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First-principles based theory of spin-orbit coupling induced triplet pairing: Application to the superconducting ground state of rhenium

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Abstract – Recent μSR measurements revealed that spontaneous magnetism exists in the superconducting state of rhenium and it also appears in other rhenium based materials like Re6Zr, Re6Hf, Re6Ti. The superconducting state of these materials show s-wave-like properties and the pairing mechanism is most likely driven by electron-phonon coupling. In this paper we take elemental rhenium as a testbed and investigate its ground state. By developing an LCAO formalism for the solution of the spin-generalized Bogoliubov-de Gennes equation we use every details of the first-principles band-structure together with spin-orbit coupling. In this paper we provide a possible explanation of the spontaneous time-reverseal symmetry breaking in the superconducting ground state of rhenium by arguing that taking into account the orbital degrees of freedom, spin-orbit coupling is inducing even-parity odd-orbital spin triplet Cooper pairs, and Cooper pairs' migration between the equal-spin triplet states may lower the total energy. We show how magnetism emerges and the structure of the gap changes as a function of the triplet component of the interaction strength.

In condensed matter theory ferromagnetism serves as the basic example for spontaneously broken time-reverseal symmetry (TRS). In the Stoner model, the shift between the different spin branches carries a cost in kinetic energy and a gain in Coulomb energy. When the Coulomb gain dominates, the ferromagnetic phase transition occurs spontaneously through electron migration between the down-spin and up-spin Fermi surfaces. This simple picture relates ferromagnetism to higher density of states at the Fermi level. It has recently been argued that a similar mechanism, involving Cooper pair migration instead of migration of individual electrons, may cause spontaneous magnetization in non-unitary triplet superconductors [1-4]. In contrast, conventional superconductivity and magnetism are considered to be incompatible.

Here we investigate theoretically the possibility of a similar phenomenon in the ground state of elemental rhenium. This system is believed to be a conventional superconductor [5] yet recently, and surprisingly, experimental evidence has been found that its superconducting state breaks time-reversal symmetry (TRS) [6]. Our calculation describes the superconducting ground state of rhenium taking into account the quantitative details and complexity of its band structure, including multi-orbital physics and Spin-Orbit Coupling (SOC). For this purpose we have developed a Linear Combination of Atomic Orbitals (LCAO) formalism (in SIESTA [7-9]) to solve the spin-generalized Bogoliubov-de Gennes (SBdG) equations [10]. We introduce superconductivity via a conven-
tional, BCS-like pairing potential which matches the correct value of the energy gap $\Delta$. We find that through non-linear couplings induced by SOC an additional order parameter emerges in the triplet channel. We introduce a pairing interaction in this additional channel and investigate the ground-state phase diagram as a function of its strength $\Lambda_{sOT}$, treated as an adjustable parameter. We discuss the implications of our results for the interpretation of the recent experiments [6].

Broken time-reversal symmetry (TRS) has been discovered in many superconductors [4,11], chiefly using muon-spin relaxation ($\mu$SR), confirmed in some cases by SQUID magnetometry and/or the optical Kerr effect. Examples include heavy-fermion superconductors like UBe$_{13}$, UP$_{13}$, Sr$_2$RuO$_4$, filled skutterudites, filled La$_7$(Ir, Rh)$_1$[14, 15], the La-Ni based triplet superconductors LaNiC$_2$ [16] and LaNiGa$_2$ [1] and the Re-based systems Re$_6$ [17] and Re$_0$[18]. Elemental Re and Re$_0$$_0$Nb$_2$$_0$$_0$ [6].

The standard symmetry analysis [32] implies that the order parameter at the superconducting critical temperature $T_c$ must correspond to one of the irreducible representations of the symmetry group of the crystal. While this often leaves open many possibilities, in the cases of La$_7$(Ir, Rh)$_1$, Re$_6$, and Re$_0$[18] whose crystal structures have very low symmetry it constrains the available pairing states greatly. Coupled to the observation of nodeless, two-gap behaviour in both systems [3,33] it led to the proposal of an equal-spin triplet pairing function with even parity under momentum reversal $\mathbf{k} \rightarrow -\mathbf{k}$ but odd parity under orbital exchange [3]. This internally-antisymmetric nonunitary triplet (INT) theory has been shown to be in quantitative agreement with experiments [4] and predicts an unusual spin-splitting of the electronic Density of States (DOS) [4]. The Re-based TRS breaking superconductors are also multi-band and fully-gapped suggesting similar physics may be at play. On the other hand, in these systems there are other symmetry-allowed possibilities and physics may be at play. On the other hand, in these systems there are other symmetry-allowed possibilities and there is no two-gap behaviour as would be expected in a Cooper pair migration scenario. This has led to other proposals including the loop super-current (LSC) scenario which requires several distinct, but symmetry-related sites within the unit cell [34,35]. The LSC scenario, however, does not naturally apply to elemental rhenium due to its simpler crystal structure. Here we revisit an INT-type theory for the case of rhenium - specifically, the coexistence of INT pairs with conventional singlet pairing.

First we describe the normal state band structure of rhenium. All our calculations are carried out with the SIESTA package [7], which we generalized for the superconducting state (see in the Supplemental Material). Rhenium has a hexagonal close-packed crystal structure with Space Group P6$_3$/mmc (No. 194) and lattice parameters $a = b = 278.1$ pm and $c = 449.7$ pm [36]. There are two atoms in the unit cell (shown in Fig. 1) together with the corresponding coordinate system), and the Re atoms fill the Wyckoff positions of 2c site: $(1/3,2/3,1/4)$ and $(2/3,1/3,3/4)$. In order to achieve a sufficiently quantitative description of the band structure we have used a double-zeta polarized basis set involving 30 atomic orbitals of the rhenium atom. The electronic exchange-correlation energy is treated in the Local Spin Density Approximation (LSDA) with the Ceperley-Alder exchange-correlation energy functional [37]. Norm-conserving pseudopotentials are used for interactions between ions and electrons. The Brillouin zone is sampled using the Monkhorst-Pack scheme with $(24 \times 24 \times 24)$ k-points for the electronic properties in the normal state.

