Effects of impurities on the upper critical field H_{c2} in superconductors without inversion symmetry

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We calculate the upper critical field $H_{c2}(T)$ due to the orbital pair breaking in disordered superconductors without inversion symmetry. Differences from the usual centrosymmetric case are highlighted. The linearized gap equations in magnetic field, with the singlet and triplet pairing channels mixed by impurity scattering, are solved exactly for a cubic crystal.

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I. INTRODUCTION

Recently, superconductivity has been discovered in a number of compounds lacking inversion symmetry, such as $CePt_3Si$ (Ref. 1), UIr (Ref. 2), $CeRhSi_3$ (Ref. 3), $CeIrSi_3$ (Ref. 4), $Li_2(Pd_{3-x}Pt_x)B$ (Ref. 5), and many others. Much of the theoretical work in the field has focused on searching for the features which are specific to noncentrosymmetric systems. These include the magnetoelectric effect,[6–8] a large residual spin susceptibility and reduced paramagnetic limiting,[7,9–12] and various nonuniform superconducting states.[13–16]

In this paper we study the effects of the absence of inversion symmetry on the upper critical field $H_{c2}(T)$ at arbitrary temperature. We assume the pairing to be of the Bardeen-Cooper-Schrieffer (BCS) type and include only the orbital pair breaking. The main qualitative difference from the centrosymmetric case is that the spin-orbit (SO) coupling of electrons with the crystal lattice changes the nature of single-electron states, lifting spin degeneracy of the energy bands. Then even scalar impurities can mix the singlet and triplet channels in the Cooper pair propagator, thus making the theory considerably more complicated. The derivation of the H_{c2} equations for arbitrary noncentrosymmetric crystal symmetry is presented in Sec. II below, with some of the technical details relegated to Appendixes A and B. In Sec. III, we apply the general equations to a cubic superconductor with the point group $\mathbb{G}=\mathbf{O}$. Assuming that both the band structure and the SO coupling are fully isotropic, we are able to exactly solve the coupled equations for the singlet and triplet channels, obtain the H_{c2} equation in a closed form, and derive analytical expressions for the upper critical field in the "dirty" limit. This isotropic model clearly shows the deviations from the usual, i.e., centrosymmetric BCS, case, for which the upper critical field was calculated in the classic papers by Helfand, Werthamer, and Hohenberg in the 1960s (Refs. 17 and 18). Section IV contains a discussion of our results.

The magnetic phase diagram of noncentrosymmetric superconductors has been discussed previously in several works. The upper critical field for a clean three-dimensional Rashba superconductor was calculated in Ref. 15 while the effects of disorder in the Ginzburg-Landau regime were studied in Ref. 19. Two-dimensional case, in which only the paramagnetic pair breaking is present, was considered in Ref. 20. Recently, H_{c2} at all temperatures was calculated in Ref. 21, neglecting the impurity-induced triplet channel in the pair propagator in the limit when the SO band splitting is small compared with the Fermi energy. In this paper, we relax this last condition and include both the singlet and triplet channels. Throughout the paper we use the units in which $\hbar=k_B=1$.

II. DERIVATION OF H_{c2} EQUATIONS: GENERAL CASE

Let us consider a noncentrosymmetric superconductor with the Hamiltonian given by $H=H_0+H_{\rm imp}+H_{\rm int}$. The first term,

$$H_0=\sum_{\boldsymbol{k}}[\epsilon_0(\boldsymbol{k})\delta_{\alpha\beta}+\boldsymbol{\gamma}(\boldsymbol{k})\boldsymbol{\sigma}_{\alpha\beta}]a^\dagger_{\boldsymbol{k}\alpha}a_{\boldsymbol{k}\beta}, \tag{1}$$

describes noninteracting electrons in the crystal lattice potential, where $\alpha,\beta=\uparrow,\downarrow$ label spin projections, $\epsilon_0(\boldsymbol{k})$ is the quasiparticle energy counted from ϵ_F, and $\hat{\boldsymbol{\sigma}}$ are the Pauli matrices. In Eq. (1) and everywhere below, summation over repeated spin indices is implied while summations over spatial and band indices are always shown explicitly. The second term, with $\boldsymbol{\gamma}(\boldsymbol{k})=-\boldsymbol{\gamma}(-\boldsymbol{k})$, describes a Rashba-type (or antisymmetric) SO coupling of electrons with the crystal lattice.[22] If a usual SO coupling (which is present even in centrosymmetric crystals) is included, then α, β in Eq. (1) should be interpreted as pseudospin projections. Diagonalization of H_0 yields two nondegenerate bands labeled by the helicity $\lambda=\pm$:

$$\xi_\lambda(\boldsymbol{k})=\epsilon_0(\boldsymbol{k})+\lambda|\boldsymbol{\gamma}(\boldsymbol{k})|. \tag{2}$$

The Fermi velocities in the two bands are given by $\boldsymbol{v}_\lambda(\boldsymbol{k})=\partial\xi_\lambda/\partial\boldsymbol{k}$. The Fermi-level densities of states are defined in the usual way by $N_\lambda=\mathcal{V}^{-1}\Sigma_{\boldsymbol{k}}\delta[\xi_\lambda(\boldsymbol{k})]$ ($\mathcal{V}$ is the system volume), and the difference between N_+ and N_- is characterized by a parameter

$$\delta=\frac{N_+-N_-}{N_++N_-}. \tag{3}$$

If the SO coupling is small compared with the Fermi energy, then $\delta\sim\mathcal{O}(E_{\rm SO}/\epsilon_F)$, where $E_{\rm SO}=2\max_{\boldsymbol{k}}|\boldsymbol{\gamma}(\boldsymbol{k})|$ is a measure of the SO band splitting.

Scattering of electrons at isotropic scalar impurities is introduced according to

$$H_{\rm imp} = \int d^3\boldsymbol{r} U(\boldsymbol{r}) \psi_\alpha^\dagger(\boldsymbol{r}) \psi_\alpha(\boldsymbol{r}). \tag{4}$$

The random potential $U(\boldsymbol{r})$ has zero mean and is characterized by the correlator $\langle U(\boldsymbol{r})U(\boldsymbol{r}')\rangle = n_{\rm imp}U_0^2\delta(\boldsymbol{r}-\boldsymbol{r}')$, where $n_{\rm imp}$ is the impurity concentration and U_0 has the meaning of the strength of an individual pointlike impurity. The field operators are given by $\psi_\alpha(\boldsymbol{r}) = \mathcal{V}^{-1/2}\Sigma_{\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{r}} a_{\boldsymbol{k}\alpha}$.

Neglecting the paramagnetic pair breaking, which is a good assumption in many bulk noncentrosymmetric materials, the effect of a uniform external magnetic field $\boldsymbol{H}$ is described by the Peierls substitution[23]

$$\hat{h} = \epsilon_0(\boldsymbol{K}) + \boldsymbol{\gamma}(\boldsymbol{K})\hat{\boldsymbol{\sigma}} + U(\boldsymbol{r}), \tag{5}$$

where $\boldsymbol{K} = -i\boldsymbol{\nabla} + (e/c)\boldsymbol{A}(\boldsymbol{r})$ and e is the absolute value of the electron charge.

