



Singular Temperature Dependence of the Equation of State of Superconductors with Spin-Orbit Interaction in Low-Temperature Region – II

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Received: 28 February 2018 / Accepted: 23 March 2018 / Published online: 26 April 2018
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Abstract

We extend a previous study of the space and temperature dependence of the order parameter in an ultrathin superconducting film in a longitudinal magnetic field to the vicinity of the critical transition surface. In these films, the spin-orbit interaction can be sizeable. The calculations are restricted to the low-temperature regime. Special attention is given to the zero temperature limit where the state with the maximum value of the critical field is investigated for the given strength of the spin-orbit interaction.

Keywords Superconductivity · Inhomogeneous state · Spin-orbit interaction · Order parameter · Singularity in low temperature region

1 Introduction

Very thin film deposited on a substrate can be in a superconducting state [1, 2], even in very strong longitudinal magnetic fields and with strong spin-orbit interactions. In paper [1], single atomic layer films of Pb on Si(111) substrate have been studied. Superconducting transition temperature was 1.83 K. The upper critical field was estimated to be 1450 G. The experimental data for order parameter Δ are in a good agreement with the BCS theory. In the paper [2], the superconductivity with T_c above 100K in the FeSe on the substrate SrTiO₃ was estimated. The temperature dependence of critical current J_c was fitted to the Ginzburg-Landau functional. It was found that J_c decreased with increasing magnetic field up to 11T at 3K.

The order parameter Δ in such a system is the function of three parameters: magnetic field, spin-orbit interaction, temperature. Equation $\Delta = 0$ creates surface in this space: critical transition surface. The critical transition surface on

the subspace spanned by magnetic field, spin-orbit interaction, and temperature was investigated in a low-temperature region in papers [3, 4]. The point $T = 0$ is a singular point for such a system. It is expected that near the transition surface the behavior of the order parameter also will be nontrivial and will attract special interest for experimental investigations. In this paper, we present the results of theoretical investigation of the space and temperature dependence of the order parameter in the vicinity of critical transition surface. Note that critical values of the longitudinal magnetic field and spin-orbit interaction in the inhomogeneous state are nearly twice as large as the same values are for homogeneous state. We investigate the state starting from the state with the maximal value of the critical magnetic field for fixed value of the spin-orbit interaction at $T = 0$.

2 Equation System for the Superconducting Order Parameter

For a thin superconducting film, deposited on a substrate, the spin-orbit interaction can be taken in the form [5, 6]

$$\hat{V}_{SO} = \frac{-i\hbar^2}{2m^2c^2} \left(\left[\frac{\partial U}{\partial \mathbf{r}} \times \frac{\partial}{\partial \mathbf{r}} \right] \hat{\mathbf{S}} \right) \quad (1)$$

where $\hat{\mathbf{S}}$ is the spin operator of an electron, m is the electron mass, c is the speed of light, and U is the self-consistent

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potential. In normal metals, the Green's function is a 2×2 matrix and satisfied the equation

$$\left(\frac{\partial}{\partial \tau} + \hat{L} \right) \hat{G} = \delta(\mathbf{r} - \mathbf{r}') \delta(\tau - \tau') \quad (2)$$

where τ is imaginary time and the operator \hat{L} is

$$\hat{L} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{r}^2} + \hat{V}_{SO} - \mu - \frac{e\hbar}{mc} (\mathbf{H}\mathbf{S}) . \quad (3)$$

The last term is the Zeeman energy, μ is the chemical potential, and \mathbf{H} is an in-plane external magnetic field. The eigenfunctions of operator \hat{L} are of the form

$$\begin{pmatrix} \psi_1^{(n)} \\ \psi_2^{(n)} \end{pmatrix} = \exp \left(\frac{ip_x}{\hbar} x + \frac{ip_y}{\hbar} y \right) \chi_n(z) \begin{pmatrix} f_1^{(n)} \\ f_2^{(n)} \end{pmatrix} . \quad (4)$$

The $\chi_n(z)$ are normalized eigenfunctions of the operator

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + U(z) \right) \chi_n(z) = \epsilon_n \chi_n(z), \quad n = 0, 1, 2, \dots \quad (5)$$

In the subspace with given values of p_x , p_y , and n , the vector $(f_1^{(n)}, f_2^{(n)})$ is a solution of the equation

$$\begin{bmatrix} -\frac{\hbar^2}{4m^2c^2} \hat{\alpha}_n & 0 & p_x + ip_y \\ p_x - ip_y & 0 & 0 \\ 0 & h_x - ih_y & 0 \end{bmatrix} \begin{pmatrix} f_1^{(n)} \\ f_2^{(n)} \end{pmatrix} = \lambda^{(n)} \begin{pmatrix} f_1^{(n)} \\ f_2^{(n)} \end{pmatrix} . \quad (6)$$

with

$$\hat{\alpha}_n = \int_{-\infty}^{\infty} dz \frac{\partial U}{\partial z} |\chi_n(z)|^2, \quad h = \mu_B \mathbf{H}, \quad \mu_B = \frac{e\hbar}{2mc} . \quad (7)$$

Eigenvalues $\lambda^{(n)}$ are

$$\lambda_{\pm}^{(n)} = \pm \sqrt{\frac{(\tilde{\alpha}_n)^2}{4} v_F^2 p^2 + h^2 + (h_x p_y - h_y p_x) v_F \cdot \tilde{\alpha}_n} . \quad (8)$$

where

$$\tilde{\alpha}_n = \hat{\alpha}_n \frac{\hbar}{2m^2 c^2 v_F} . \quad (9)$$

and v_F is Fermi velocity.

The eigenfunctions $f_{\pm}^{(n)}$ are found to be

$$\begin{aligned} f_+^{(n)} &= \frac{1}{\sqrt{2}} \left[1; -\frac{1}{\lambda_+^{(n)}} \left(\frac{\tilde{\alpha} v_F}{2} (p_y - ip_x) + (h_x + ih_y) \right) \right] \\ f_-^{(n)} &= \frac{1}{\sqrt{2}} \left[-\frac{1}{\lambda_-^{(n)}} \left(\frac{\tilde{\alpha} v_F}{2} (p_y + ip_x) + (h_x - ih_y) \right); 1 \right] . \end{aligned} \quad (10)$$

In a normal metal, Green's function decomposes into four blocks (see also, consideration of normal metal without spin-orbit interaction [7])

$$\begin{pmatrix} \hat{G}_{++}^{(0)} & 0 \\ 0 & \hat{G}_{--}^{(0)} \end{pmatrix},$$

and satisfies the equation

$$\begin{pmatrix} \frac{\partial}{\partial \tau} + \hat{L} & 0 \\ 0 & \frac{\partial}{\partial \tau} - \hat{L} \end{pmatrix} \begin{pmatrix} \hat{G}_{++}^{(0)} \\ \hat{G}_{--}^{(0)} \end{pmatrix} = \delta(\mathbf{r} - \mathbf{r}') \delta(\tau - \tau') . \quad (11)$$