The orbitals which contribute most significantly to the Fermi surface are the Re 5$d$ and 6$p$ orbitals and their contribution is summarized quantitatively in Table 1. The calculated DOS for one spin at the Fermi level is 0.454 states/eV/unit cell not significantly different from the value of 0.37 states/eV/unit cell found in Ref. [38]. The Fermi surface is shown in Fig. 2. It contains five sheets, including closed-hole sections (Fig. 2a-c), an open electron sheet (Fig. 2d), and a closed electron piece (Fig. 2e) which is in good agreement with the results published in Ref. [38]. Since the hexagonal close-packed structure contains two atoms per unit cell, the total number of electrons and holes must be equal. In Fig. 2 the Fermi velocities $v_F$ are also shown [39] and reflects a significant anisotropy.

Quite generally, the superconducting order parameter (spin-dependent anomalous density) is given by

$$\chi^{\alpha \beta}(\mathbf{r}, \mathbf{r}') = \langle \Psi^\alpha(\mathbf{r}) \Psi^\beta(\mathbf{r}') \rangle$$

where $\alpha, \beta$ are spin indices (\uparrow) and $\Psi^\alpha(\mathbf{r})$ is annihilation field operator for an electron with spin $\alpha$ at $\mathbf{r}$. In order
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Fig. 2: (Color online) Fermi surface sheets (a-e) and the merged Fermi surface (f) of rhenium with the absolute value of Fermi velocities (in atomic units) superimposed as a color scale.

to describe superconductivity we add to the exchange-correlation functional $\Omega_{xc}[\rho, \mathbf{m}]$ a quadratic term in the order parameter:

$$
\Omega_{xc}[\rho, \mathbf{m}, \chi] = \Omega_{xc}^{\text{LSDA}}[\rho, \mathbf{m}]
- \int \! \! d\mathbf{r} \int \! \! d\mathbf{r}' \int \! \! d\mathbf{x} \int \! \! d\mathbf{x}' \sum_{i,j=S,T,\Lambda,T'} \chi_i^x(\mathbf{r}, \mathbf{r}'; \Lambda) \Lambda_j^{\Lambda}(\mathbf{r}, \mathbf{r}' \cdot \mathbf{x}, \mathbf{x}') \chi_j^x(\mathbf{x}, \mathbf{x}').
$$

Here $\Omega_{xc}^{\text{LSDA}}[\rho, \mathbf{m}]$ is the normal-state exchange-correlation functional in the local spin-density approximation (LSDA) and we have introduced the Balian-Werthamer parametrisation of the order parameter in singlet ($S$) and triplet ($T$) components, $\chi = [\chi^S + \chi^T, \sigma] \Lambda \sigma_y$, where $\chi^T = (\chi^{T_x}, \chi^{T_y}, \chi^{T_z})$ and $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ ($\sigma_i$ is the $i$th Pauli matrix). Due to fermionic antisymmetry the order parameter $\chi$ is odd under the exchange of all the labels of the two electrons. It follows that the singlet component $\chi^S$ and the triplet component $\chi^T$ must be even and odd, respectively, under the exchange or the particle coordinates. In the absence of SOC this precludes mixed singlet-triplet pairing whereas when SOC cannot be neglected they can in principle coexist - irrespective of whether the crystal has a centre of inversion. At the superconducting transition temperature, however, a further distinction emerges: due to the requirement that the superconducting instability corresponds to an irreducible representation of the point group of the crystal, the order parameter just below $T_c$ must have a well-defined parity under the exchange of coordinates, which means that it must be either purely-singlet or purely-triplet. Nevertheless in the ground state non-linear mixing of singlet and triplet may occur in both centrosymmetric and noncentrosymmetric superconductors. It is that possibility that we investigate here.

In a single-band system even and odd under coordinate exchange is the same as, in reciprocal space, even and odd, respectively, under the parity operation $\mathbf{k} \rightarrow -\mathbf{k}$. In contrast, for multi-orbital superconductors one also has to consider the symmetry under exchange of orbital indices and there are in total 4 possibilities (ignoring odd-frequency pairing) which are summarised in Table 2.

Note that the overall Parity × Orbital symmetry is still always even for the singlet component and odd for the triplets, meaning that the above arguments about mixing of singlet and triplet in centrosymmetric vs noncentrosymmetric superconductors still apply. Nevertheless the extra freedom to achieve the correct symmetry of the wave function by using the orbital index allows interesting phenomena, including purely-triplet states that possess BCS-like features such as a fully-gapped spectrum (the case of the INT state [3,4]). Here we enquire about the possibility of mixed singlet-triplet states with full gap and broken TRS in rhenium.

<table>
<thead>
<tr>
<th>Parity</th>
<th>Orbital</th>
<th>Spin</th>
<th>Product</th>
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<td>Odd</td>
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<td>Triplet</td>
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Table 2: Symmetry classes of even-frequency Cooper pairs

For elemental rhenium the symmetry analysis which could pin down the possible structures of the order parameter is complicated by the non-symmorphic structure [6]. Nevertheless in view of the BCS-like properties reported for this material [5], our starting point (working in a localised atomic orbital basis) is a local, on-site, intra-orbital, site- and $\mathbf{k}$-independent pairing potential $\Delta$ leading to a finite anomalous density [1]. Thus we do not aim to describe the gap anisotropy which would require introducing the effect of electron-phonon coupling into the band structure [43,45]. The technical details of the calculation are given in the Supplemental Material and here we describe our results.