We describe the pairing interaction by a BCS-like Hamiltonian:

$$H_{\rm int} = -V\int d^3\boldsymbol{r} \psi_\uparrow^\dagger(\boldsymbol{r})\psi_\downarrow^\dagger(\boldsymbol{r})\psi_\downarrow(\boldsymbol{r})\psi_\uparrow(\boldsymbol{r}), \tag{6}$$

where $V>0$ is the coupling constant. In this model, the superconducting order parameter is represented by a single complex function $\eta(\boldsymbol{r})$ (see Ref. 24). The critical temperature at a given field, or inversely the upper critical field $H_{c2}(T)$ at a given temperature, is found from the condition that the linearized gap equation,

$$\left[\frac{1}{V} - T{\sum_n}' \hat{X}(\omega_n)\right]\eta(\boldsymbol{r}) = 0, \tag{7}$$

has a nontrivial solution. Here $\omega_n = (2n+1)\pi T$ is the fermionic Matsubara frequency (the prime in the second term means that the summation is limited to $|\omega_n| \le \omega_c$, where ω_c is the BCS frequency cutoff) and the operator $\hat{X}(\omega_n)$ is defined by the following kernel:

$$X(\boldsymbol{r},\boldsymbol{r}';\omega_n) = \frac{1}{2}\langle {\rm tr}\ \hat{g}^\dagger \hat{G}(\boldsymbol{r},\boldsymbol{r}';\omega_n)\hat{g}\hat{G}^T(\boldsymbol{r},\boldsymbol{r}';-\omega_n)\rangle_{\rm imp}, \tag{8}$$

where $\hat{g} = i\hat{\sigma}_2$. The angular brackets denote the impurity averaging, and $\hat{G}(\boldsymbol{r},\boldsymbol{r}';\omega_n)$ is the Matsubara Green's functions of electrons in the normal state, which satisfies the equation

$$(i\omega_n - \hat{h})\hat{G}(\boldsymbol{r},\boldsymbol{r}';\omega_n) = \delta(\boldsymbol{r}-\boldsymbol{r}'), \tag{9}$$

where the single-particle Hamiltonian $\hat{h}$ is given by expression (5).

At zero field, Eq. (9) yields the following expression for the average Green's function:

$$\hat{G}_0(\boldsymbol{k},\omega_n) = \sum_{\lambda=\pm} \hat{\Pi}_\lambda(\boldsymbol{k}) G_\lambda(\boldsymbol{k},\omega_n), \tag{10}$$

where

$$\hat{\Pi}_\lambda(\boldsymbol{k}) = \frac{1+\lambda\hat{\boldsymbol{\gamma}}(\boldsymbol{k})\hat{\boldsymbol{\sigma}}}{2} \tag{11}$$

are the band projection operators ($\hat{\boldsymbol{\gamma}} = \boldsymbol{\gamma}/|\boldsymbol{\gamma}|$), and

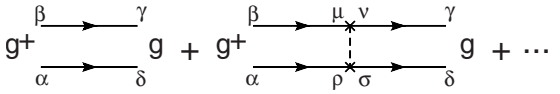

FIG. 1. Impurity ladder diagrams in the Cooper channel. Lines with arrows correspond to the average Green's functions of electrons, $\hat{g} = i\hat{\sigma}_2$, and the impurity (dashed) lines are defined in the text [see Eq. (15)].

$$G_\lambda(\boldsymbol{k},\omega_n) = \frac{1}{i\omega_n - \xi_\lambda(\boldsymbol{k}) + i\Gamma\ {\rm sgn}\ \omega_n} \tag{12}$$

are the electron Green's functions in the band representation. Here $\xi_\lambda(\boldsymbol{k})$ is the quasiparticle dispersion in the λth band [see Eq. (2)], $\Gamma = 1/2\tau$ is the elastic-scattering rate, $\tau = (2\pi n_{\rm imp}U_0^2 N_F)^{-1}$ is the electron mean-free time due to impurities, and

$$N_F = \frac{N_+ + N_-}{2}. \tag{13}$$

The impurity average of the product of two Green's functions in Eq. (8) can be represented graphically by the ladder diagrams (see Fig. 1). We assume the disorder that is sufficiently weak for the diagrams with crossed impurity lines to be negligible (see Ref. 25). In order to solve Eq. (7) at nonzero field, we introduce an impurity-renormalized gap function $\hat{D}(\boldsymbol{r},\omega_n)$, which is a matrix in the spin space satisfying the following integral equation

$$\begin{aligned}\hat{D}(\boldsymbol{r},\omega_n) = {}& \eta(\boldsymbol{r})\hat{g} + \frac{1}{2}n_{\rm imp}U_0^2\hat{g}\int d^3\boldsymbol{r}'\ {\rm tr}\ \hat{g}^\dagger\hat{G}(\boldsymbol{r},\boldsymbol{r}';\omega_n) \\ & \times\hat{D}(\boldsymbol{r}',\omega_n)\hat{G}^T(\boldsymbol{r},\boldsymbol{r}';-\omega_n) \\ & + \frac{1}{2}n_{\rm imp}U_0^2\hat{\boldsymbol{g}}\int d^3\boldsymbol{r}'\ {\rm tr}\ \hat{\boldsymbol{g}}^\dagger\hat{G}(\boldsymbol{r},\boldsymbol{r}';\omega_n) \\ & \times\hat{D}(\boldsymbol{r}',\omega_n)\hat{G}^T(\boldsymbol{r},\boldsymbol{r}';-\omega_n),\end{aligned} \tag{14}$$

where $\hat{G}(\boldsymbol{r},\boldsymbol{r}';\omega_n)$ are the disorder-averaged solutions of Eq. (9). The above equation can be easily derived from the impurity ladder diagrams in Fig. 1 by representing each "rung" of the ladder as a sum of spin-singlet and spin-triplet terms:

$$n_{\rm imp}U_0^2\delta_{\mu\nu}\delta_{\rho\sigma} = \frac{1}{2}n_{\rm imp}U_0^2 g_{\mu\rho}g^\dagger_{\sigma\nu} + \frac{1}{2}n_{\rm imp}U_0^2\boldsymbol{g}_{\mu\rho}\boldsymbol{g}^\dagger_{\sigma\nu}, \tag{15}$$

where $\hat{\boldsymbol{g}} = i\hat{\boldsymbol{\sigma}}\hat{\sigma}_2$.