From (3), (8), (10), and (11), we obtain

$$\begin{aligned} \hat{G}_{++}^{(0)} &= T \sum_{\omega} \sum_n \chi_n(z) \chi_n^*(z') \\ &\times \sum_{\lambda_+^{(n)} = \infty}^{\infty} \frac{dp_x dp_y}{(2\pi\hbar)^2} \left(f(\mathbf{p})^{(n)} \left(f(\mathbf{p})^{(n)} \right)^+ \right)_+ \\ &\times \frac{\exp \left(\frac{i\mathbf{p}}{\hbar} (\mathbf{r} - \mathbf{r}') \right) \exp(-i\omega(\tau - \tau'))}{-i\omega + \frac{\mathbf{p}^2}{2m} + \epsilon_n - \mu + \lambda_+^{(n)}(\mathbf{p})} \\ \hat{G}_{--}^{(0)} &= T \sum_{\omega} \sum_n \chi_n(z) \chi_n^*(z') \\ &\times \sum_{\lambda_-^{(n)} = \infty}^{\infty} \frac{dp_x dp_y}{(2\pi\hbar)^2} \left(f(\mathbf{p})^{(n)} \left(f(\mathbf{p})^{(n)} \right)^+ \right)_- \\ &\times \frac{\exp \left(\frac{i\mathbf{p}}{\hbar} (\mathbf{r} - \mathbf{r}') \right) \exp(-i\omega(\tau - \tau'))}{-i\omega - \frac{\mathbf{p}^2}{2m} - \epsilon_n + \mu - \lambda_-^{(n)}(\mathbf{p})} . \end{aligned} \quad (12)$$

In (12), quantity $\left(f(\mathbf{p})^{(n)} \left(f(\mathbf{p})^{(n)} \right)^+ \right)_{\pm}$ is matrix 2×2 with usual matrix product. In order to have a strong enough spin-orbit interaction, the film thickness should be very small (i.e., of the order of interatomic distances). Then, the energy distance in ϵ_n is large. This circumstance enables us to keep only the term $n = 0$ in the sum over n . The function (10) forms a complete basis in terms of which we can express the electron-electron interaction as

$$H_{\text{int}} = \frac{1}{2} \int d^3 \mathbf{r} d^3 \mathbf{r}' V(\mathbf{r} - \mathbf{r}') (\psi_v^+(\mathbf{r}) (\psi_{\mu}^+(\mathbf{r}') \psi_{\mu}(\mathbf{r}')) \psi_v(\mathbf{r})) \quad (13)$$

with indexes $v, \mu = \pm$. We assume below that the potential V is δ -function like: $V(\mathbf{r} - \mathbf{r}') = V_0 \delta(\mathbf{r} - \mathbf{r}')$. We consider Cooper pairing of the type $\langle \psi_+(\mathbf{r}) \psi_-(\mathbf{r}') \rangle$ – electrons only, i.e., Cooper pairs formed from different Fermi surfaces [7, 8].

In superconductor, Green's function \tilde{G} is matrix (4×4) and satisfies the equation

$$\begin{aligned}\tilde{G} &= \begin{pmatrix} \hat{G}_{++} & \hat{F} \\ \hat{F}^+ & \hat{G}_{--} \end{pmatrix}, \quad \begin{pmatrix} \frac{\partial}{\partial \tau} + \hat{L} & \hat{\Delta} \\ \hat{\Delta}^+ & \frac{\partial}{\partial \tau} - \hat{L} \end{pmatrix} \\ \tilde{G} &= \delta(\mathbf{r} - \mathbf{r}')\delta(\tau - \tau') .\end{aligned}\quad (14)$$

The operator $\hat{\Delta}(\mathbf{r})$ is [3]

$$\hat{\Delta}(\mathbf{r}) = \Delta(\mathbf{r}) \begin{pmatrix} 1; 0 \\ 0; 1 \end{pmatrix} Tr \quad (15)$$

where Tr denotes taking the trace. The self-consistency equation is

$$\Delta = |V_0| \cdot Tr \hat{F}(\mathbf{r}, \mathbf{r}, \tau = \tau') .\quad (16)$$

Equation system (12), (14), (15), (16) is a complete equation system for order parameter.

3 Inhomogeneous Pairing Near Critical Transition Surface

We solve the system of equations for the order parameter $\Delta(\mathbf{r})$ near the critical transition surface by the perturbation theory. From (14), we obtain

$$\begin{aligned}\hat{G}_{++} &= \hat{G}_{++}^{(0)} + \hat{G}_{++}^{(0)} \hat{\Delta} \hat{G}_{--}^{(0)} \hat{\Delta}^+ \hat{G}_{++}^{(0)} ; \\ \hat{G}_{--} &= \hat{G}_{--}^{(0)} + \hat{G}_{--}^{(0)} \hat{\Delta}^+ \hat{G}_{++}^{(0)} \hat{\Delta} \hat{G}_{--}^{(0)} ; \\ \hat{F}^+ &= -\hat{G}_{--}^{(0)} \hat{\Delta}^+ \left[\hat{G}_{++}^{(0)} + \hat{G}_{++}^{(0)} \hat{\Delta} \hat{G}_{--}^{(0)} \hat{\Delta}_0^+ \hat{G}_{++}^{(0)} \right] ; \\ \hat{F} &= -\hat{G}_{++}^{(0)} \hat{\Delta} \left[\hat{G}_{--}^{(0)} + \hat{G}_{--}^{(0)} \hat{\Delta}^+ \hat{G}_{++}^{(0)} \hat{\Delta} \hat{G}_{--}^{(0)} \right] .\end{aligned}\quad (17)$$

Such perturbation procedure can be easily continued up to the infinity. The behavior of the inhomogeneous order parameter near the critical surface is singular. As a result, a partial summation of “dangerous” terms should be made in the expansion (17). To do this, we express the order parameter $\Delta(\mathbf{r})$ in the inhomogeneous state in the form of a Fourier series

$$\Delta(r) = \alpha_1 \cos((\mathbf{Q}\mathbf{r})/\hbar) + \alpha_2 \cos(3(\mathbf{Q}\mathbf{r})/\hbar) + \alpha_3 \cos(5(\mathbf{Q}\mathbf{r})/\hbar) + \dots \quad (18)$$

All terms inside the fifth order perturbation theory are presented in explicit form in “Appendix”. In each order of perturbation theory (see (17)), the value of separate element is determined by the product of phase factors $\exp(ik_j(\mathbf{Q}\mathbf{r}_j)/\hbar)$ (k_j —integer number). For the term of function $Tr \hat{F}(\mathbf{r}, \mathbf{r}, \tau = \tau')$, proportional to $\cos((\mathbf{Q}\mathbf{r})/\hbar)$, the largest value in each order of perturbation theory arises only from correlated product with phase factor equal to $\exp\{i\mathbf{Q}[(\mathbf{r}_1 - \mathbf{r}_2) + \dots + (\mathbf{r}_{2K-1} - \mathbf{r}_{2K})] + \mathbf{r}_{2K+1}\}$ (or to complex conjugate). For the term of function $Tr \hat{F}(\mathbf{r}, \mathbf{r}, \tau = \tau')$ proportional to $\cos(3(\mathbf{Q}\mathbf{r})/\hbar)$, the largest value in each order of perturbation theory arises from correlated product with phase factor of type $\exp\{i\mathbf{Q}[r_1 + (\mathbf{r}_2 - \mathbf{r}_3) + \dots + (\mathbf{r}_{2K-2} - \mathbf{r}_{2K-1})] + \mathbf{r}_{2K} + \mathbf{r}_{2K+1}\}$ (or complex conjugate). For other terms, similar rules exist also.