Given its large SOC, rhenium has been used as a platform to build hybrid systems with nanoscale iron islands which host Majorana fermions [11,22]. These experiments did not reveal significant gap anisotropy of rhenium, supporting our assumption of a constant $\Delta$ in the singlet channel.
between every pair of Re inter-orbital with the same strength, in absolute value, EOT attraction takes place on-site, however this one is

We solve the SBdG equations with SIESTA using the observed constant pairing potential $\Delta = 0.28$ meV \cite{11} in the spin singlet channel. The Brillouin zone is sampled again using the Monkhorst-Pack scheme, however much finer $k$-mesh is needed regarding the small value of the superconducting gap, namely we used $(240 \times 240 \times 240)$ $k$-points. Interestingly, the self-consistent solution of the Bogoliubov-de Gennes equations yields finite anomalous density in the EOT channel in addition to the expected EES pairing (using the abbreviations in Table 2). We speculate that this is a similar effect to how SOC can induce spin polarization in nonmagnetic 3D crystals when the inversion symmetry is not broken since spin polarization effects originate fundamentally from specific atomic site asymmetries, rather than from the asymmetry of the crystal space–group \cite{46}. We have found that around 9% percent of the spin singlet anomalous charge is mixed into the EOT channel in equal rates into the $S_z = 1, 0, -1$ triplet components (this ratio is obtained from integrating the anomalous densities in the Brillouin zone). In Fig. 3, we have plotted the distribution of the mixing in the orbital basis which shows correlation with the partial DOS, namely the larger DOS indicates more mixed triplet charge on the corresponding orbitals.

The presence of EOT pairing alongside the expected EES suggests that our original kernel interaction was too simplistic. Indeed SOC is expected to mix the interaction into the triplet channel \cite{47}. We thus introduce an additional interaction strength $\Lambda_{EOT}$ corresponding to EOT states as a phenomenological parameter. We assume the EOT attraction takes place on-site, however this one is inter-orbital with the same strength, in absolute value, between every pair of Re $d$ orbitals shown in Fig. 3. We assume different values of $\Lambda_{EOT}$ and solve the SBdG equations self-consistently, calculating the quasiparticle DOS and the size of the magnetic moment. The results are shown in Fig. 4. We find four distinct ground states: in the first phase (Fig. 4a), for small values of $\Lambda_{EOT}$, the fully gapped structure is preserved. Above a certain value of $\Lambda_{EOT}$ the profile of DOS becomes parabolic which is a clear sign of point nodes appearing in the gap structure (Fig. 4b) but there is still no magnetism (Fig. 4c). Such a gap structure would be manifested in the specific heat following power law for small temperatures, which is not observed \cite{5}. More interestingly above $\Lambda_{EOT} = 0.38$ eV we find different charges corresponding to the $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ EOT states (Fig. 4b) and a net magnetization (Fig. 4e). Moreover, the magnetised superconducting state is also separated into two phases indicated by two types of gap structures (Figs. 4c and d). Both magnetic phases are fully gapped but they are significantly different. We found a narrow region of $\Lambda_{EOT}$ where the underlying reason for magnetism is the shift between the two gaps in the two different spin channels (Fig. 4d). The state at higher values of $\Lambda_{EOT}$ is similar to the INT state believed to be realised in LaNiGa$_2$ \cite{4} and LaNiC$_2$ \cite{18}, where magnetism emerges from different gap sizes in the different spin channels (Fig. 4). However, the two gaps do not resolve perfectly in the spin up and spin down channels here due to the presence of coupling between the spin channels by both the singlet pairing potential and spin-orbit coupling. In Fig. 4(d) the size of the magnetic moment is shown as a function of the EOT interaction strength $\Lambda_{EOT}$. Note that the crossing between the two magnetic phases is indicated by a concave-to-convex function transition. The intermediate magnetic Phase III has to our knowledge never been observed before in calculations and is one of our main results.

In LaNiC$_2$ and LaNiGa$_2$ it was shown that a purely triplet INT state (an EOT state in the language of Table 2) is compatible with the experimental observations \cite{13,4,49}. The difference with rhenium is that here the pairing takes place principally in the singlet channel and the triplet pairing is a (non-negligible) perturbation. That a fully-gapped, TRS-breaking ground state can still be obtained under these circumstances is our other main result. Furthermore, in both cases Cooper pair migration is the underlying physical reason for net magnetism which lowers the total energy. The idea of Cooper pair migration between equal-spin triplet states was introduced by K. Miyake in Ref. \cite{2} for Sr$_2$RuO$_4$ and it is the microscopic mechanism behind the generic coupling of triplet pairing to magnetisation discussed in Ref. \cite{1}.

The presence of an EOT pairing density even in the absence of an EOT pairing interaction justifies the introduction of the additional, phenomenological parameter $\Lambda_{EOT}$. Extending our calculations to finite temperature would be a highly desirable next step. Since our EES and EOT states have different symmetry under inversion, in general they will have different critical temperatures, whereas a single critical temperature is observed experimentally. On the other hand the EOT state might act as a subdominant order parameter - similarly to the relationship between triplet pairing and magnetisation in LaNiGa$_2$ \cite{1}.
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Fig. 4: (Color online) Electronic density of states in the superconducting states of rhenium corresponding to the four phases (a-d) and the magnetic moment as a function of the interaction strength in the triplet channel (e) where the phases are separated with vertical dashed lines. SOC is inducing Even-parity Odd-orbital spin Triplet (EOT) states which is coupled back to the SBdG equations with the EOT interaction strength treated as a phenomenological tunable parameter. The self-consistent solutions for the EOT states reveal four phases: a) fully gapped quasiparticle spectrum without magnetization ($\Lambda_{EOT} < 0.1$ eV), b) nodal gap structure with point nodes without magnetization (0.1 eV $< \Lambda_{EOT} < 0.38$ eV), c) fully gapped quasiparticle spectrum with shifted spin-resolved Von-Hove peaks leading to net magnetization (0.38 eV $< \Lambda_{EOT} < 0.6$ eV), d) fully gapped quasiparticle spectrum with two different spin-polarized gap sizes leading to net magnetization ($\Lambda_{EOT} > 0.6$ eV). The plots in panels (a-d) correspond to $\Lambda_{EOT} = 0.0546$ eV, 0.218 eV, 0.437 eV and 0.820 eV, respectively.

The investigation of singlet-triplet mixing in centrosymmetric materials is in its infancy. We mention that Spin- and Angle-Resolved Photoemission Spectroscopy measurements [50] already suggested the coexistence of spin singlet and spin triplet Cooper pairs in case of Sr$_2$RuO$_4$ (which has centrosymmetric crystal structure) which could be responsible for the observed Knight shift related to in-plane fields [51]. Similar effect was also proposed in Ref. [52].

