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Memorandum

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Pippard's non-local effect in the case of diffuse scattering

A weak external magnetic field acts on the ground state of the superconductor as a perturbation. Within a perturbation expansion one can show [1, 2, 3] that the following non-local relation between the supercurrent density $\boldsymbol{j}$ and the vector potential $\boldsymbol{A}$ holds (in Coulomb gauge $\nabla\cdot\boldsymbol{A} = 0$):

$$j_\alpha(\boldsymbol{r}) = -\sum_\beta \int \underbrace{\left[R_{\alpha\beta}(\boldsymbol{r}-\boldsymbol{r}') - \frac{e^2 n_\mathrm{S}}{m^*}\,\delta(\boldsymbol{r}-\boldsymbol{r}')\delta_{\alpha\beta}\right]}_{=:\,K_{\alpha\beta}(\boldsymbol{r}-\boldsymbol{r}')} A_\beta(\boldsymbol{r}')\,\mathrm{d}\boldsymbol{r}' \tag{1}$$

where e is the electron charge, n_S the supercarrier density, m^* the effective electron mass, and $\nabla\wedge\boldsymbol{A} = \boldsymbol{B}$. The first term in the square brackets, $R_{\alpha\beta}$, describes the paramagnetic response, whereas the second reflects the diamagnetic one. $K_{\alpha\beta}$ is called the kernel. If the wave function of the electronic ground-state were "rigid" with respect to all perturbations (rather than only those which lead to transverse excitations) $R_{\alpha\beta}$ would be identically zero and Eq.(1) would reduce to the local $\boldsymbol{j}$-$\boldsymbol{A}$ relation

$$j_\alpha(\boldsymbol{r}) = -\frac{1}{\mu_0\lambda_\mathrm{L}^2} A_\alpha(\boldsymbol{r}) \tag{2}$$

with μ_0 the magnetic permeability of the vaccum. This combined with the Maxwell equation $\nabla\wedge\boldsymbol{B} = \mu_0\boldsymbol{j}$ yields, at a plane superconductor-vacuum interface, the result of an exponentially suppressed magnetic field

$$B(z) = B_\mathrm{ext}\,\exp(-z/\lambda_\mathrm{L}) \tag{3}$$

with the London penetration depth $\lambda_\mathrm{L} = \sqrt{\dfrac{m^*}{\mu_0 e^2 n_\mathrm{S}}}$, which is the well known result.

However, $R_{\alpha\beta}$ has a range of the order of the diameter of the Cooper pairs, *i.e.* of the coherence length ξ. The magnetic penetration depth sets the length scale for the decay of the magnetization; for $\lambda \gg \xi$ the spatial variation of the vector potential $\boldsymbol{A}$ over the superconducting pairs is negligible and the one-parameter local description of Eq.(2) holds. If $\xi \gtrsim \lambda$ the full non-local description has to be taken into account.

Using the Maxwell equation and the relation between $\boldsymbol{A}$ and $\boldsymbol{B}$, Eq.(1) transforms to an integro-differential equation

$$\left[\nabla\wedge\nabla\wedge\boldsymbol{A}\right]_\alpha(\boldsymbol{r}) = -\sum_\beta \int K_{\alpha\beta}(\boldsymbol{r}-\boldsymbol{r}')A_\beta(\boldsymbol{r}')\mathrm{d}^3r' \tag{4}$$

This equation can be solved if the boundary conditions are known. For two different boundary conditions Eq.(4) has been discussed [4, 5, 6, 7], which are:

- Specular Reflection, *i.e.* the electrons, Cooper pairs are perfectly reflected from the interface (incoming angle = outgoing angle). In this case Eq.(4) can be simplified by the aim of Fourier transform methods.

- Diffuse scattering, *i.e.* the electrons, Cooper pairs lose all their memory upon scattering on the interface.

The *diffuse scattering* case is mathematical the more difficult one and will be discussed here. The boundary condition for diffuse scattering at the interface and further assuming a isotropic kernel leads to

$$\nabla \wedge \nabla \wedge \boldsymbol{A}(\boldsymbol{r}) = -\int_0^D \left[\iint_0^\infty K(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{A}(\boldsymbol{r}')\,\mathrm{d}^2 r'_{xy} \right] \mathrm{d}r'_z \tag{5}$$

assuming a thin film of thickness D. This simplifies to

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2} A_y(z) = \int_0^D K(|z-z'|) A_y(z)\,\mathrm{d}z \tag{6}$$

with the Pippard kernel

$$K(|z|) = \frac{3}{4}\frac{1}{\xi_0 \lambda^2} \int_1^\infty \left(\frac{1}{t} - \frac{1}{t^3}\right) e^{-|z|t/\xi}\,\mathrm{d}t \tag{7}$$