Partial summation over these terms can be made in all orders of perturbation theory. As result to the function $F_1(\mathbf{r}, \mathbf{r}, \tau = \tau')$, we obtain the next value (see “Appendix”)

$$\begin{aligned}F_1(\mathbf{r}, \mathbf{r}, \tau = \tau') &= T \sum_{\omega} |\chi_0(z)|^2 \int_{-\infty}^{+\infty} \frac{md\xi}{(2\pi\hbar)^2} \int_0^{2\pi} d\varphi \\ &\left\{ \frac{\alpha_1}{2} \cos\left(\frac{(\mathbf{Q}\mathbf{r})}{\hbar}\right) \left(\frac{1}{\xi^2 - (i\omega - \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2 + \alpha_1^2/4} + \frac{1}{\xi^2 - (i\omega + \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2 + \alpha_1^2/4} \right) \right. \\ &+ \frac{\alpha_2}{2} \cos\left(\frac{3(\mathbf{Q}\mathbf{r})}{\hbar}\right) \left(\frac{1}{\xi^2 - (i\omega - \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} + \frac{1}{\xi^2 - (i\omega + \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} \right) \\ &+ \frac{\alpha_3}{2} \cos\left(\frac{5(\mathbf{Q}\mathbf{r})}{\hbar}\right) \left(\frac{1}{\xi^2 - (i\omega - \frac{5(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} + \frac{1}{\xi^2 - (i\omega + \frac{5(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} \right) \left. \right\} \\ &- T \sum_{\omega} \chi_0(z) \chi_0^*(z) \int_{-\infty}^{+\infty} \frac{md\xi}{(2\pi\hbar)^2} \int_0^{2\pi} d\varphi\end{aligned}$$

$$\begin{aligned}
& \left\{ \frac{\alpha_1^3}{8} \cos\left(\frac{3(\mathbf{Qr})}{\hbar}\right) \left(\frac{1}{\xi^2 - \left(i\omega - \frac{3(\mathbf{PQ})}{2m} - \lambda\right)^2} \cdot \frac{1}{\xi^2 - \left(i\omega + \frac{(\mathbf{PQ})}{2m} - \lambda\right)^2 + \alpha_1^2/4} \right. \right. \\
& + \frac{1}{\xi^2 - \left(i\omega + \frac{3(\mathbf{PQ})}{2m} - \lambda\right)^2} \cdot \frac{1}{\xi^2 - \left(i\omega - \frac{(\mathbf{PQ})}{2m} - \lambda\right)^2 + \alpha_1^2/4} \Bigg) \\
& + \frac{\alpha_1^3}{4} \cos\left(\frac{(\mathbf{Qr})}{\hbar}\right) \left[\frac{1}{\left(-i\omega + \xi - \frac{3(\mathbf{PQ})}{2m} + \lambda\right) \left(i\omega + \xi - \frac{(\mathbf{PQ})}{2m} - \lambda\right) \left(\xi^2 - \left(i\omega - \frac{(\mathbf{PQ})}{2m} - \lambda\right)^2 + \alpha_1^2/4\right)} \right. \\
& \left. \left. + \frac{1}{\left(-i\omega + \xi + \frac{3(\mathbf{PQ})}{2m} + \lambda\right) \left(i\omega + \xi + \frac{(\mathbf{PQ})}{2m} - \lambda\right) \left(\xi^2 - \left(i\omega + \frac{(\mathbf{PQ})}{2m} - \lambda\right)^2 + \alpha_1^2/4\right)} \right] \right\} \quad (19)
\end{aligned}$$

here (\mathbf{PQ}) is a scalar product of vector \mathbf{P} on Fermi surface and vector \mathbf{Q} , φ is angle between \mathbf{P} and \mathbf{H} , $\lambda = \lambda_+$.

Terms F_2 , F_3 can be considered as a small correction to the quantity $\text{Tr } \hat{F}(r, r, \tau = \tau')$. As a result, general equation to the order parameter near critical transition surface is

$$\alpha_1 \cos\left(\frac{(\mathbf{Qr})}{\hbar}\right) + \alpha_2 \cos\left(\frac{3(\mathbf{Qr})}{\hbar}\right) = |V_0| \cdot F_1 \quad (20)$$

Equations (19), (20) enable us to obtain expressions for free energy F on the subspace of the periodic function (18). The free energy F is in such a case a function of the parameters $\{\alpha_1, \alpha_2; \dots; P Q / 2m\}$. For any value of temperature T , the parameter $P Q / 2m$ can be found from the equation

$$\frac{\partial F}{\partial (P Q / 2m)} = 0. \quad (21)$$

here $P = P_F$.

The system of equations (20) itself can be found from extremum condition of functional F over parameters $\{\alpha_1, \alpha_2; \dots\}$, i.e.,

$$\frac{\partial F}{\partial \alpha_j} = 0, \quad \{\alpha_j = 1, 2, \dots\}. \quad (22)$$

Below, we will consider low-temperature region $T \ll P Q / 2m$.

Note that integrals in (19) can be written down in a form more simple for integration. To do this, we note that in a low-temperature region the main contribution to the

integrals arises from regions of φ close to $\pi/2$, with a_- in denominator of integrals, or in the regions near the points $\{\varphi_0 = -\arcsin(|R_2|); \varphi_1 = -\pi - \varphi_0\}$ if in denominator of integrals stay a_+ . The quantities a_{\pm} are equal to

$$a_{\pm} = \frac{p_F Q}{2m} \sin \varphi \pm \lambda. \quad (23)$$

In the vicinity of point $\varphi = \frac{\pi}{2}$, we have

$$\begin{aligned}
\varphi &= \frac{\pi}{2} + \delta\varphi; \quad \sin \varphi = 1 - \frac{\delta\varphi^2}{2}; \\
a_- &= -\frac{h}{2\sqrt{\gamma_1}} \left\{ \frac{1-R_2}{2} (\delta\varphi)^2 + \frac{\delta\gamma_1}{\gamma_1} \right\}; \quad \frac{h}{2\sqrt{\gamma_1}} \frac{\delta\gamma_1}{\gamma_1} = -\pi T \beta
\end{aligned} \quad (24)$$

The quantities $\{\delta\gamma_1/\gamma_1, \beta\}$ have been found in paper [4]. For $T = 0$, eight branches are found in paper [3] with different values of \mathbf{Q} on the plane of parameters (γ_1, γ_2) , where

$$\gamma_1 = \left(\frac{2h}{v_F Q} \right)^2, \quad \gamma_2 = \left(\frac{\tilde{\alpha} \epsilon_F}{h} \right)^2 \quad (25)$$

Optimal are branches I, II. These branches are parametrized by one parameter $R_2 (-1 < R_2 < -1/2)$. Parameter γ_2 we consider as given. And for small values of T (not equal to 0), we can put [4]

$$\frac{\delta\gamma_1}{\gamma_1} = -\beta Z \frac{1-R_2}{2} \quad (26)$$

The quantity β is dimensionless function of Z . Definition of function Z and exact equation for β are given in (49). In main approximation, we have

$$\beta = \frac{1}{\pi} \ln \left(\frac{\pi}{(1 - R_2)\sqrt{Z}} \right) \quad (27)$$

In the vicinity of point $\varphi_0 = -\arcsin(|R_2|)$, we have

$$\begin{aligned} \sin \varphi &= R_2 + \sqrt{1 - R_2^2} \delta\varphi; \\ a_+ &= \frac{h}{\sqrt{\gamma_1}} \left\{ -\sqrt{1 - R_2^2} \frac{1 - R_2}{2R_2} \delta\varphi - \frac{\delta\gamma_1 R_2}{2\gamma_1} \right\}. \end{aligned} \quad (28)$$

And in the vicinity of point $\varphi_1 = -\pi + \arcsin(|R_2|)$, we obtain

$$\begin{aligned} \sin \varphi &= R_2 - \sqrt{1 - R_2^2} \delta\varphi; \\ a_+ &= \frac{h}{\sqrt{\gamma_1}} \left\{ \sqrt{1 - R_2^2} \frac{1 - R_2}{2R_2} \delta\varphi - \frac{\delta\gamma_1 R_2}{2\gamma_1} \right\}. \end{aligned} \quad (29)$$

