega) = \int d\epsilon' \Delta_{s}^{s} B_{-}(\epsilon, \epsilon', \omega) \quad (A33) \]
\[ B^{s*}(\epsilon, \omega) = \int d\epsilon' \Delta_{s}^{s*} B_{-}(\epsilon, \epsilon', \omega) \quad (A34) \]
\[ B^{t}(\epsilon, \omega) = \int d\epsilon' \Delta_{s}^{t} B_{+}(\epsilon, \epsilon', \omega) \quad (A35) \]
\[ B^{t*}(\epsilon, \omega) = \int d\epsilon' \Delta_{s}^{t*} B_{+}(\epsilon, \epsilon', \omega) \quad (A36) \]

and thus, Eq. (A6) becomes on the real axis (omitting the arguments \(\epsilon, \omega\))

\[ \tilde{\sigma}_{\sigma} = \left( (\epsilon + \Sigma_{\epsilon} + \text{sign}(\sigma) A_{\sigma}^{\epsilon})^{2} + (B_{\sigma}^{s} + \text{sign}(\sigma) B_{\sigma}^{t}) (B_{\sigma}^{s*} + \text{sign}(\sigma) B_{\sigma}^{t*}) \right)^{1/2}. \quad (A37) \]

Now we can finally obtain the retarded GF with the equations from Eqs. (A2) to (A5) together with Eq. (A6) for \(\tilde{\sigma}_{\sigma}(\epsilon)\) in terms of \(B\) and the corresponding SE parts constructed from real and imaginary part close to the real axis. Then we can evaluate the DOS according to

\[ \rho_{\alpha}(\omega) = -2 \int d\epsilon \delta(\omega - \epsilon) \lim_{\eta \to 0} \lim_{\epsilon \to \omega} G_{n\sigma}(\epsilon) \phi(\epsilon) \quad (A8) \]

We obtain the local DOS \(\rho_{\alpha}(\omega, r)\) simply by replacing \(\phi(\epsilon)\) with the local double DOS \(\phi_{r}(\epsilon, r) = \int_{k_{\sigma}} \phi(\epsilon, \mathbf{r})|^{2}\).

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