Seeking solution of Eq. (14) in the form

$$\hat{D}(\boldsymbol{r},\omega_n) = d_0(\boldsymbol{r},\omega_n)\hat{g} + \boldsymbol{d}(\boldsymbol{r},\omega_n)\hat{\boldsymbol{g}}, \tag{16}$$

we obtain a system of four integral equations for $d_a(\boldsymbol{r},\omega_n)$, where $a = 0,1,2,3$:

$$\sum_{b=0}^{3}[\delta_{ab} - \Gamma\hat{\mathcal{Y}}_{ab}(\omega_n)]d_b(\boldsymbol{r},\omega_n) = \eta(\boldsymbol{r})\delta_{a0}. \tag{17}$$

Here the operators $\hat{\mathcal{Y}}_{ab}(\omega_n)$ are defined by the kernels

$$\mathcal{Y}_{ab}(\boldsymbol{r},\boldsymbol{r}';\omega_n) = \frac{1}{2\pi N_F}\mathrm{tr}\,\hat{g}_a^\dagger \hat{G}(\boldsymbol{r},\boldsymbol{r}';\omega_n)\hat{g}_b\hat{G}^T(\boldsymbol{r},\boldsymbol{r}';-\omega_n), \tag{18}$$

with $\hat{g}_0=\hat{g}$. We see that, in addition to the spin-singlet component d_0 of the impurity-renormalized gap function, impurity scattering can also induce a nonzero spin-triplet component $\boldsymbol{d}$. The linearized gap equation [see Eq. (7)] contains only the former: Using Eq. (17), we obtain

$$\frac{1}{N_F V}\eta(\boldsymbol{r}) - \pi T\sum_n{}' \frac{d_0(\boldsymbol{r},\omega_n)-\eta(\boldsymbol{r})}{\Gamma} = 0. \tag{19}$$

It is easy to see that the triplet component does not appear in the centrosymmetric case. Indeed, in the absence of the Zeeman interaction, the spin structure of the Green's function is trivial: $G_{\alpha\beta}(\boldsymbol{r},\boldsymbol{r}';\omega_n)=\delta_{\alpha\beta}G(\boldsymbol{r},\boldsymbol{r}';\omega_n)$. Then it follows from Eq. (18) that $\hat{\mathcal{Y}}_{ab}(\omega_n)=\delta_{ab}\hat{\mathcal{Y}}(\omega_n)$; therefore $d_0=(1-\Gamma\hat{\mathcal{Y}})^{-1}\eta$ and $\boldsymbol{d}=0$.

It should also be noted that, due to our choice of the pairing Hamiltonian [Eq. (6)], the order parameter has only the singlet component $\eta(\boldsymbol{r})$. In general, the pairing interaction contains not only the singlet but also the triplet as well as the mixed channels,[24] resulting in the order parameter having both the singlet and triplet components, which are mixed even in the absence of impurities. In this case, the gap equations become more complicated.

The next step is to find the spectrum of the operators $\hat{\mathcal{Y}}_{ab}(\omega_n)$. The orbital effect of the magnetic field is described by a phase factor in the average electron Green's function: $\hat{G}(\boldsymbol{r},\boldsymbol{r}';\omega_n)=\hat{G}_0(\boldsymbol{r}-\boldsymbol{r}';\omega_n)e^{i\varphi(\boldsymbol{r},\boldsymbol{r}')}$, where $\hat{G}_0$ is the average Green's function in the normal state at zero field, $\varphi(\boldsymbol{r},\boldsymbol{r}')=(e/c)\int_{\boldsymbol{r}}^{\boldsymbol{r}'}\boldsymbol{A}(\boldsymbol{r})d\boldsymbol{r}$, and the integration is performed along a straight line connecting $\boldsymbol{r}$ and $\boldsymbol{r}'$ (Ref. 25). The "phase-only" approximation is legitimate if the temperature is not very low so that the Landau-level quantization can be neglected. Using the identity $e^{2i\varphi(\boldsymbol{r},\boldsymbol{r}')}\eta(\boldsymbol{r}')=e^{-i(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{D}}\eta(\boldsymbol{r})$, where $\boldsymbol{D}=-i\boldsymbol{\nabla}+(2e/c)\boldsymbol{A}$, we obtain

$$\hat{\mathcal{Y}}_{ab}(\omega_n) = \overline{\mathcal{Y}}_{ab}(\boldsymbol{q},\omega_n)|_{\boldsymbol{q}\to\boldsymbol{D}}, \tag{20}$$

where

$$\overline{\mathcal{Y}}_{ab}(\boldsymbol{q},\omega_n) = \frac{1}{2\pi N_F}\int\frac{d^3\boldsymbol{k}}{(2\pi)^3}\mathrm{tr}\,\hat{g}_a^\dagger\hat{G}_0(\boldsymbol{k}+\boldsymbol{q},\omega_n)\hat{g}_b\hat{G}_0^T(-\boldsymbol{k},-\omega_n). \tag{21}$$

Substituting here the Green's function (10) and calculating the spin traces, we obtain for the singlet-singlet term

$$\overline{\mathcal{Y}}_{00}(\boldsymbol{q},\omega_n) = \frac{1}{2}\sum_\lambda \rho_\lambda\left\langle\frac{1}{|\omega_n|+\Gamma+i\boldsymbol{v}_\lambda(\boldsymbol{k})\boldsymbol{q}\ \mathrm{sgn}\ \omega_n/2}\right\rangle_\lambda, \tag{22}$$

where

$$\rho_\pm = \frac{N_\pm}{N_F} = 1\pm\delta \tag{23}$$

are the fractional densities of states in the two bands and $\langle(\ldots)\rangle_\lambda$ denotes the Fermi-surface averaging in the λth band. Similarly, for the singlet-triplet mixing terms, we obtain

$$\overline{\mathcal{Y}}_{0i}(\boldsymbol{q},\omega_n) = \overline{\mathcal{Y}}_{i0}(\boldsymbol{q},\omega_n) = \frac{1}{2}\sum_\lambda \lambda\rho_\lambda\left\langle\frac{\hat{\gamma}_i(\boldsymbol{k})}{|\omega_n|+\Gamma+i\boldsymbol{v}_\lambda(\boldsymbol{k})\boldsymbol{q}\ \mathrm{sgn}\ \omega_n/2}\right\rangle_\lambda \tag{24}$$

We see that the mixing occurs due to the SO coupling and vanishes at $\boldsymbol{\gamma}\to 0$, when $\rho_+=\rho_-=1$ and $\boldsymbol{v}_+=\boldsymbol{v}_-=\boldsymbol{v}_F$. Finally, the triplet-triplet terms can be represented as follows:

$$\overline{\mathcal{Y}}_{ij}(\boldsymbol{q},\omega_n) = \overline{\mathcal{Y}}_{ij}^{(1)}(\boldsymbol{q},\omega_n) + \overline{\mathcal{Y}}_{ij}^{(2)}(\boldsymbol{q},\omega_n), \tag{25}$$

where

$$\overline{\mathcal{Y}}_{ij}^{(1)}(\boldsymbol{q},\omega_n) = \frac{1}{2}\sum_\lambda \rho_\lambda\left\langle\frac{\hat{\gamma}_i(\boldsymbol{k})\hat{\gamma}_j(\boldsymbol{k})}{|\omega_n|+\Gamma+i\boldsymbol{v}_\lambda(\boldsymbol{k})\boldsymbol{q}\ \mathrm{sgn}\ \omega_n/2}\right\rangle_\lambda \tag{26}$$

and

$$\overline{\mathcal{Y}}_{ij}^{(2)}(\boldsymbol{q},\omega_n) = \frac{1}{2\pi N_F}\sum_\lambda\int\frac{d^3\boldsymbol{k}}{(2\pi)^3}(\delta_{ij}-\hat{\gamma}_i\hat{\gamma}_j-i\lambda e_{ijl}\hat{\gamma}_l) \times G_\lambda(\boldsymbol{k}+\boldsymbol{q},\omega_n)G_{-\lambda}(-\boldsymbol{k},-\omega_n). \tag{27}$$