In this paper we have shown a possible explanation for the time-reverseal symmetry breaking in the superconducting ground state of s-wave-like, fully gapped superconductors with significant SOC by taking rhenium as a testbed for our investigations. Instead of the traditional
route of ignoring the microscopic complexity of Fermi surfaces, we considered the first-principles electronic band structure of rhenium which has five bands crossing the Fermi level. We have modeled the superconducting state by taking the experimental gap in the spin singlet channel for the solution of the SBdG equations, treating spin-orbit coupling on the same footing both in the normal and in the superconducting state. Spin-orbit coupling induced significant even-parity odd-orbital spin triplet states (the mixing ratio is 9% compared to the spin singlet component). In our theory the triplet component of the pairing interaction \( \Lambda_{EOT} \) is introduced phenomenologically and its origin is uncertain. It is known that the presence of SOC (which as we have seen gives rise to the anomalous triplet densities even without a triplet interaction) can conspire with electron-phonon correlations to give rise to triplet pairing [47]. It is also known that Hund’s coupling can induce EOT states [53,54], so spin-orbit coupling could be crucial but may not be the only cause for the appearance of EOT states. By solving self-consistently the SBdG equations we have found magnetic phases above a certain value of the triplet pairing interaction \( \Lambda_{EOT} \) with fully gapped structures in agreement with the experimental result. The desirable step is to quantitatively account for the spontaneous TRS breaking in rhenium which requires finite temperature calculations including the specific heat based on a more sophisticated exchange correlation functional.

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Supplemental Material. — The spin-generalized form of the Bogoliubov-de Gennes (SBdG) equations is required if we would like to include the effects of magnetism, spin-orbit coupling, and it is also necessary for the description of unconventional (non-s-wave) superconductivity. Recent studies [3,4,18,55–65] in several materials, including the Iron based superconductors, half-Heusler compounds, UPt3 and Sr3RuO4 and other recently discovered TRS breaking superconductors have also pointed out the importance of orbital degrees of freedom of electrons in determining the superconducting order parameter. An important observation is that the appearance of unconventional pairing scenarios does not always lead to TRS breaking suggesting that the microscopic details of the Fermi surface are crucial in understanding the relation between magnetism and superconductivity. Therefore the Linear Combination of Atomic Orbitals (LCAO) method as implemented in the SIESTA package seems to be a great candidate to combine different pairing models of superconductors based on their first-principles band structure. Here we provide the details of the LCAO formalism for the solution of the SBdG equations allowing the combination of the first-principles band structure with different pairing models describing the superconducting state.

Spin density-functional theory for superconductors. As a consequence of the anticommutation rules, the superconducting order parameter [Eq. (1) in the article] obeys

\[
\chi^{\alpha\beta}(r,r') = -\chi^{\beta\alpha}(r',r). \tag{3}
\]

The following Balian-Werthamer (BW) representation of the superconducting order parameter will be used:

\[
\chi(r,r') = \begin{pmatrix}
X^S(r,r') \\
X^T_x(r,r') \\
X^T_y(r,r') \\
X^T_z(r,r')
\end{pmatrix}, \tag{4}
\]

where

\[
X^S(r,r') = \frac{\chi^\downarrow\downarrow(r,r') - \chi^\uparrow\uparrow(r,r')}{2}, \tag{5a}
\]

\[
X^T_x(r,r') = \frac{\chi^\downarrow\downarrow(r,r') - \chi^\uparrow\uparrow(r,r')}{2}, \tag{5b}
\]

\[
X^T_y(r,r') = \frac{\chi^\downarrow\downarrow(r,r') + \chi^\uparrow\uparrow(r,r')}{2i}, \tag{5c}
\]

\[
X^T_z(r,r') = \frac{\chi^\downarrow\downarrow(r,r') + \chi^\uparrow\uparrow(r,r')}{2}. \tag{5d}
\]

The order parameter of a spin singlet superconductor is symmetric under parity inversion and antisymmetric under the exchange of spin labels, while the order parameter of a triplet superconductor is antisymmetric under parity.
inversion and symmetric under the exchange of spin labels. Hence,
\[ \chi'(r, r') = (-1)^{\Pi_i} \chi'(r', r), \]
(6)
where \( \Pi_i = 0 \) for the spin singlet component \( (i = S) \) and \( \Pi_i = 1 \) for the spin triplet component \( (i = (T_x, T_y, T_z)) \). However in the orbital basis this statement needs more clarification and in fact taking into account the orbital degrees of freedom it is entirely possible that even in an inversion-symmetric crystal spin singlet and spin triplet superconductivity do coexist. There is evidence that in noncentrosymmetric superconductors spin-orbit coupling can mix singlet and triplet states \[66, \]
however such mixing effect was also suggested by ARPES measurements for the centrosymmetric crystal of \( \text{Sr}_2\text{RuO}_4 \) \[50. \]