Now, we define three integrals $\{J, J_1, J_2\}$ that are parts of integrals in (19).

$$\begin{aligned} J &= T \sum_{\omega} (\chi_0(z))^2 \int_{-\infty}^{\infty} \frac{d\xi}{(2\pi\hbar)^2} \int_0^{2\pi} d\varphi \left\{ \left(\frac{1}{\xi^2 + \frac{\alpha_1^2}{4} - (i\omega - a_+)^2} + \frac{1}{\xi^2 + \frac{\alpha_1^2}{4} - (i\omega + a_-)^2} \right) \right. \\ &\quad \left. - \left(\frac{1}{\xi^2 - (i\omega - a_+)^2} + \frac{1}{\xi^2 - (i\omega + a_-)^2} \right) \right\} \\ J_1 &= T \sum_{\omega} (\chi_0(z))^2 \int_{-\infty}^{\infty} \frac{d\xi}{(2\pi\hbar)^2} \int_0^{2\pi} d\varphi \left\{ \frac{\xi^2 - (i\omega + a_-)^2}{\xi^2 - (i\omega - \frac{3(PQ)}{2m} - \lambda)^2} \left(\frac{1}{\xi^2 - (i\omega + a_-)^2} - \frac{1}{\xi^2 + \frac{\alpha_1^2}{4} - (i\omega + a_-)^2} \right) \right. \\ &\quad \left. + \frac{\xi^2 - (i\omega - a_+)^2}{\xi^2 - (i\omega + \frac{3(PQ)}{2m} - \lambda)^2} \left(\frac{1}{\xi^2 - (i\omega - a_+)^2} - \frac{1}{\xi^2 + \frac{\alpha_1^2}{4} - (i\omega - a_+)^2} \right) \right\} \\ J_2 &= T \sum_{\omega} (\chi_0(z))^2 \int_{-\infty}^{\infty} \frac{d\xi}{(2\pi\hbar)^2} \int_0^{2\pi} d\varphi \left\{ \frac{-i\omega + \xi + a_+}{(-i\omega + \xi - \frac{3(PQ)}{2m} + \lambda)} \left(\frac{1}{\xi^2 - (i\omega - a_+)^2} - \frac{1}{\xi^2 + \frac{\alpha_1^2}{4} - (i\omega - a_+)^2} \right) \right. \\ &\quad \left. + \frac{-i\omega + \xi - a_-}{(-i\omega + \xi + \frac{3(PQ)}{2m} + \lambda)} \left(\frac{1}{\xi^2 - (i\omega + a_-)^2} - \frac{1}{\xi^2 + \frac{\alpha_1^2}{4} - (i\omega + a_-)^2} \right) \right\} \end{aligned} \quad (30)$$

More simple for calculations are derivatives of integrals $\{J, J_1, J_2\}$ over parameter α_1 . With help from (24), (28), (29), (30), we obtain

$$\begin{aligned} \frac{\partial J}{\partial \alpha_1} &= T \sum_{\omega} |\chi_0|^2 \int_{-\infty}^{\infty} \frac{d\xi}{(2\pi\hbar)^2} \frac{\partial}{\partial \alpha_1} \left\{ \left(\frac{2\sqrt{\gamma_1}}{h} \frac{2}{1 - R_2} \right)^{1/2} \int_{-\infty}^{\infty} dt \frac{1}{\xi^2 + \frac{\alpha_1^2}{4} - \left[i\omega - \left(t^2 + \frac{h}{2\sqrt{\gamma_1}} \frac{\delta\gamma_1}{\gamma_1} \right) \right]^2} \right. \\ &\quad \left. - 2 \left(\frac{2|R_2|}{1 - R_2} \frac{\sqrt{\gamma_1}}{h\sqrt{1 - R_2^2}} \right) \int_{-\infty}^{\infty} dt \frac{1}{\left(t - i\omega + \sqrt{\xi^2 + \alpha_1^2/4} \right) \left(t - i\omega - \sqrt{\xi^2 + \alpha_1^2/4} \right)} \right\}. \end{aligned} \quad (31)$$

The last integral in (31) is equal to 0. That is, the main contribution arises only from term with a_- in denominator.

$$\begin{aligned} -\frac{2}{\alpha_1} \frac{\partial}{\partial \alpha_1} \left(\frac{2}{\alpha_1} \frac{\partial J_1}{\partial \alpha_1} \right) &= T \sum_{\omega} |\chi_0(z)|^2 \int_{-\infty}^{\infty} \frac{d\xi}{(2\pi\hbar)^2} \int_0^{2\pi} d\varphi \frac{\xi^2 - (i\omega + a_-)^2}{\xi^2 - \left(i\omega - \frac{3(\mathbf{PQ})}{2m} - \lambda\right)^2} \\ &\cdot \frac{2}{\left(\xi^2 + \frac{\alpha_1^2}{4} - (i\omega + a_-)^2\right)^3} \\ -\frac{2}{\alpha_1} \frac{\partial}{\partial \alpha_1} \left(\frac{2}{\alpha_1} \frac{\partial J_2}{\partial \alpha_1} \right) &= T \sum_{\omega} |\chi_0(z)|^2 \int_{-\infty}^{\infty} \frac{d\xi}{(2\pi\hbar)^2} \int_0^{2\pi} d\varphi \frac{-i\omega + \xi - a_-}{-i\omega + \xi + \frac{3(\mathbf{PQ})}{2m} + \lambda} \\ &\cdot \frac{2}{\left(\xi^2 + \frac{\alpha_1^2}{4} - (i\omega + a_-)^2\right)^3}. \end{aligned} \quad (32)$$

Main contribution in the integral value arises from the point ($\varphi = \frac{\pi}{2}$), where we will put

$$\varphi = \frac{\pi}{2} + \delta\varphi, \quad \sin \varphi = 1 - (\delta\varphi)^2/2, \quad \delta\varphi = \left(\frac{2\sqrt{\gamma_1}}{h} \frac{2}{1-R_2} \right)^{1/2} t. \quad (33)$$

Equations (31), (32), and (33) enable us to calculate the value of all integrals (J, J_1, J_2) and complete estimation of equation for order parameter in low-temperature region.

4 Subregion of Low-Temperature Region $\alpha_1 > 2\pi T\beta$

The low-temperature region $P_F Q/m \gg \pi T$ decays on two subregions: $\alpha_1 > 2\pi T\beta$ and $\alpha_1 \ll 2\pi T\beta$. We will consider first the region $\alpha_1 > 2\pi T\beta$. In this region, we obtain from (31)

$$\begin{aligned} \frac{\partial J}{\partial \alpha_1} &= \langle |\chi_0(z)|^2 \rangle \left(\frac{2\sqrt{\gamma_1}}{h} \frac{2}{1-R_2} \right)^{1/2} \frac{\partial}{\partial \alpha_1} \int_{-\infty}^{\infty} \frac{d\xi}{(2\pi\hbar)^2} \int_{-\infty}^{\infty} dt \\ &\times \left\{ \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{1}{\xi^2 + \frac{\alpha_1^2}{4} + (\omega + i(t^2 - \pi T\beta))^2} \right. \\ &+ \left[\frac{T}{2i} \int dy (tg(\pi y) - i) + \frac{T}{2i} \int dy (tg(\pi y) + i) \right] \\ &\left. \times \frac{1}{\xi^2 + \frac{\alpha_1^2}{4} - [i2\pi Ty - (t^2 - \pi T\beta)]^2} \right\}. \end{aligned} \quad (34)$$

Here the arrow means the integration contour and points indicate the poles of $tg(\pi y)$.