The singlet impurity scattering channel, which is described by the first term in expression (15), causes only the scattering of intraband pairs between the bands. In contrast, the triplet impurity scattering can create also interband pairs, which are described by $\overline{\mathcal{Y}}_{ij}^{(2)}$. It is easy to show that if the SO band splitting exceeds both ω_c and Γ then the second (interband) term in Eq. (25) is smaller than the first (intraband) one (see Appendix A). Note that in real materials, E_{SO} ranges from tens to hundreds of meV (see Ref. 26 for $CePt_3Si$, and Ref. 27 for Li_2Pd_3B and Li_2Pt_3B). On the other hand, there is still considerable uncertainty as to the values of ω_c, especially in heavy-fermion compounds, such as $CePt_3Si$. The typical energy of phonons responsible for the pairing in Li_2Pd_3B was estimated in Ref. 27 to be 20 meV while the SO band splitting is 30 meV (reaching 200 meV in Li_2Pt_3B).

The critical temperature of the phase transition into a uniform superconducting state at zero field can be found by setting $\boldsymbol{q}=0$ in the above expressions. According to Eq. (24), the singlet and triplet channels are decoupled. Then it follows from Eqs. (22) and (17) that $d_0(\omega_n)=(1+\Gamma/|\omega_n|)\eta$. Substituting this into Eq. (19), we obtain

$$\frac{1}{N_F V} - \pi T\sum_n{}'\frac{1}{|\omega_n|} = 0, \tag{28}$$

which yields the superconducting critical temperature:

$$T_{c0} = \frac{2e^{\mathbb{C}}}{\pi}\omega_c e^{-1/N_F V}, \tag{29}$$

where $\mathbb{C}\simeq 0.577$ is Euler's constant. We see that there is an analog of Anderson's theorem in noncentrosymmetric superconductors with a BCS-contact pairing interaction: the zero-field critical temperature is not affected by scalar disorder.[19]

In the presence of magnetic field, neglecting the interband contributions to the triplet pair propagator, we obtain

$$\overline{\mathcal{Y}}_{ab}(\boldsymbol{q},\omega_n) = \frac{1}{2}\sum_{\lambda}\rho_\lambda\left\langle \frac{\Lambda_{\lambda,a}(\boldsymbol{k})\Lambda_{\lambda,b}(\boldsymbol{k})}{|\omega_n| + \Gamma + i\boldsymbol{v}_\lambda(\boldsymbol{k})\boldsymbol{q}\ \mathrm{sgn}\ \omega_n/2}\right\rangle_\lambda, \tag{30}$$

where

$$\Lambda_{\lambda,a}(\boldsymbol{k}) = \begin{cases} 1, & a=0, \\ \lambda\hat{\gamma}_a(\boldsymbol{k}), & a=1,2,3. \end{cases} \tag{31}$$

Next we use in Eq. (30) the identity $x^{-1}=\int_0^\infty du\ e^{-xu}$, and make the substitution $\boldsymbol{q}\to\boldsymbol{D}$ [see Eq. (20)] in the exponent to represent $\hat{\mathcal{Y}}_{ab}(\omega_n)$ as a differential operator of infinite order:

$$\hat{\mathcal{Y}}_{ab}(\omega_n) = \frac{1}{2}\int_0^\infty du\ e^{-u(|\omega_n|+\Gamma)}\sum_\lambda \rho_\lambda \hat{\mathcal{O}}_\lambda^{ab}, \tag{32}$$

where

$$\hat{\mathcal{O}}_\lambda^{ab} = \langle \Lambda_{\lambda,a}(\boldsymbol{k})\Lambda_{\lambda,b}(\boldsymbol{k})e^{-iu\boldsymbol{v}_\lambda(\boldsymbol{k})\boldsymbol{D}\ \mathrm{sgn}\ \omega_n/2}\rangle_\lambda. \tag{33}$$

In order to solve Eq. (17) with the operators $\hat{\mathcal{Y}}_{ab}(\omega_n)$ given by expression (32), we follow the procedure described in Ref. 17. We choose the z axis along the external field, so that $\boldsymbol{H}=H\hat{z}$ and introduce the operators

$$a_\pm = \ell_H\frac{D_x \pm iD_y}{2}, \quad a_3 = \ell_H D_z, \tag{34}$$

where $\ell_H=\sqrt{c/eH}$ is the magnetic length. It is easy to check that $a_+=a_-^\dagger$ and $[a_-,a_+]=1$; therefore $a_\pm$ have the meaning of the raising and lowering operators while $a_3=a_3^\dagger$ commutes with both of them: $[a_3,a_\pm]=0$. It is convenient to expand both the order parameter η and the impurity-renormalized gap functions d_a in the basis of Landau levels $|N,p\rangle$, which satisfy

$$a_+|N,p\rangle = \sqrt{N+1}|N+1,p\rangle, \tag{35}$$

$$a_-|N,p\rangle = \sqrt{N}|N-1,p\rangle$$

$$a_3|N,p\rangle = p|N,p\rangle,$$

where $N=0,1,\ldots$, and p is a real number. We have

$$\eta(\boldsymbol{r}) = \sum_{N,p}\eta_{N,p}\langle \boldsymbol{r}|N,p\rangle, \quad d_a(\boldsymbol{r},\omega_n) = \sum_{N,p} d_{N,p}^a(\omega_n)\langle \boldsymbol{r}|N,p\rangle. \tag{36}$$

According to Eq. (17), the expansion coefficients satisfy the following algebraic equations:

$$\sum_{N',p',b}[\delta_{ab}\delta_{NN'}\delta_{pp'} - \Gamma\langle N,p|\hat{\mathcal{Y}}_{ab}(\omega_n)|N',p'\rangle]d_{N',p'}^b(\omega_n) = \delta_{a0}\eta_{N,p}. \tag{37}$$

Substituting the solutions of these equations into

$$\frac{1}{N_F V}\eta_{N,p} - \pi T\sum_n{}' \frac{d_{N,p}^0(\omega_n) - \eta_{N,p}}{\Gamma} = 0 \tag{38}$$

[see Eq. (19)] and setting the determinant of the resulting linear equations for $\eta_{N,p}$ to zero, one arrives at an equation for the upper critical field.