The concept of spontaneously broken gauge symmetry caused by superconducting order parameter can easily be introduced in the framework of density functional theory. By introducing the grand canonical potential \( \Omega[\rho, \mathbf{m}, \chi] \) as a functional of the charge density \( \rho(r) \), the magnetization density \( \mathbf{m}(r) \), and the anomalous density \( \chi(r, r') \), it can be shown that it is minimized by
\[ \rho(r) = \sum_{\alpha, n} f(\varepsilon_n) |u_n^\alpha(r)|^2 + \sum_{\alpha, n} f(-\varepsilon_n) |v_n^\alpha(r)|^2, \]
(7a)
\[ m_{\{x,y,z\}}(r) = \sum_{\alpha, \beta, n} f(\varepsilon_n) u_n^\alpha(r) v_n^\beta(r) \] \[ + \sum_{\alpha, \beta, n} f(-\varepsilon_n) u_n^\beta(r) v_n^\alpha(r)^*, \]
(7b)
\[ \chi^{\alpha\beta}(r, r') = \sum_{\alpha, \beta, n} f(\varepsilon_n) u_n^\alpha(r) v_n^\beta(r')^* + \sum_{\alpha, \beta, n} f(-\varepsilon_n) u_n^\beta(r) v_n^\alpha(r')^*, \]
(7c)
with the following orthonormality and completeness relations
\[ \sum_{\alpha} \int dr [u_n^\alpha(r)^* u_n^\alpha(r) + v_n^\alpha(r)^* v_n^\alpha(r)] = \delta_{mn}, \]
(8a)
\[ \sum_{\alpha} \int dr [u_n^\alpha(r)^* u_n^\beta(r) + v_n^\alpha(r)^* v_n^\beta(r)] = 0, \]
(8b)
\[ \sum_n [u_n^\alpha(r) u_n^\alpha(r')^* + v_n^\alpha(r) v_n^\alpha(r')^*] = \delta^{\alpha\beta}(r - r'), \]
(8c)
\[ \sum_n [u_n^\alpha(r) v_n^\beta(r')^* + v_n^\alpha(r) u_n^\beta(r')^*] = 0. \]
(8d)
Here \( f(\varepsilon_n) \) is the Fermi-Dirac function describing the occupation of electrons, while \( 1 - f(\varepsilon_n) = f(-\varepsilon_n) \) describes the occupation of holes. \( u_n^\alpha(r), v_n^\beta(r) \) are the electron and hole components (respectively) of the following

Bogoliubov-de Gennes eigenvalue problem
\[ \int dr' \hat{H}_{\text{BdG}}(r, r') \begin{pmatrix} u_n^\alpha(r') \\ v_n^\alpha(r') \\ u_n^\beta(r') \\ v_n^\beta(r') \end{pmatrix} = \varepsilon_n \begin{pmatrix} u_n^\alpha(r) \\ v_n^\alpha(r) \\ u_n^\beta(r) \\ v_n^\beta(r) \end{pmatrix}, \]
(9)
where
\[ \hat{H}_{\text{BdG}}(r, r') = \left( \hat{H}_c(r) \delta(r - r') - \Delta_{\text{eff}}(r, r') \right), \]
(10)
and
\[ \hat{H}_c(r) = \left( -\nabla^2 + V_{\text{eff}}(r) - \mu \right) \hat{u}_2 + \hat{\sigma} \mathbf{B}_{\text{eff}}(r) + \hat{V}_{\text{PS}} + \hat{H}_{\text{rel}}, \]
(11)
\( \mu \) is the chemical potential, \( \hat{\sigma} \) are the Pauli matrices and \( \hat{H}_{\text{rel}} \) contains the scalar-relativistic and spin-orbit coupling terms. The relativistic contributions related to the pairing potential (anomalous Darwin term, anomalous spin-orbit coupling) will be neglected due to their very small values \[67,68. \]

The effective single-electron potential \( V_{\text{eff}}(r) \), exchange field \( \mathbf{B}_{\text{eff}}(r) \), and the effective (complex) pairing potential \( \Delta_{\text{eff}}(r, r') \) are determined by
\[ V_{\text{eff}}(r) = \int \frac{\rho(r')}{|r - r'|} dr' + \frac{\delta \Omega_{\text{ext}}[\rho, \mathbf{m}, \chi]}{\delta \rho(r)} \]
(12a)
\[ \mathbf{B}_{\text{eff}}(r) = \mathbf{B}_{\text{ext}}(r) + \frac{\delta \Omega_{\text{ext}}[\rho, \mathbf{m}, \chi]}{\delta \mathbf{m}(r)}, \]
(12b)
\[ \Delta_{\text{eff}}(r, r') = \sum_{i=S, T_x, T_y, T_z} d_i(r, r') \sigma_i \delta \sigma_y, \]
(12c)
\[ d_i(r, r') = d^i_{\text{ext}}(r, r') + \frac{\delta \Omega_{\text{ext}}[\rho, \mathbf{m}, \chi]}{\delta \chi(r, r')^*}, \]
(12d)
where \( \mathbf{B}_{\text{ext}}(r) \) is the external exchange field, and the effective pairing potential \( \Delta_{\text{eff}}(r, r') \) is recasted according to the BW representation of the superconducting order parameter. Here \( \sigma_i \) labels the spin singlet and triplet components in the BW representation. The notations \( \sigma_S, \sigma_{T_x}, \sigma_{T_y}, \sigma_{T_z} \) represent, respectively, the \( 2 \times 2 \) identity matrix and the \( \sigma_x, \sigma_y, \) and \( \sigma_z \) Pauli matrices. \( d^i_{\text{ext}}(r, r') \) may be regarded as an external pairing potential. However, this external field only acts to break the symmetry (here the gauge symmetry) of the system. This is a merely mathematical tool and does not have physical meaning. (Practically, it always goes to zero during the self-consistent cycles. This scheme is analogous to introducing a weak magnetic field to fix the direction of spontaneous magnetization of a ferromagnet.)

The SBdG equation has the particle-hole symmetry, namely, by replacing the eigenvector \( [u_n(r), v_n(r)]^T \) in the
spin-generalized BdG equation with \( [\mathbf{v}^*(\mathbf{r}), \mathbf{u}^*(\mathbf{r})]^T \) leads to the to the equivalent negative eigenvalue \(-\varepsilon_\mathbf{m}\). It shall be noted that this symmetry is different from the non-relativistic, non-magnetic case for spin singlet superconductors, since singlet pairing is mixing different spin channels close to the Fermi level. However, by investigating the different spin branches without exchange field and triplet components, the original \((4 \times 4)\) SBdG Hamiltonian is decoupled and separated into a pair of BdG Hamiltonians \((2 \times 2)\) which has the expected particle-hole symmetry, namely the replacement of the eigenvector \([u^\alpha_n(\mathbf{r}), v^\alpha_n(\mathbf{r})]^T\) with \([-v^\alpha_n(\mathbf{r})^*, u^\alpha_n(\mathbf{r})^*]^T\) leads to the equivalent negative eigenvalue.