The same situation takes place for integrals $\{J_1, J_2\}$. We have

In the range $\alpha_1 > 2\pi T\beta$, we obtain from (34)

$$\begin{aligned} \frac{\partial J}{\partial \alpha_1} &= \langle |\chi_0(z)|^2 \rangle \left(\frac{2\sqrt{\gamma_1}}{h} \frac{2}{1-R_2} \right)^{1/2} \int_{-\infty}^{\infty} \frac{d\xi}{(2\pi\hbar)^2} \frac{\partial}{\partial \alpha_1} \\ &\left\{ \frac{R}{\sqrt{\xi^2 + \alpha_1^2/4}} - \int_0^R \frac{dt}{\sqrt{\xi^2 + \alpha_1^2/4}} \frac{\exp(-(R^2 - t^2)/T)}{1 + \exp(-(R^2 - t^2)/T)} \right. \\ &- \int_0^{\infty} \frac{dt}{\sqrt{\xi^2 + \alpha_1^2/4}} \frac{\exp(-\left(t^2 + \sqrt{\xi^2 + \alpha_1^2/4} - \pi T\beta\right)/T)}{1 + \exp(-\left(t^2 + \sqrt{\xi^2 + \alpha_1^2/4} - \pi T\beta\right)/T)} \\ &\left. + \int_R^{\infty} \frac{dt}{\sqrt{\xi^2 + \alpha_1^2/4}} \frac{\exp(-(t^2 - R^2)/T)}{1 + \exp(-(t^2 - R^2)/T)} \right\} \end{aligned} \quad (35)$$

$$\text{where } R = \left(\sqrt{\xi^2 + \alpha_1^2/4} + \pi T\beta \right)^{1/2}.$$

The second and fourth terms in (35) strongly cancel each other. Expansion is going over powers of (T/R^2) . As result, we obtain

$$\begin{aligned} &- \int_0^R dt \frac{\exp(-(R^2 - t^2)/T)}{1 + \exp(-(R^2 - t^2)/T)} \\ &+ \int_R^{\infty} dt \frac{\exp(-(t^2 - R^2)/T)}{1 + \exp(-(t^2 - R^2)/T)} = -\frac{T^2}{4 \cdot R^3} \zeta_{(2)}, \\ &\int_{-\infty}^{\infty} d\xi \int_0^{\infty} \frac{dt}{\sqrt{\xi^2 + \alpha_1^2/4}} \frac{\exp(-\left(t^2 + \sqrt{\xi^2 + \alpha_1^2/4} - \pi T\beta\right)/T)}{1 + \exp(-\left(t^2 + \sqrt{\xi^2 + \alpha_1^2/4} - \pi T\beta\right)/T)} \\ &= \frac{\pi T}{\sqrt{\alpha_1}} \ln \left(1 + \exp \left(-\left(\frac{\alpha_1}{2T} - \pi\beta \right) \right) \right) \end{aligned} \quad (36)$$

Final answer for the function J in the region $\alpha_1 > 2\pi T\beta$ is

$$J = \left\langle |\chi_0(z)|^2 \right\rangle \left(\frac{2\sqrt{\gamma_1}}{h} \frac{2}{1 - R_2} \right)^{1/2} \frac{1}{(2\pi\hbar)^2} \cdot \left\{ J^{(2)} - \frac{\pi T}{\sqrt{\alpha_1}} \ln \left[1 + \exp \left(- \left(\frac{\alpha_1}{2T} - \pi\beta \right) \right) \right] - \frac{\zeta(2)T^2}{2} \int_0^\infty \frac{d\xi}{R^3 \sqrt{\xi^2 + \frac{\alpha_1^2}{4}}} \right\} \quad (37)$$

here $\zeta(x)$ —is Riemann ζ function, and function $J^{(2)}$ is given by equation

$$\begin{aligned} \frac{\partial J^{(2)}}{\partial \alpha_1} &= 2 \int_0^\infty d\xi \frac{\partial}{\partial \alpha_1} \left(\frac{R}{\sqrt{\xi^2 + \alpha_1^2/4}} \right) \\ &= -\frac{1}{\sqrt{2\alpha_1}} \int_0^\infty dy \frac{\sqrt{y^2 + 1} + 4\pi T\beta/\alpha_1}{(y^2 + 1)^{3/2} \left(\sqrt{y^2 + 1} + 2\pi T\beta/\alpha_1 \right)^{1/2}}. \end{aligned} \quad (38)$$

It has series expansion over parameter $(2\pi T\beta/\alpha_1)$

$$J^{(2)} = -\sqrt{2\alpha_1} C_1 + \sqrt{2\alpha_1} \cdot \frac{3\pi T\beta}{\alpha_1} C_2 + \dots \quad (39)$$

with coefficients C_1, C_2 equal to

$$\begin{aligned} C_1 &= \int_0^\infty \frac{dy}{(y^2 + 1)^{5/4}} = \sqrt{2} \left[(2 - \sqrt{2}) + \sum_{K=1}^\infty B_K \right] = 1.198134; \\ B_1 &= \frac{1}{3}, \quad B_K = -B_{K-1} \frac{(K - 5/4)(K - 1/2)}{K(K - 1/4)}; \\ C_2 &= \int_0^\infty \frac{dy}{(y^2 + 1)^{7/4}} = \frac{\sqrt{2}}{3} \sum_{K=0}^\infty \tilde{B}_K = 0.874015; \end{aligned}$$

$$\begin{aligned} \tilde{B}_0 &= 2, \quad \tilde{B}_K = -\tilde{B}_{K-1} \cdot \frac{(K - 1/2)}{K} \cdot \frac{(K - 3/4)}{K + 1/4}; \quad K \geq 1 \\ \int_0^\infty \frac{dy}{(y^2 + 1)^{9/4}} &= \frac{3}{5} C_1; \quad \int_0^\infty \frac{dy}{(y^2 + 1)^{11/4}} = \frac{5}{7} C_2; \dots \end{aligned} \quad (40)$$

The last integral in (37) also has series expansion over parameter $2\pi T\beta/\alpha_1$.

$$\begin{aligned} \int_0^\infty \frac{d\xi}{R^3 \sqrt{\xi^2 + \alpha_1^2/4}} &= \left(\frac{2}{\alpha_1} \right)^{3/2} \int_0^\infty \frac{dy}{(y^2 + 1)^{5/4} \left(1 + \frac{2\pi T\beta}{\alpha_1 \sqrt{y^2 + 1}} \right)^{3/2}} \\ &= \left(\frac{2}{\alpha_1} \right)^{3/2} \left[C_1 - \frac{3\pi T\beta}{\alpha_1} C_2 \dots \right]. \end{aligned} \quad (41)$$