III. CUBIC CASE

In the general case, i.e., for arbitrary crystal symmetry and electronic band structure, the procedure outlined in the previous section does not yield an equation for $H_{c2}(T)$ in a closed form since all the Landau levels are coupled and one has to diagonalize infinite matrices. In order to make progress, we focus on the case of a noncentrosymmetric cubic superconductor with the point group $\mathbb{G}=\mathbf{O}$, which describes, for instance, the crystal symmetry of $Li_2(Pd_{1-x},Pt_x)_3B$. The simplest expression for the SO coupling compatible with all symmetry requirements has the following form:

$$\boldsymbol{\gamma}(\boldsymbol{k}) = \gamma_0\boldsymbol{k}, \tag{39}$$

where γ_0 is a constant. We assume a parabolic band: $\epsilon_0(\boldsymbol{k})=\boldsymbol{k}^2/2m^*-\epsilon_F$, where m^* is the effective mass, $\epsilon_F=k_0^2/2m^*$, and k_0 is the Fermi wave vector in the absence of the SO coupling. The band dispersion functions are given by

$$\xi_\lambda(\boldsymbol{k}) = \frac{k^2-k_0^2}{2m^*} + \lambda|\gamma_0|k, \tag{40}$$

so that the SO band splitting is isotropic and given by $E_{\mathrm{SO}}=2|\gamma_0|k_0$. It is convenient to characterize the SO coupling strength by a dimensionless parameter $\varrho=E_{\mathrm{SO}}/4\epsilon_F$. While the two Fermi surfaces have different radii, $k_{F,\lambda}=k_0(\sqrt{1+\varrho^2}-\lambda\varrho)$, the Fermi velocities are the same: $\boldsymbol{v}_\lambda(\boldsymbol{k})=v_F\hat{\boldsymbol{k}}$, where $v_F=k_0\sqrt{1+\varrho^2}/m^*$. For the parameter δ, which characterizes the difference between the band densities of states [see Eq. (3)], we have $|\delta|=2\varrho\sqrt{1+\varrho^2}/(1+2\varrho^2)$. We assume that

$$\delta_c \ll |\delta| \le 1, \tag{41}$$

where $\delta_c=\max(\omega_c,\Gamma)/\epsilon_F\ll 1$. While the first inequality is equivalent to the condition $E_{\mathrm{SO}}\gg\max(\omega_c,\Gamma)$, which ensures the smallness of the interband contribution to the Cooper impurity ladder (see Appendix A), the second one is always satisfied with $|\delta|\to 1$ corresponding to the rather unrealistic limit of extremely strong SO coupling, $\varrho\to\infty$.

In order to solve the gap equations, we make a change of variables in the triplet component:

$$d_\pm(\boldsymbol{r},\omega_n) = \frac{d_1(\boldsymbol{r},\omega_n) \pm id_2(\boldsymbol{r},\omega_n)}{\sqrt{2}}.$$

Then, Eq. (17) takes the following form:

$$\begin{pmatrix} 1-\Gamma\hat{\mathcal{Y}}_{00} & -\Gamma\hat{\mathcal{Y}}_{03} & -\Gamma\hat{\mathcal{Y}}_{0-} & -\Gamma\hat{\mathcal{Y}}_{0+} \\ -\Gamma\hat{\mathcal{Y}}_{03} & 1-\Gamma\hat{\mathcal{Y}}_{33} & -\Gamma\hat{\mathcal{Y}}_{3-} & -\Gamma\hat{\mathcal{Y}}_{3+} \\ -\Gamma\hat{\mathcal{Y}}_{0+} & -\Gamma\hat{\mathcal{Y}}_{3+} & 1-\Gamma\hat{\mathcal{Z}} & -\Gamma\hat{\mathcal{Z}}_{+} \\ -\Gamma\hat{\mathcal{Y}}_{0-} & -\Gamma\hat{\mathcal{Y}}_{3-} & -\Gamma\hat{\mathcal{Z}}_{-} & 1-\Gamma\hat{\mathcal{Z}} \end{pmatrix} \begin{pmatrix} d_0 \\ d_3 \\ d_+ \\ d_- \end{pmatrix} = \begin{pmatrix} \eta \\ 0 \\ 0 \\ 0 \end{pmatrix}, \tag{42}$$

where

$$\hat{\mathcal{Y}}_{0\pm} = \frac{\hat{\mathcal{Y}}_{01} \pm i\hat{\mathcal{Y}}_{02}}{\sqrt{2}}, \quad \hat{\mathcal{Y}}_{3\pm} = \frac{\hat{\mathcal{Y}}_{13} \pm i\hat{\mathcal{Y}}_{23}}{\sqrt{2}}, \quad \hat{\mathcal{Z}} = \frac{\hat{\mathcal{Y}}_{11} + \hat{\mathcal{Y}}_{22}}{2},$$

$$\hat{\mathcal{Z}}_{\pm} = \frac{\hat{\mathcal{Y}}_{11} \pm 2i\hat{\mathcal{Y}}_{12} - \hat{\mathcal{Y}}_{22}}{2},$$

with $\hat{\mathcal{Y}}_{ab} = \hat{\mathcal{Y}}_{ba}$ given by Eq. (32).

According to Sec. II, one has to know the matrix elements of the operators $\hat{\mathcal{Y}}_{ab}(\omega_n)$ in the basis of the Landau levels $|N,p\rangle$. After some straightforward algebra (see Appendix B), we obtain the following expressions for the nonzero matrix elements:

$$\langle N,p|\hat{\mathcal{Y}}_{00}(\omega_n)|N,p\rangle = y^{00}_{N,p}(\omega_n),$$

$$\langle N,p|\hat{\mathcal{Y}}_{03}(\omega_n)|N,p\rangle = y^{03}_{N,p}(\omega_n),$$

$$\langle N,p|\hat{\mathcal{Y}}_{33}(\omega_n)|N,p\rangle = y^{33}_{N,p}(\omega_n),$$

$$\langle N,p|\hat{\mathcal{Z}}(\omega_n)|N,p\rangle = z_{N,p}(\omega_n),$$

where

$$y^{00}_{N,p}(\omega_n) = \int_0^\infty du\ e^{-u(|\omega_n|+\Gamma)} \int_0^1 ds\ \cos(pvs) e^{-v^2(1-s^2)/2} \times L_N[v^2(1-s^2)], \tag{43}$$

$$y^{03}_{N,p}(\omega_n) = -i\delta \int_0^\infty du\ e^{-u(|\omega_n|+\Gamma)} \int_0^1 ds\ s\ \sin(pvs) e^{-v^2(1-s^2)/2} \times L_N[v^2(1-s^2)], \tag{44}$$

$$y^{33}_{N,p}(\omega_n) = \int_0^\infty du\ e^{-u(|\omega_n|+\Gamma)} \int_0^1 ds\ s^2\ \cos(pvs) e^{-v^2(1-s^2)/2} \times L_N[v^2(1-s^2)], \tag{45}$$

$$z_{N,p}(\omega_n) = \frac{1}{2} \int_0^\infty du\ e^{-u(|\omega_n|+\Gamma)} \int_0^1 ds(1-s^2) \times \cos(pvs) e^{-v^2(1-s^2)/2} L_N[v^2(1-s^2)], \tag{46}$$