It is also noteworthy that the superconducting order parameter \(\chi(\mathbf{r}, \mathbf{r'})\) should not be confused with the pairing potential \(d(\mathbf{r}, \mathbf{r'})\). In general, e.g. in a heterostructure, \(\chi(\mathbf{r}, \mathbf{r'})\) can exist in a crystal even in the case of \(d(\mathbf{r}, \mathbf{r'}) = 0\), since the proximity effect induces the superconducting order parameter \(\chi(\mathbf{r}, \mathbf{r'})\) but not the pairing potential \(d(\mathbf{r}, \mathbf{r'})\).

By construction the vector \(d(\mathbf{r}, \mathbf{r'})\) describing the pairing potential has the same symmetry properties as the superconducting order parameter \(\chi(\mathbf{r}, \mathbf{r'})\). Therefore, in case of triplet superconductors \(d(\mathbf{r}, \mathbf{r'})\) can not be local in real space because of the antisymmetric behaviour, while this approximation can be made in conventional, s-wave superconductors. It should be noted that the singlet \(d_S(\mathbf{r}, \mathbf{r'})\) transforms as a scalar under rotation, while \((d_{T_x}(\mathbf{r}, \mathbf{r'}), d_{T_y}(\mathbf{r}, \mathbf{r'}), d_{T_z}(\mathbf{r}, \mathbf{r'}))^T\) transforms as a vector.

Generally, the superconducting contributions to the grand canonical potential can be approximated by the following kernel integral

\[
\Omega_{xc}[\rho, \mathbf{m}, \chi] = \Omega_{xc}^{\text{SDA}}[\rho, \mathbf{m}] - \int \mathbf{dr} \int \mathbf{dr}' \int d\mathbf{x} \int d\mathbf{x}' \sum_{i,j} \chi_i^{\dagger}(\mathbf{r}, \mathbf{r}')\chi_j(\mathbf{x}, \mathbf{x}') \chi_j^{\dagger}(\mathbf{x}, \mathbf{x}'),
\]

where

\[
d(\mathbf{r}, \mathbf{r'}) = d_{\text{ext}}(\mathbf{r}, \mathbf{r'}) + \int d\mathbf{x} \int d\mathbf{x}' \sum_j \Lambda_{ij}(\mathbf{r}, \mathbf{r'}; \mathbf{x}, \mathbf{x}') \chi_j^{\dagger}(\mathbf{x}, \mathbf{x}'),\]

(13)

where the kernel is hermitian

\[
\Lambda_{ij}(\mathbf{r}, \mathbf{r'}; \mathbf{x}, \mathbf{x}') = \Lambda_{ji}(\mathbf{x}', \mathbf{x}; \mathbf{r'}, \mathbf{r})^*.
\]

(15)

According to conventional BCS theory the electron-phonon coupling can be modeled by fully local interorbital pairing potential between opposite spins. Albeit, the full first-principles calculations of the pairing potential shows that there are also non-local corrections (in real space) due to electron-phonon coupling \([69]\). We can conclude it is very unlikely that electron-phonon coupling could stabilize a dominant triplet pairing state without SOC \([47]\). There are several classes of candidates for triplet superconductivity \((^3\text{He}, \text{Sr}_2\text{RuO}_4,\) non-centrosymmetric superconductors, heavy fermions). We should note here that due to strong SOC, spin is not a good quantum number in the f-electron based heavy fermions (their possible ,,spin-triplet pairing” may be rather named as ,,odd-parity” pairing based on the symmetry of the radial part). In fact, this serves the reason for using the Balian-Werthamer parametrization of the order parameter and pairing potential, since by generalizing this construction (multiplication of the Pauli matrices with the nonrelativistic time-reversal matrix) to the relativistic case (multiplication of Dirac matrices with the relativistic time-reversal matrix) we can obtain the order parameters which obey the Lorentz-invariance requirement \([67][68]\).

**Tight-binding representation of Spin generalized BdG equations.** SIESTA uses strictly confined basis orbitals which are zero beyond a given radius. These orbitals for an atom \(I\) located at \(\mathbf{R}_I\) can be expressed as

\[
\varphi^{\text{Imp}}(\mathbf{r}) = \delta^{I\text{Imp}}(\mathbf{r}) \varphi^{\text{Imp}}(\mathbf{r}_I),
\]

where \(\mathbf{r}_I = \mathbf{r} - \mathbf{R}_I\), and \(l, m\) are the usual angular momentum indices, and \(q\) labels the orbitals with the same angular momentum but with different radial dependence. Hereafter, the more compact notation \(\mu\) stands in for the full set of orbital indices \(l, m, q\). In spin space the local orbitals are introduced as

\[
\varphi^{\mu\alpha}(\mathbf{r}) = \varphi^{\text{Imp}}(\mathbf{r}) \otimes [\alpha]
\]

(17)

where \(\alpha\) is the spin label. In SIESTA the local orbitals \(\varphi^{\mu\alpha}(\mathbf{r})\) are chosen to be real, however, for generality we still use the conjugate notation, hence, the electron and hole components read as

\[
u^\mu_n(\mathbf{r}) = \sum_\mu \varphi^\mu(\mathbf{r}) u^\mu_n,\]

(18a)

\[
u^\alpha_n(\mathbf{r}) = \sum_\mu \varphi^\mu(\mathbf{r})^* v^\mu_n.\]

(18b)

This choice of the basis preserves the original structure of the SBdG equations, and it leads to the SBdG equation in the local orbital representation

\[
\sum_{\mu\alpha} \left( -H^{\nu_\mu\beta\alpha}_e(\mathbf{r}) - \Delta^{\nu_\mu\beta\alpha}_e \right) (u^\mu_n)^* v^\alpha_n = 0,
\]

(19)

where the matrix elements are

\[
H^{\nu_\mu\beta\alpha}_e = H^{\nu_\mu\beta\alpha}_e - \varepsilon_n S^{\nu_\mu\beta\alpha},\]

(20a)

\[
H^{\nu_\mu\beta\alpha}_e = \int d\mathbf{r'} \varphi^{\nu_\mu}(\mathbf{r'})^* H^{\beta\alpha}_e(\mathbf{r'}) \varphi^{\nu_\mu}(\mathbf{r}),\]

(20b)

\[
S^{\nu_\mu\beta\alpha} = \int d\mathbf{r'} \varphi^{\nu_\mu}(\mathbf{r'})^* \varphi^{\nu_\mu}(\mathbf{r}),\]

(20c)

\[
\Delta^{\nu_\mu\beta\alpha}_e = \int d\mathbf{r'} \varphi^{\nu_\mu}(\mathbf{r'})^* \Delta^{\nu_\mu\beta\alpha}_e(\mathbf{r'}, \mathbf{r}) \varphi^{\nu_\mu}(\mathbf{r}).\]

(20d)
with the following property of the gap function
\( \Delta_{\text{eff}}(\kappa) = \sum_{\mu} \epsilon^{\mu}_{x} \varphi^\ast_{\mu}(\kappa) \chi(\kappa) \).