In the same way, we calculate the value of integrals $\{J_1, J_2\}$ from (32). We have

$$\begin{aligned} J_1 &= \left\langle |\chi_0(z)|^2 \right\rangle \cdot \left(\frac{2\sqrt{\gamma_1}}{h} \frac{2}{1 - R_2} \right)^{1/2} \frac{1}{(2\pi\hbar)^2} \left(\frac{m}{2P_F Q} \right)^2 \\ &\quad \left\{ \frac{\alpha_1^2}{4} \left(\frac{T^2 \zeta(2)}{2} \int_0^\infty \frac{d\xi}{R^3 \sqrt{\xi^2 + \alpha_1^2/4}} \right. \right. \\ &\quad \left. \left. + \frac{\pi T}{\sqrt{\alpha_1}} \ln \left[1 + \exp \left(- \left(\frac{\alpha_1}{2T} - \pi\beta \right) \right) \right] \right) + J_1^{(2)} \right\} \end{aligned} \quad (42)$$

where function $J_1^{(2)}$ is solution of equation

$$\begin{aligned} \frac{2}{\alpha_1} \frac{\partial}{\partial \alpha_1} \left(\frac{2}{\alpha_1} \frac{\partial J_1^{(2)}}{\partial \alpha_1} \right) &= 2 \left(\frac{2}{\alpha_1} \right)^{3/2} \int_0^\infty \frac{dy}{(y^2 + 1)^{5/2}} \\ &\quad \times (y^2 + 1/4) \left(\sqrt{y^2 + 1} + \frac{2\pi T\beta}{\alpha_1} \right)^{1/2} \end{aligned} \quad (43)$$

Function $J_1^{(2)}$ has series expansion over parameter $2\pi T\beta/\alpha_1$. We obtain from (43)

$$J_1^{(2)} = \frac{22}{50} C_1 \sqrt{2} \alpha_1^{5/2} - \frac{13}{21} \sqrt{2} \pi T \beta C_2 \cdot \alpha_1^{3/2} + \dots \quad (44)$$

Function J_2 is equal to (in the range $\alpha_1 > 2\pi T\beta$)

$$\begin{aligned} J_2 = & - \left\langle |\chi_0(z)|^2 \right\rangle \frac{1}{(2\pi\hbar)^2} \left(\frac{2\sqrt{\gamma_1}}{h} \frac{2}{1-R_2} \right)^{1/2} \frac{m}{2P_F Q} \\ & \left\{ -\frac{T^2 \zeta_{(2)}}{2} \int_0^\infty \frac{d\xi}{R^3} + \frac{\pi T \sqrt{\alpha_1}}{2} \ln \right. \\ & \left. \left[1 + \exp \left(-\left(\frac{\alpha_1}{2T} - \pi\beta \right) \right) \right] + J_2^{(2)} \right\} \quad ; \quad J_2^{(2)} = 0 \end{aligned} \quad (45)$$

The integral in (45) is equal to

$$\begin{aligned} \int_0^\infty \frac{d\xi}{R^3} &= \left(\frac{2}{\alpha_1} \right)^{1/2} \int_0^\infty \frac{dy}{\left(\sqrt{y^2+1} + \frac{2\pi T \beta}{\alpha_1} \right)^{3/2}}; \\ \int_0^\infty \frac{dy}{(y^2+1)^{3/4}} &= 3 \int_0^\infty \frac{dy}{(y^2+1)^{7/4}} = 3C_2. \end{aligned} \quad (46)$$

5 Subregion $\alpha_1 < 2\pi T\beta$

Consider now the low-temperature subregion restricted by condition $\alpha_1 < 2\pi T\beta$. In this case, we will use the equation, estimated in [4].

$$\begin{aligned} & \frac{i}{2} \int_{-\infty}^\infty dt \left\{ \psi' \left(\frac{1}{2} + \frac{i}{2}(t^2 - \beta) \right) - \psi' \left(\frac{1}{2} - \frac{i}{2}(t^2 - \beta) \right) \right\} \\ &= 2\pi^2 \sum_{K=1}^\infty (-)^{K+1} \sqrt{K} \exp(-\pi K \beta) \\ & \int_{-\infty}^\infty dt \left\{ \psi'' \left(\frac{1}{2} + \frac{i}{2}(t^2 - \beta) \right) + \psi'' \left(\frac{1}{2} - \frac{i}{2}(t^2 - \beta) \right) \right\} \\ &= 8\pi^3 \sum_{K=1}^\infty (K)^{3/2} (-)^K \exp(-\pi K \beta) \end{aligned} \quad (47)$$

In main approximation over parameter $\alpha_1/(2\pi T\beta)$, we obtain from (30)

$$\begin{aligned} J &= \frac{\alpha_1^2}{32} \frac{\sqrt{\pi T}}{(2\pi T)^2} \left\langle |\chi_0(z)|^2 \right\rangle \frac{1}{(2\pi\hbar)^2} \left(\frac{2\sqrt{\gamma_1}}{h} \frac{2}{1-R_2} \right)^{1/2} \\ & \int_{-\infty}^\infty dt \left\{ \psi'' \left(\frac{1}{2} + \frac{i}{2}(t^2 - \beta) \right) + \psi'' \left(\frac{1}{2} - \frac{i}{2}(t^2 - \beta) \right) \right\}. \end{aligned} \quad (48)$$

The quantity β is solution of equation [4]

$$\sum_{K=1}^\infty (-)^{K+1} \sqrt{K} \exp(-\pi K \beta) = \frac{1-R_2}{\pi} \sqrt{Z} \quad ; \quad Z = \frac{4\pi T \sqrt{\gamma_1}}{h(1-R_2)}. \quad (49)$$

From (47), (48), and (49), we obtain

$$J = -\frac{\pi \alpha_1^2}{4T} \left(\frac{\sqrt{\gamma_1}}{h} \right) \frac{\left\langle |\chi_0(z)|^2 \right\rangle}{(2\pi\hbar)^2} \quad ; \quad \alpha_1 \ll 2\pi T\beta. \quad (50)$$

From (32), it follows that

$$\begin{aligned} -\frac{2}{\alpha_1} \frac{\partial}{\partial \alpha_1} \left(\frac{2}{\alpha_1} \frac{\partial J_1}{\partial \alpha_1} \right) &= J \cdot \frac{8}{\alpha_1^2} \left(\frac{m}{2P_F Q} \right)^2; \\ J_1 &= \frac{\pi \alpha_1^4}{16T} \left(\frac{m}{2P_F Q} \right)^2 \frac{\left\langle |\chi_0(z)|^2 \right\rangle}{(2\pi\hbar)^2} \left(\frac{\sqrt{\gamma_1}}{h} \right). \end{aligned} \quad (51)$$

In the same approximation, we obtain the next equation for function J_2

$$\begin{aligned} J_2 &= - \left\langle |\chi_0(z)|^2 \right\rangle \left(\frac{m}{2P_F Q} \right) \frac{\alpha_1^2}{16\sqrt{\pi T}} \left(\frac{2\sqrt{\gamma_1}}{h} \cdot \frac{2}{1-R_2} \right)^{1/2} \frac{1}{(2\pi\hbar)^2} \frac{i}{2} \\ & \cdot \int_{-\infty}^\infty dt \left(\psi' \left(\frac{1}{2} + \frac{i}{2}(t^2 - \beta) \right) - \psi' \left(\frac{1}{2} - \frac{i}{2}(t^2 - \beta) \right) \right). \end{aligned} \quad (52)$$

Final expression for value of quantity J_2 , following from (47) and (52), is

$$J_2 = - \left\langle |\chi_0|^2 \right\rangle \frac{1}{(2\pi\hbar)^2} \left(\frac{m}{2P_F Q} \right) \frac{\pi \alpha_1^2}{2} \left(\frac{\sqrt{\gamma_1}}{h} \right). \quad (53)$$