$v = (v_F\ \mathrm{sgn}\ \omega_n / 2\ell_H)u$, and $L_N(x)$ are the Laguerre polynomials of degree N. Similarly, we obtain

$$\langle N,p|\hat{\mathcal{Y}}_{0-}(\omega_n)|N+1,p\rangle = \langle N+1,p|\hat{\mathcal{Y}}_{0+}(\omega_n)|N,p\rangle = \tilde{y}^0_{N,p}(\omega_n),$$

$$\langle N,p|\hat{\mathcal{Y}}_{3-}(\omega_n)|N+1,p\rangle = \langle N+1,p|\hat{\mathcal{Y}}_{3+}(\omega_n)|N,p\rangle = \tilde{y}^3_{N,p}(\omega_n),$$

$$\langle N,p|\hat{\mathcal{Z}}_{-}(\omega_n)|N+2,p\rangle = \langle N+2,p|\hat{\mathcal{Z}}_{+}(\omega_n)|N,p\rangle = \tilde{z}_{N,p}(\omega_n),$$

where

$$\tilde{y}^0_{N,p}(\omega_n) = -i\delta \frac{1}{\sqrt{2(N+1)}} \int_0^\infty du\ e^{-u(|\omega_n|+\Gamma)} \int_0^1 ds\ v \times (1-s^2)\cos(pvs) e^{-v^2(1-s^2)/2} L^{(1)}_N[v^2(1-s^2)], \tag{47}$$

$$\tilde{y}^3_{N,p}(\omega_n) = -\frac{1}{\sqrt{2(N+1)}} \int_0^\infty du\ e^{-u(|\omega_n|+\Gamma)} \int_0^1 ds\ vs \times (1-s^2)\sin(pvs) e^{-v^2(1-s^2)/2} L^{(1)}_N[v^2(1-s^2)], \tag{48}$$

$$\tilde{z}_{N,p}(\omega_n) = -\frac{1}{2\sqrt{(N+1)(N+2)}} \int_0^\infty du\ e^{-u(|\omega_n|+\Gamma)} \int_0^1 ds\ v^2 \times (1-s^2)^2\cos(pvs) e^{-v^2(1-s^2)/2} L^{(2)}_N[v^2(1-s^2)], \tag{49}$$

and $L^{(\alpha)}_N(x)$ are the generalized Laguerre polynomials.

It follows from the above expressions that the Landau levels are decoupled, and for $\eta(\boldsymbol{r}) = \eta\langle \boldsymbol{r}|N,p\rangle$ (η is a constant), the solution of Eq. (42) has the following form:

$$\begin{pmatrix} d_0(\boldsymbol{r},\omega_n) \\ d_3(\boldsymbol{r},\omega_n) \\ d_+(\boldsymbol{r},\omega_n) \\ d_-(\boldsymbol{r},\omega_n) \end{pmatrix} = \begin{pmatrix} d^0_{N,p}(\omega_n)\langle \boldsymbol{r}|N,p\rangle \\ d^3_{N,p}(\omega_n)\langle \boldsymbol{r}|N,p\rangle \\ d^+_{N,p}(\omega_n)\langle \boldsymbol{r}|N+1,p\rangle \\ d^-_{N,p}(\omega_n)\langle \boldsymbol{r}|N-1,p\rangle \end{pmatrix}. \tag{50}$$

For given N and p, the coefficients are found from the equations

$$\sum_{b=0,3,\pm} \mathcal{M}_{ab}(N,p;\omega_n) d^b_{N,p}(\omega_n) = \delta_{a0}\eta, \tag{51}$$

where

$$\hat{\mathcal{M}}(N,p;\omega_n)=\begin{pmatrix} 1-\Gamma y^{00}_{N,p} & -\Gamma y^{03}_{N,p} & -\Gamma \tilde{y}^{0}_{N,p} & -\Gamma \tilde{y}^{0}_{N-1,p} \\ -\Gamma y^{03}_{N,p} & 1-\Gamma y^{33}_{N,p} & -\Gamma \tilde{y}^{3}_{N,p} & -\Gamma \tilde{y}^{3}_{N-1,p} \\ -\Gamma \tilde{y}^{0}_{N,p} & -\Gamma \tilde{y}^{3}_{N,p} & 1-\Gamma z_{N+1,p} & -\Gamma \tilde{z}_{N-1,p} \\ -\Gamma \tilde{y}^{0}_{N-1,p} & -\Gamma \tilde{y}^{3}_{N-1,p} & -\Gamma \tilde{z}_{N-1,p} & 1-\Gamma z_{N-1,p} \end{pmatrix}. \tag{52}$$

Substituting the solution of Eq. (51) in Eq. (38), and using Eqs. (28) and (29) to eliminate both the frequency cutoff and the coupling constant, we obtain an equation implicitly relating the magnetic field and the transition temperature at given N and p:

$$\ln\frac{T_{c0}}{T}=\pi T\sum_n\left\{\frac{1}{|\omega_n|}-\frac{[\hat{\mathcal{M}}^{-1}(N,p;\omega_n)]_{00}-1}{\Gamma}\right\}. \tag{53}$$

The upper critical field $H_{c2}(T)$ is obtained by maximizing the solution of this equation with respect to both N and p.

Note that the matrix elements of $\hat{\mathcal{M}}$ which are responsible for the singlet-triplet mixing, i.e., $y^{03}_{N,p}$, $\tilde{y}^{0}_{N,p}$, and $\tilde{y}^{0}_{N-1,p}$, are all proportional to δ [see Eqs. (44) and (47)]. Therefore, at $|\delta|\ll 1$ the singlet and triplet channels are effectively decoupled. Neglecting the corrections of the order of δ^2, we obtain from Eq. (51) that $[\hat{\mathcal{M}}^{-1}(N,p;\omega_n)]_{00}=(1-\Gamma y^{00}_{N,p})^{-1}$. Substituting this into Eq. (53), we recover the Helfand-Werthamer expressions[17] with the maximum critical field corresponding to $N=p=0$ at all temperatures. Thus, in the weak SO coupling limit the absence of inversion symmetry does not bring about any new features in $H_{c2}(T)$, compared with the centrosymmetric case (as long as the paramagnetic pair breaking is not included, see Ref. 21).