Then the orbital representation of the densities are determined by
\[
\begin{align*}
\rho_{\alpha\beta}(\kappa) &= \sum_{\mu} \varphi^\mu_{\alpha}(\kappa) \varphi^\mu_{\beta}(\kappa), \\
m_{\alpha\beta}(\kappa) &= \sum_{\mu} \varphi^\mu_{\alpha}(\kappa) \varphi^\mu_{\beta}(\kappa), \tag{21a, 21b}
\end{align*}
\]

\[
\begin{align*}
\chi_{\alpha\beta}(\kappa) &= \sum_{\mu} \varphi^\mu_{\alpha}(\kappa) \chi_{\alpha\beta}(\kappa), \tag{21c}
\end{align*}
\]

where
\[
\begin{align*}
\rho_{\alpha\beta}(\kappa) &= \sum \frac{f(\epsilon_{\alpha}(\kappa) - \epsilon_{\beta}(\kappa))}{\epsilon_{\alpha}(\kappa) - \epsilon_{\beta}(\kappa)} \varphi^\mu_{\alpha}(\kappa) \varphi^\mu_{\beta}(\kappa), \tag{22a}
\end{align*}
\]
\[
\begin{align*}
m_{\alpha\beta}(\kappa) &= \sum \frac{f(\epsilon_{\alpha}(\kappa) - \epsilon_{\beta}(\kappa))}{\epsilon_{\alpha}(\kappa) - \epsilon_{\beta}(\kappa)} \varphi^\mu_{\alpha}(\kappa) \varphi^\mu_{\beta}(\kappa), \tag{22b}
\end{align*}
\]
\[
\begin{align*}
\chi_{\alpha\beta}(\kappa) &= \sum \frac{f(\epsilon_{\alpha}(\kappa) - \epsilon_{\beta}(\kappa))}{\epsilon_{\alpha}(\kappa) - \epsilon_{\beta}(\kappa)} \varphi^\mu_{\alpha}(\kappa) \varphi^\mu_{\beta}(\kappa). \tag{22c}
\end{align*}
\]

The normalization of the eigenvector reads as
\[
\sum_{\alpha} \left[ \left( \varphi^\mu_{\alpha}(\kappa) \right)^\ast \varphi^\mu_{\alpha}(\kappa) \right] = 1 \quad \forall n. \tag{23}
\]

Then the local orbital BW representation of \( \chi \) can easily be obtained from the \( \chi_{\alpha\beta} \) components. The corresponding pairing potentials can be obtained as
\[
\begin{align*}
a_{\mu\nu}(\kappa) &= \frac{1}{\sqrt{\pi}} \int d\kappa \int d\kappa' \chi_{\alpha\beta}(\kappa) \chi_{\alpha\beta}(\kappa'), \tag{24}
\end{align*}
\]

where
\[
\begin{align*}
\chi_{\alpha\beta}(\kappa_{\mu\nu} &:= \sum_{\mu} \varphi^\mu_{\alpha}(\kappa) \varphi^\mu_{\beta}(\kappa), \tag{25}
\end{align*}
\]

The SBdG Hamiltonian is then
\[
H_{\text{SBdG}}(\kappa) = \sum_{\mu\nu} H_{\text{SBdG}}^{\mu\nu}(\kappa) \varphi^\mu(\kappa(\kappa' - \kappa)), \tag{27}
\]

where \( \sum_{\mu\nu} \) means equivalent by translation and
\[
\begin{align*}
\sum_{\mu\nu} \left( - \left( \Delta_{\text{eff}}^\mu(\kappa) \right)^\ast \right) = \left( \Delta_{\text{eff}}^\mu(\kappa) \right) \left( u_{\mu\nu}^\ast(\kappa) \right) = 0, \tag{28}
\end{align*}
\]

Spin-orbit coupling induced triplet pairing in superconducting rhenium. The SBdG Hamiltonian is then
\[
H_{\text{SBdG}}^{\mu\nu}(\kappa) = \sum_{\mu\nu} H_{\text{SBdG}}^{\mu\nu}(\kappa) \varphi^\mu(\kappa(\kappa' - \kappa)), \tag{27}
\]

where we have used that the Fourier transform of \( f^\ast(r) \) is \( f^\ast(-k) \). For \( k \) and \( k' \) real, \( f^\ast(-k) = f(k) \). Furthermore, we've assumed that the pairing potential keeps the lattice periodicity (this is why it depends only on \( k \) and not \( k', k' \)). Here a point should be made. In the FFLO (Fulde-Ferrell-Larkin-Ovchinnikov) state Cooper pairs are formed with finite momentum. In an exchange field the Fermi surface splits into up and down parts. Thus the only way for a single Cooper pair to form is for an electron in the state \( |k + q/2, \alpha \rangle \) to pair with an electron in the state \( |k - q/2, \alpha \rangle \). So, the Cooper pair will have finite net momentum \( q \). Artificially, the \( k, k' \) dependence of the pairing potential can not be neglected, alternatively, one should use a supercell as it is also necessary for surfaces or heterostructures.