As a result, in low-temperature region $\pi T \ll P_F Q/2m$, the (20) for order parameter acquires the form

$$\begin{aligned} \alpha_1 \cos\left(\frac{(\mathbf{Q}\mathbf{r})}{\hbar}\right) + \alpha_2 \cos\left(\frac{3(\mathbf{Q}\mathbf{r})}{\hbar}\right) &= |V_0|m \left\{ \cos\left(\frac{(\mathbf{Q}\mathbf{r})}{\hbar}\right) \cdot \alpha_1(0.5 \cdot J - J_2) - \frac{\alpha_1}{2} J_1 \cos\left(\frac{(3\mathbf{Q}\mathbf{r})}{\hbar}\right) \right\} \\ &\quad + \frac{|V_0|m \langle |\chi_0(z)|^2 \rangle}{4(2\pi\hbar)^2} \left\{ \alpha_1 \cos\left(\frac{(\mathbf{Q}\mathbf{r})}{\hbar}\right) \left[4\pi \ln\left(\frac{\gamma_1(T=0)\omega_D^2}{h^2}\right) \right. \right. \\ &\quad \left. \left. + 8\pi \ln 2 - 2(1-R_2)Z \cdot \left(1 + \ln\left(\frac{\pi}{(1-R_2)\sqrt{Z}}\right) \right) \right] \right. \\ &\quad \left. + \alpha_2 \cos\left(\frac{3(\mathbf{Q}\mathbf{r})}{\hbar}\right) \left[4\pi \ln\left(\frac{\gamma_1\omega_D^2}{9h^2}\right) + 8\pi \ln 2 \right] \right\} \end{aligned} \quad (54)$$

To obtain (54), we used the value of linear on α_1 terms from paper [4] and next equation

$$\begin{aligned} T \sum_{\omega} \int_{-\infty}^{\infty} \frac{d\xi}{(2\pi\hbar)^2} \int_0^{2\pi} d\varphi \left[\frac{1}{\xi^2 - \left(i\omega - \left(\frac{3(\mathbf{P}\mathbf{Q})}{2m} + \lambda\right)\right)^2} + \frac{1}{\xi^2 - \left(i\omega + \left(\frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)\right)^2} \right] \\ = \frac{1}{2(2\pi\hbar)^2} \left\{ 4\pi \ln\left(\frac{\gamma_1\omega_D^2}{9h^2}\right) + 8\pi \ln 2 \right\}. \end{aligned} \quad (55)$$

Equation (54) gives temperature, magnetic field, and spin-orbit interaction dependence of the order parameter $\Delta(\mathbf{r})$ in low-temperature region $\pi T \ll P_F Q/2m$ near the critical surface.

6 Conclusions

We obtain explicit expression for the order parameter in two-dimensional space (thin films) in inhomogeneous state near the critical surface in low-temperature region $\pi T \ll (P_F Q)/2m$. Low-temperature region $\pi T \ll (P_F Q)/2m$ separated for two subregions: $\alpha_1 > 2\pi T\beta$ and $\alpha_1 < 2\pi T\beta$. In full subregion $\alpha_1 > 2\pi T\beta$, the relative simple general equations for all coefficients are found. In this subregion, series expansion is going over parameter $2\pi\beta T/\alpha_1$. All functions are singular in this subregion. Usual expansion over order parameter Δ near the critical point is going over integer powers of Δ similar to that as it takes place in Ginzburg-Landau approximation: after linear term, cubic term is going. In the considered region, next term has power 3/2 (see (37, 39, 50)). Such singularity will present special interest for experimental investigation. Equation (34) is valid also in subregion $\alpha_1 < 2\pi\beta T$. In this subregion, some additional restrictions arise for integration over ξ, t . Partially, in first integral (34), we obtain restriction from down $\pi T\beta - \sqrt{(\alpha_1)^2/4 + (\xi)^2} < (t)^2 < (R)^2$. In subregion $\alpha_1 << 2\pi T\beta$, expansion of all coefficients is going over

parameter $\alpha_1/2\pi T\beta$. Nontrivial key equation that enables us to relatively easily find expansion coefficients in this region is given by (47).

We present also the general equation for inhomogeneous state in full temperature region near the critical surface. The reconstruction of free energy functional on the subspace of periodic functions can be made with the help of (20).

Acknowledgements The considered problem was formulated by Prof. P. Fulde. I thank him for the permanent attention, numerous discussions, and real collaboration.

Funding Information Open access funding provided by Max Planck Society.

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Appendix

With help from (14), (17), (18), we obtain the next expression for function $\text{Tr}\hat{F}(\mathbf{r}, \mathbf{r}, \tau = \tau')$ inside fifth order perturbation theory over quantity α_1

$$\begin{aligned} \text{Tr}\hat{F}(\mathbf{r}, \mathbf{r}, \tau = \tau') &= F_1(\mathbf{r}, \mathbf{r}, \tau = \tau') + F_2(\mathbf{r}, \mathbf{r}, \tau = \tau') \\ &\quad + F_3(\mathbf{r}, \mathbf{r}, \tau = \tau') \end{aligned} \quad (\text{A1})$$

where

$$\begin{aligned}
F_1(\mathbf{r}, \mathbf{r}, \tau = \tau') = & T \sum_{\omega} \chi_0(z) \chi_0^*(z) \int_{-\infty}^{\infty} \frac{md\xi}{(2\pi\hbar)^2} \int_0^{2\pi} d\varphi \\
& \cdot \left\{ \frac{\alpha_1}{2} \cos\left(\frac{(\mathbf{Q}\mathbf{r})}{\hbar}\right) \left[\frac{1}{\xi^2 - (i\omega - \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} \left(1 - \frac{\alpha_1^2/4}{\xi^2 - (i\omega - \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} \right. \right. \right. \\
& + \frac{(\alpha_1^2/4)^2}{\left(\xi^2 - (i\omega - \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2\right)^2} \left. \right) + \frac{1}{\xi^2 - (i\omega + \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} \\
& \cdot \left. \left(1 - \frac{\alpha_1^2/4}{\xi^2 - (i\omega + \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} + \frac{(\alpha_1^2/4)^2}{\left(\xi^2 - (i\omega + \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2\right)^2} \right) \right] \\
& + \frac{\alpha_2}{2} \cos\left(\frac{3(\mathbf{Q}\mathbf{r})}{\hbar}\right) \left(\frac{1}{\xi^2 - (i\omega - \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} + \frac{1}{\xi^2 - (i\omega + \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} \right) \\
& + \frac{\alpha_3}{2} \cos\left(\frac{5(\mathbf{Q}\mathbf{r})}{\hbar}\right) \left(\frac{1}{\xi^2 - (i\omega - \frac{5(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} + \frac{1}{\xi^2 - (i\omega + \frac{5(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} \right) \Big\} \\
& - T \sum_{\omega} \chi_0(z) \chi_0^*(z) \int_{-\infty}^{\infty} \frac{md\xi}{(2\pi\hbar)^2} \int_0^{2\pi} d\varphi \\
& \cdot \left\{ \frac{\alpha_1^3}{8} \cos\left(\frac{3(\mathbf{Q}\mathbf{r})}{\hbar}\right) \left[\frac{1}{\xi^2 - (i\omega - \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} \left(\frac{1}{\xi^2 - (i\omega + \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} - \frac{\alpha_1^2/4}{\left(\xi^2 - (i\omega + \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2\right)^2} \right) \right. \right. \\
& + \frac{1}{\xi^2 - (i\omega + \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} \cdot \left(\frac{1}{\xi^2 - (i\omega - \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} - \frac{\alpha_1^2/4}{\left(\xi^2 - (i\omega - \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2\right)^2} \right) \Big] \\
& + \frac{\alpha_1^3}{4} \cos\left(\frac{(\mathbf{Q}\mathbf{r})}{\hbar}\right) \left[\frac{1}{(-i\omega + \xi - \frac{3(\mathbf{P}\mathbf{Q})}{2m} + \lambda)(i\omega + \xi - \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)} \left(\frac{1}{\xi^2 - (i\omega - \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} \right. \right. \\
& - \frac{\alpha_1^2/4}{\left(\xi^2 - (i\omega - \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2\right)^2} \Big) + \frac{1}{(-i\omega + \xi + \frac{3(\mathbf{P}\mathbf{Q})}{2m} + \lambda)(i\omega + \xi + \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)} \\
& \cdot \left. \left(\frac{1}{\xi^2 - (i\omega + \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2} - \frac{\alpha_1^2/4}{\left(\xi^2 - (i\omega + \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda)^2\right)^2} \right) \right] \Big\} \quad (\text{A2})
\end{aligned}$$