"Dirty" limit at $N=0$, $p=0$

At arbitrary magnitude of the SO band splitting, the singlet-triplet mixing makes the H_{c2} equation in noncentrosymmetric superconductors considerably more cumbersome than in the Helfand-Werthamer problem even in our "minimal" isotropic model. It is even possible that, at some values of the parameters, the maximum critical field is achieved for $N>0$ and $p\neq 0$, the latter corresponding to a disorder-induced modulation of the order parameter along the applied field. Leaving investigation of these exotic possibilities to future work, here we just consider the case $N=p=0$. Then it follows from Eqs. (50) and (51) that $d^3_{0,0}=d^-_{0,0}=0$, and $[\hat{\mathcal{M}}^{-1}(0,0;\omega_n)]_{00}=(1-\Gamma z_{1,0})/[(1-\Gamma y^{00}_{0,0})(1-\Gamma z_{1,0})-\Gamma^2(\tilde{y}^{0}_{0,0})^2]$. It is convenient to introduce the reduced temperature, magnetic field, and disorder:

$$t=\frac{T}{T_{c0}},\quad h=\frac{2H}{H_0},\quad \zeta=\frac{\Gamma}{\pi T_{c0}},$$

where $H_0=\Phi_0/\pi\xi_0^2$, $\Phi_0=\pi c/e$ is the magnetic-flux quantum, and $\xi_0=v_F/2\pi T_{c0}$ is the superconducting coherence length. In these notations, Eq. (53) yields the following equation for the upper critical field $h_{c2}(t)$:

$$\ln\frac{1}{t}=2\sum_{n\geq 0}\left[\frac{1}{2n+1}-t\frac{w_n(1-\zeta p_n)-\zeta\delta^2 q_n^2}{(1-\zeta w_n)(1-\zeta p_n)+\zeta^2\delta^2 q_n^2}\right], \tag{54}$$

where

$$w_n(t,h)=\int_0^\infty d\rho\, e^{-\tilde{\omega}_n\rho}\int_0^1 ds\, e^{-h\rho^2(1-s^2)/4},$$

$$p_n(t,h)=\int_0^\infty d\rho\, e^{-\tilde{\omega}_n\rho}\int_0^1 ds\frac{1-s^2}{2}\times\left[1-\frac{h}{2}\rho^2(1-s^2)\right]e^{-h\rho^2(1-s^2)/4},$$

$$q_n(t,h)=\int_0^\infty d\rho\, e^{-\tilde{\omega}_n\rho}\int_0^1 ds\sqrt{\frac{h}{4}}\rho(1-s^2)e^{-h\rho^2(1-s^2)/4}, \tag{55}$$

where $\tilde{\omega}_n=(2n+1)t+\zeta$.

In the clean limit, i.e., at $\zeta\to 0$, or if the SO band splitting is negligibly small, i.e., at $\delta\to 0$, one recovers from Eq. (54) the Helfand-Werthamer equation for a centrosymmetric superconductor. Thus the absence of inversion symmetry affects the upper critical field only if disorder is present. One can expect that the effect will be most pronounced in the dirty limit, $\zeta\gg 1$. [Note that, according to Eq. (41), the disorder strength should satisfy $\zeta\ll(\epsilon_F/T_{c0})|\delta|$.] We shall see that in this limit h_{c2} scales as ζ, which allows one to use the Taylor expansions of the exponentials in Eq. (55):

$$w_n(t,h)\simeq\frac{1}{\tilde{\omega}_n}\left(1-\frac{h}{3\tilde{\omega}_n^2}\right),$$

$$p_n(t,h)\simeq\frac{1}{3\tilde{\omega}_n}\left(1-\frac{6h}{5\tilde{\omega}_n^2}\right),$$

$$q_n(t,h)\simeq\frac{\sqrt{h}}{3\tilde{\omega}_n^2}.$$

Using the fact that the main contribution to the Matsubara sum in Eq. (54) comes from $(2n+1)t\ll\zeta$, we arrive at a well-known universal equation, which describes the magnetic pair breaking in superconductors:[28]

$$\ln\frac{1}{t}=\Psi\left(\frac{1}{2}+\frac{\sigma}{t}\right)-\Psi\left(\frac{1}{2}\right), \tag{56}$$

where $\Psi(x)$ is the digamma function, and

$$\sigma=\frac{2+\delta^2}{12\zeta}h \tag{57}$$

characterizes the pair-breaker strength. Note that the corresponding expression in the centrosymmetric case is different: $\sigma_{CS}=h/6\zeta$ (Ref. 17). Analytical expressions for the upper critical field can be obtained in the weak-field limit near the critical temperature:

$$h_{c2}|_{t\to 1}=\frac{24\zeta}{(2+\delta^2)\pi^2}(1-t), \tag{58}$$

and also at low temperatures:

$$h_{c2}|_{t=0}=\frac{3e^{-\mathbb{C}}}{2+\delta^2}\zeta. \tag{59}$$

We see that the SO band splitting in the noncentrosymmetric case enhances the orbital pair breaking.

IV. CONCLUSIONS

We have derived equations for the upper critical field in noncentrosymmetric superconductors with the orbital pair breaking. Although for a BCS-contact pairing interaction the order parameter has just the singlet component, one has to include also the triplet pairing channel in the gap equations due to impurity scattering. In a cubic crystal (the point group $\mathbb{G}=\mathbf{O}$), in which both the electron dispersion and the SO coupling are isotropic, the gap equations are shown to be diagonal in the Landau-level basis with the singlet and triplet channels still mixed together. For the order parameter corresponding to the lowest Landau level without any modulation along the applied field, we have obtained the H_{c2} equation in a closed form and solved it in the dirty limit, in which the effects of the absence of inversion symmetry are expected to be most pronounced. The effect on the upper critical field of the singlet-triplet mixing, which is responsible for the deviations from the Helfand-Werthamer theory, is found to be proportional to δ^2.

Application of our theory to real noncentrosymmetric superconductors of cubic symmetry, such as $Li_2(Pd_{3-x}Pt_x)B$, is complicated by the fact that the Fermi surfaces as well as the SO band splitting are strongly anisotropic. Using the maximum values of the SO band splitting from Ref. 27, one can estimate the corrections to $H_{c2}(T)$ due to the singlet-triplet mixing to be of the order of several percent.

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APPENDIX A: INTERBAND VS INTRABAND CONTRIBUTIONS

In this appendix, we estimate the relative magnitudes of the intraband and interband contributions to the triplet pair propagator [Eq. (25)] in the limit when the SO coupling is strong compared with both the cut-off energy ω_c and the elastic-scattering rate Γ. Let us consider an isotropic band with $\boldsymbol{\gamma}(\boldsymbol{k})=\gamma_0\boldsymbol{k}$ in a cubic crystal. Neglecting for simplicity the differences between the densities of states and the Fermi velocities in the two bands: $\rho_+=\rho_-=1$ and $\boldsymbol{v}_+=\boldsymbol{v}_-=\boldsymbol{v}_F$, and setting $\boldsymbol{q}=0$, we obtain from Eqs. (26) and (27)

$$\overline{\mathcal{Y}}^{(1)}_{ij}(\boldsymbol{q}=0,\omega_n)=\frac{\langle\hat{\gamma}_i\hat{\gamma}_j\rangle_{\hat{\boldsymbol{k}}}}{|\omega_n|+\Gamma}=\frac{\delta_{ij}}{3(|\omega_n|+\Gamma)}\equiv\mathcal{Y}_{\text{intra}}(\omega_n)\delta_{ij},$$

and

$$\overline{\mathcal{Y}}^{(2)}_{ij}(\boldsymbol{q}=0,\omega_n)=\frac{1}{2}\sum_{\lambda}\left\langle\frac{\delta_{ij}-\hat{\gamma}_i\hat{\gamma}_j}{|\omega_n|+\Gamma+i\lambda|\boldsymbol{\gamma}|\text{sgn }\omega_n}\right\rangle_{\hat{\boldsymbol{k}}}$$

$$=\frac{2\delta_{ij}}{3(|\omega_n|+\Gamma)(1+r^2)}\equiv\mathcal{Y}_{\text{inter}}(\omega_n)\delta_{ij},$$

where $r(\omega_n)=E_{\text{SO}}/2(|\omega_n|+\Gamma)$. Due to the BCS cutoff, the maximum value of ω_n is equal to ω_c; therefore $r_{\min}\sim E_{\text{SO}}/\max(\omega_c,\Gamma)\gg 1$. From this it follows that

$$\max_n\frac{\mathcal{Y}_{\text{inter}}(\omega_n)}{\mathcal{Y}_{\text{intra}}(\omega_n)}=\frac{2}{1+r^2_{\min}}\sim\left[\frac{\max(\omega_c,\Gamma)}{E_{\text{SO}}}\right]^2\ll 1.$$

Therefore the interband contribution is small compared with the intraband one at all Matsubara frequencies.