The orbital representation of the densities in momentum space reads as
\[
\begin{align*}
\rho_{\alpha\beta}(\kappa) &= \sum \frac{f(\epsilon_{\alpha}(\kappa) - \epsilon_{\beta}(\kappa))}{\epsilon_{\alpha}(\kappa) - \epsilon_{\beta}(\kappa)} \varphi^\mu_{\alpha}(\kappa) \varphi^\mu_{\beta}(\kappa), \tag{29a}
\end{align*}
\]

Therefore, the wave functions may be written as
\[
\begin{align*}
u_{\mu}(\kappa, r) &= \sum_{\mu} \varphi_{\mu}(r) u_{\mu}(\kappa) e^{i \kappa R}, \tag{26a}
\end{align*}
\]

\[
\begin{align*}
v_{\nu}(\kappa, r) &= \sum_{\mu} \varphi_{\mu}(r) v_{\mu}(\kappa) e^{i \kappa R}, \tag{26b}
\end{align*}
\]
The pairing potential also has the same symmetry, which can be written as
\[ \Delta_{\text{eff}}(k) = -\Delta_{\text{eff}}^*(-k), \] (31)
where the transposition \( T \) is with respect to both the orbital and spin indices, while the particle-hole symmetry in momentum space reads as
\[ u(\varepsilon n, k) = -v^*(\varepsilon n, -k). \] (32)

The number of electrons in the primitive cell is
\[ N = \sum_{i} \sum_{\alpha} \int_{\text{BZ}} \text{d}k S^{i\alpha}(k) \delta^{ij} \rho^{\alpha,\beta}(k), \] (33)
while in \( k \)-space the normalization of the eigenvector can be written as
\[ \sum_{i} \sum_{\alpha} (u_{i\alpha}^*(k))^{*} S^{i\alpha}(k) u_{i\alpha}^*(k) \]
\[ + \sum_{i} \sum_{\alpha} (v_{i\alpha}^*(k))^{*} (S^{i\alpha})(-k)^* v_{i\alpha}^*(k) = 1 \quad \forall n, \forall k. \] (34)

In general, the pairing potential can be obtained from the kernel and the order parameter in the following way
\[ d^{i\alpha}(k) = d_{\text{ext}}^{i\alpha}(k) + \sum_{j} \sum_{(\mu\nu)} \int_{\text{BZ}} \text{d}k' \Lambda^{ij}_{\mu\nu,\mu'\nu'}(k, k') \chi_{j,\mu'\nu'}. \] (35)

In our calculations we will assume that the kernel is local meaning that
\[ \Lambda^{ij}_{\mu\nu,\mu'\nu'} = \delta^{ij} \delta_{\mu\nu} \delta_{\mu'\nu'} \Lambda^{i}_{\mu\nu}. \] (36)

In this approach we get the following convolution integral for the pairing potential
\[ d^{i\alpha}(k) = d_{\text{ext}}^{i\alpha}(k) + \int_{\text{BZ}} \text{d}k' \Lambda^{i}_{\mu\nu}(k - k') \chi^{i,\mu\nu}(k'), \] (37)
where
\[ \Lambda^{i}_{\mu\nu}(k) = \sum_{\mu'\nu'} \Lambda^{i}_{\mu\nu} \epsilon_{k(R_{\mu'}, -R_{\nu})}. \] (38)

Here the kernel can be strongly \( k \) dependent even if \( \Lambda^{i}_{\mu\nu} \) is site-diagonal. In general to model an exotic pairing state the \( \Lambda^{i}_{\mu\nu} \) interaction strengths can be treated as adjustable parameters what we fit to get the experimental \( T_c \) and gap, then without further parameters the theory could be applied to calculate other quantities, and investigate other effects (e.g., surfaces, proximity with other exotic materials). It is expected that very small number of \( \Lambda^{i}_{\mu\nu} \) parameters will be enough to describe the experimental facts (like transition temperature, gap, specific heat, penetration depth). The main reason for optimism is the physical meaning of these parameters, namely,
\[ \Lambda^{i}_{\mu\nu} = \int \text{d}r \int \text{d}r' |\phi^{i}(r)|^2 \Lambda^{i}(r, r') |\phi^{i}(r')|^2 \] (39)

determine the sites and orbitals involved in the pairing mechanism in every spin channels. Similar strategy was proposed in Ref. [70] for spin singlet superconductivity and applied successfully in many cases including multiband superconductors [71] and heterostructures [56][63] as well.

Practically, we start from the normalization to the experimental static effective Kohn-Sham potentials \( (V_{\text{eff}}, \mathbf{B}_{\text{eff}}) \). In the case of rhenum we have assumed a spin singlet pairing potential (which leads to the experimental value of the gap), then the same \( \Lambda_{\text{EOT}} \) interaction strength was assumed for the even-parity odd-orbital spin triplet (EOT) states induced by SOC. The SBdG equations have to be solved self-consistently for the \( \Lambda_{\text{EOT}} \) interaction strength. To allow possible redistribution of EOT Cooper pairs we assumed a corresponding finite \( d^{\text{EOT}} \) external pairing potential what goes to zero during the self-consistent cycles.

Other quantity of interest is the Projected density of states for electrons and holes with spin \( \alpha \) on orbital \( \nu \), respectively:
\[ D^{\alpha \nu}(\varepsilon) = \sum_{i} \sum_{\nu \alpha} \left( u_{i\alpha}^{\nu}(k) \right)^* S^{i\alpha}(k) u_{i\alpha}^{\nu}(k) \delta(\varepsilon - \varepsilon_n(k)), \] (40a)
\[ D^{\alpha \nu}(\varepsilon) = D^{\alpha \nu}(-\varepsilon), \] (40b)
where \( N_k \) is the number of bands at \( k \). If the gap has a line of zeros on a three-dimensional Fermi surface the DOS should be linear around the Fermi level (for an isolated point node it is parabolic). We mention that the quasi-particle DOS can be directly related to the specific heat [10]. In the fully gapped case the specific heat is exponential at low temperatures. If the gap has a line of zeros on a three-dimensional Fermi surface it should follow a power law \( \sim T^2 \). For an isolated point node it also follows a power law but with different exponent \( \sim T^3 \). In fact the anisotropy of gaps is usually concluded by fitting BCS theory to specific heat measurements, however this method should not be considered as a reliable tool for unconventional superconductors and the specific heat calculation based on the self-consistent solution of the spin-generalized BdG equations is necessary.

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