$$\begin{aligned}
F_2(\mathbf{r}, \mathbf{r}, \tau = \tau') = & T \sum_{\omega} \chi_0(z) \chi_0^*(z) \int_{-\infty}^{\infty} \frac{md\xi}{(2\pi\hbar)^2} \int_0^{2\pi} d\varphi \frac{\alpha_1^5}{32} \left\{ \cos\left(\frac{(\mathbf{Q}\mathbf{r})}{\hbar}\right) \right. \\
& \cdot \left[4 \cdot \left(\frac{1}{\left(i\omega + \xi - \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^3 \left(-i\omega + \xi + \frac{(\mathbf{P}\mathbf{Q})}{2m} + \lambda\right)^2 \left(-i\omega + \xi - \frac{3(\mathbf{P}\mathbf{Q})}{2m} + \lambda\right)} \right. \right. \\
& + \frac{1}{\left(i\omega + \xi + \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^3 \left(-i\omega + \xi - \frac{(\mathbf{P}\mathbf{Q})}{2m} + \lambda\right)^2 \left(-i\omega + \xi + \frac{3(\mathbf{P}\mathbf{Q})}{2m} + \lambda\right)} \left. \right) \\
& + 3 \left(\frac{1}{\xi^2 - \left(i\omega - \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2 \left(\xi^2 - \left(i\omega + \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right)^2} \right. \\
& + \frac{1}{\left(\xi^2 - \left(i\omega + \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right) \left(\xi^2 - \left(i\omega - \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right)^2} \left. \right] + 2 \cos\left(\frac{3(\mathbf{Q}\mathbf{r})}{\hbar}\right) \\
& \cdot \left[\left(\frac{1}{\left(i\omega + \xi + \frac{5(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right) \left(\xi^2 - \left(i\omega - \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right) \left(-i\omega + \xi + \frac{3(\mathbf{P}\mathbf{Q})}{2m} + \lambda\right) \left(\xi^2 - \left(i\omega + \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right)} \right. \right. \\
& + \frac{1}{\left(i\omega + \xi - \frac{5(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right) \left(\xi^2 - \left(i\omega + \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right) \left(-i\omega + \xi - \frac{3(\mathbf{P}\mathbf{Q})}{2m} + \lambda\right) \left(\xi^2 - \left(i\omega - \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right)} \left. \right) \\
& + \left(\frac{1}{\left(\xi^2 - \left(i\omega - \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right) \left(\xi^2 - \left(i\omega + \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right) \left(-i\omega + \xi + \frac{3(\mathbf{P}\mathbf{Q})}{2m} + \lambda\right) \left(i\omega + \xi + \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)} \right. \\
& + \frac{1}{\left(\xi^2 - \left(i\omega + \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right) \left(\xi^2 - \left(i\omega - \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right) \left(-i\omega + \xi - \frac{3(\mathbf{P}\mathbf{Q})}{2m} + \lambda\right) \left(i\omega + \xi - \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)} \left. \right] \\
& + \cos\left(\frac{5(\mathbf{Q}\mathbf{r})}{\hbar}\right) \left(\frac{1}{\left(\xi^2 - \left(i\omega - \frac{5(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right) \left(\xi^2 - \left(i\omega + \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right) \left(\xi^2 - \left(i\omega - \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right)} \right. \\
& + \left. \frac{1}{\left(\xi^2 - \left(i\omega + \frac{5(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right) \left(\xi^2 - \left(i\omega - \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right) \left(\xi^2 - \left(i\omega + \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right)} \right) \right\} \quad (\text{A3})
\end{aligned}$$

$$\begin{aligned}
F_3(\mathbf{r}, \mathbf{r}, \tau = \tau') = & -T \sum_{\omega} \chi_0(z) \chi_0^*(z) \int_{-\infty}^{\infty} \frac{md\xi}{(2\pi\hbar)^2} \int_0^{2\pi} d\varphi \frac{\alpha_1^2 \alpha_2}{8} \left\{ 3 \cos\left(\frac{(\mathbf{Q}\mathbf{r})}{\hbar}\right) \right. \\
& \cdot \left(\frac{1}{\left(\xi^2 - \left(i\omega + \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right) \left(\xi^2 - \left(i\omega - \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right)} + \frac{1}{\left(\xi^2 - \left(i\omega - \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right) \left(\xi^2 - \left(i\omega + \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right)} \right) \\
& + 2 \cos\left(\frac{3(\mathbf{Q}\mathbf{r})}{\hbar}\right) \left[\frac{1}{\xi^2 - \left(i\omega - \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2} \cdot \left(\frac{1}{\left(i\omega + \xi + \frac{5(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right) \left(-i\omega + \xi - \frac{(\mathbf{P}\mathbf{Q})}{2m} + \lambda\right)} \right. \right. \\
& + \frac{1}{\left(i\omega + \xi - \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right) \left(-i\omega + \xi - \frac{(\mathbf{P}\mathbf{Q})}{2m} + \lambda\right)} + \frac{1}{\left(i\omega + \xi - \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right) \left(-i\omega + \xi - \frac{5(\mathbf{P}\mathbf{Q})}{2m} + \lambda\right)} \Big) \\
& + \frac{1}{\xi^2 - \left(i\omega + \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2} \cdot \left(\frac{1}{\left(i\omega + \xi - \frac{5(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right) \left(-i\omega + \xi + \frac{(\mathbf{P}\mathbf{Q})}{2m} + \lambda\right)} \right. \\
& + \frac{1}{\left(i\omega + \xi + \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right) \left(-i\omega + \xi + \frac{(\mathbf{P}\mathbf{Q})}{2m} + \lambda\right)} + \frac{1}{\left(i\omega + \xi + \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right) \left(-i\omega + \xi + \frac{5(\mathbf{P}\mathbf{Q})}{2m} + \lambda\right)} \Big) \Big] + \cos\left(\frac{5(\mathbf{Q}\mathbf{r})}{\hbar}\right) \\
& \cdot \left[\left(\frac{1}{\left(\xi^2 - \left(i\omega - \frac{5(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right) \left(\xi^2 - \left(i\omega + \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right)} + \frac{1}{\left(\xi^2 - \left(i\omega + \frac{5(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right) \left(\xi^2 - \left(i\omega - \frac{3(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right)} \right) \right. \\
& + 2 \left(\frac{1}{\left(\xi^2 - \left(i\omega - \frac{5(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right) \left(-i\omega + \xi - \frac{3(\mathbf{P}\mathbf{Q})}{2m} + \lambda\right) \left(i\omega + \xi - \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)} \right. \\
& \left. \left. \left. + \frac{1}{\left(\xi^2 - \left(i\omega + \frac{5(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)^2\right) \left(-i\omega + \xi + \frac{3(\mathbf{P}\mathbf{Q})}{2m} + \lambda\right) \left(i\omega + \xi + \frac{(\mathbf{P}\mathbf{Q})}{2m} - \lambda\right)} \right) \right] \right\} \quad (\text{A4})
\end{aligned}$$

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