APPENDIX B: CALCULATION OF $\langle N,p|\hat{\mathcal{Y}}_{ab}(\omega_n)|N',p'\rangle$

The operators $\hat{\mathcal{Y}}_{ab}(\omega_n)$ are given by expression (32). For a spherical Fermi surface and $\boldsymbol{\gamma}(\boldsymbol{k})=\gamma_0\boldsymbol{k}$, we obtain from Eq. (33)

$$\hat{\mathcal{O}}^{ab}_{\lambda}=\frac{1}{2}\int_0^{\pi}d\theta\sin\theta e^{-iva_3\cos\theta}\times\int_0^{2\pi}\frac{d\phi}{2\pi}\Phi^{ab}_{\lambda}(\theta,\phi)e^{-iv(e^{-i\phi}a_++e^{i\phi}a_-)\sin\theta}, \tag{B1}$$

where $v=(v_F\text{ sign }\omega_n/2\ell_H)u$, and $\Phi^{ab}_{\lambda}(\theta,\phi)=\Lambda_{\lambda,a}(\boldsymbol{k})\Lambda_{\lambda,b}(\boldsymbol{k})$, with $\Lambda_{\lambda,0}(\boldsymbol{k})=1$ and $\Lambda_{\lambda,i}(\boldsymbol{k})=\lambda\hat{k}_i$ for $i=1,2,3$ [see Eq. (31)]. Using the well-known operator identity $e^{A+B}=e^{-[A,B]/2}e^Ae^B$, which holds if the commutator of A and B is a c number, and expanding the exponentials in powers of $a_{\pm}$, we obtain

$$\hat{\mathcal{Y}}_{ab}(\omega_n)=\frac{1}{4}\sum_{\lambda}\rho_{\lambda}\int_0^{\infty}du\ e^{-u(|\omega_n|+\Gamma)}\int_0^{\pi}d\theta\times\sin\theta e^{-iva_3\cos\theta}e^{-(v^2/2)\sin^2\theta}\hat{\mathcal{L}}^{ab}_{\lambda}(\theta), \tag{B2}$$

where

$$\hat{\mathcal{L}}^{ab}_{\lambda}(\theta)=\sum_{n,m=0}^{\infty}\frac{(-iv\sin\theta)^{n+m}}{n!\,m!}\times\left[\int_0^{2\pi}\frac{d\phi}{2\pi}\Phi^{ab}_{\lambda}(\theta,\phi)e^{i(m-n)\phi}\right]a_+^na_-^m. \tag{B3}$$

Below we perform the detailed calculations for $\hat{\mathcal{Y}}_{00}$ and

$\hat{\mathcal{Y}}_{0-}=(\hat{\mathcal{Y}}_{01}-i\hat{\mathcal{Y}}_{02})/\sqrt{2}$. Other matrix elements can be considered in a similar fashion.

$\hat{\mathcal{Y}}_{00}$: Since $\Phi_\lambda^{00}(\theta,\phi)=1$, the ϕ integral on the right-hand side of Eq. (B3) is equal to δ_{nm}, and

$$\hat{\mathcal{L}}_\lambda^{00}(\theta)=\sum_{n=0}^{\infty}\frac{(-v^2\sin^2\theta)^n}{(n!)^2}a_+^n a_-^n.$$

It is easy to show using Eq. (35) that $a_+^n a_-^n|N,p\rangle=[N!/(N-n)!]|N,p\rangle$ for $n\leq N$, and zero otherwise. Therefore,

$$\hat{\mathcal{L}}_\lambda^{00}(\theta)|N,p\rangle=\sum_{n=0}^{N}\frac{N!}{(n!)^2(N-n)!}(-v^2\sin^2\theta)^n|N,p\rangle$$
$$=L_N(v^2\sin^2\theta)|N,p\rangle,$$

where $L_N(x)$ is the Laguerre polynomial of degree N. Substituting this into Eq. (B2), using the fact that $\rho_+ + \rho_- = 2$, and introducing $s=\cos\theta$, we obtain: $\langle N,p|\hat{\mathcal{Y}}_{00}(\omega_n)|N,p\rangle = y_{N,p}^{00}(\omega_n)$, where $y_{N,p}^{00}(\omega_n)$ is given by Eq. (43).

$\hat{\mathcal{Y}}_{0-}$: Since $\Phi_\lambda^{0-}(\theta,\phi)=\lambda\sin\theta e^{-i\phi}/\sqrt{2}$, one has $m=n+1$ on the right-hand side of Eq. (B3), and

$$\hat{\mathcal{L}}_\lambda^{0-}(\theta)=\lambda\frac{\sin\theta}{\sqrt{2}}\sum_{n=0}^{\infty}\frac{(-iv\sin\theta)^{2n+1}}{n!\,(n+1)!}a_+^n a_-^{n+1}.$$

Using $a_+^n a_-^{n+1}|N+1,p\rangle=\sqrt{N+1}[N!/(N-n)!]|N,p\rangle$ (if $n\leq N$, zero otherwise), we obtain

$$\hat{\mathcal{L}}_\lambda^{0-}(\theta)|N+1,p\rangle=-i\lambda\frac{v\sin^2\theta}{\sqrt{2}}\sqrt{N+1}\sum_{n=0}^{N}\frac{N!}{(N-n)!}$$
$$\times\frac{(-v^2\sin^2\theta)^n}{n!\,(n+1)!}|N,p\rangle$$
$$=-i\lambda\frac{1}{\sqrt{2(N+1)}}v\sin^2\theta L_N^{(1)}(v^2\sin^2\theta)|N,p\rangle,$$

where $L_N^{(\alpha)}(x)$ are the generalized Laguerre polynomials (see Ref. 29)

$$L_N^{(\alpha)}(x)=\sum_{n=0}^{N}\frac{(N+\alpha)!}{(N-n)!}\frac{(-x)^n}{n!\,(n+\alpha)!}$$

(the ordinary Laguerre polynomials are recovered by setting $\alpha=0$). Substituting this into Eq. (B2) and using $\rho_+-\rho_-=2\delta$, we obtain $\langle N,p|\hat{\mathcal{Y}}_{0-}(\omega_n)|N+1,p\rangle=\tilde{y}_{N,p}^0(\omega_n)$, where is given by Eq. (47).

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