By introducing a set of dimensionless variables

$$\begin{aligned} s &= z/\xi \\ \Delta &= D/\xi \\ \alpha &= \frac{3}{4}\frac{\xi^3}{\xi_0\lambda^2} \\ F(s) &= \frac{A_y(z)}{\xi B_{\mathrm{ext}}} \\ k(|s|) &= \frac{4}{3}\xi_0\lambda^2 K(|z|) \end{aligned}$$

Eq.(7) transforms into

$$F''(s) = \alpha \int_0^\Delta k(|s-\tilde{s}|) F(\tilde{s})\,\mathrm{d}\tilde{s} \tag{8}$$

$$F'(0) = F'(\Delta) = 1 \tag{9}$$

$$F(0) = 1/2 \tag{10}$$

and $'$ is a derivative with respect to s. $F(s)$ can be written as

$$F(s) = \psi(s) - \psi(\Delta - s) \tag{11}$$

thus, it is enough to solve the equation for $\psi(s)$.

The equation was solved numerically by dividing the film thickness Δ into n intervals of the length $l = \Delta/n$. Using the abbreviation $\psi(k \cdot l) = \psi_k$, $(k = 0, \ldots, n)$, the second derivative can be approximated as

$$\psi''_k \simeq \frac{1}{l^2}\left(\psi_{k+1} - 2\psi_k + \psi_{k-1}\right) \tag{12}$$

In order to implement the right hand side of Eq.(8) efficiently, the following identities are useful

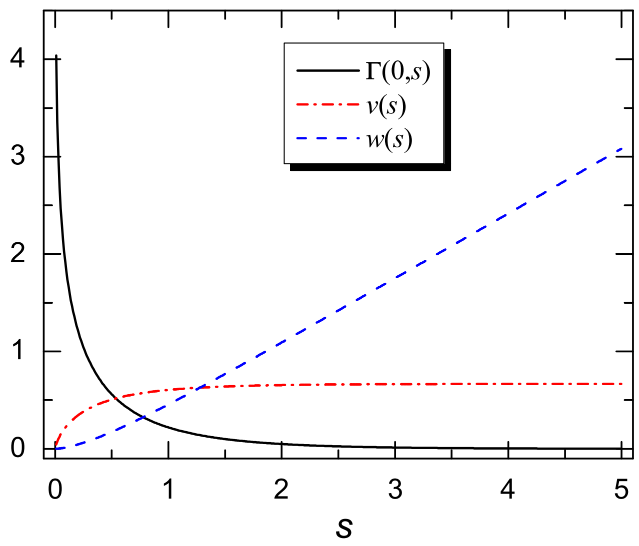

Figure 1: Shows the different relevant functions involved in the calculations.

$$v(s) = -v(-s) = \int_0^s k(|t|)\,\mathrm{d}t =$$
$$\frac{2}{3} + \frac{1}{6}\,e^{-s}\left[s(s-1)-4\right] - \frac{1}{6}s(s^2-6)\Gamma(0,s) \tag{13}$$

$$w(s) = +w(-s) = \int_0^s v(t)\,\mathrm{d}t =$$
$$\frac{1}{12}(8s-3) + \frac{1}{24}\,e^{-s}(s^3-s^2-10s+6) - \frac{1}{24}s^2(s^2-12)\Gamma(0,s) \tag{14}$$

for $s \geq 0$, and where

$$\Gamma(a,s) = \int_s^\infty t^{a-1}e^{-t}\,\mathrm{d}t \tag{15}$$

is the incomplete gamma function. The advantage of using $v(s)$ and $w(s)$ is that these functions are well behaved in the whole variable range, whereas $\Gamma(0,s)$ diverges for $s \to 0$. The functions $v(s)$ and $w(s)$ are shown in Fig.1.

Due to their definition it follows that $k(s) = v'(s) = w''(s)$ and therefore by partial integration

$$\int_0^\Delta k(|s-\tilde{s}|)\psi(\tilde{s})\,\mathrm{d}t = v(\tilde{s}-s)\psi(\tilde{s})\Big|_0^\Delta - \int_0^\Delta v(\tilde{s}-s)\psi(\tilde{s})\,\mathrm{d}t$$
$$= v_{n-i}\psi_n - v_{-i}\psi_0 - \sum_{k=0}^{n-1}\frac{1}{l}\left(\psi_{k+1}-\psi_k\right)\cdot\left(w_{k+1-i}-w_{k-i}\right). \tag{16}$$

Eqs.(12) and (16) together with Eq.(8) lead to the following set of linear equations

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$$\frac{1}{\alpha l^2}\left[\psi_{i+1} - 2\psi_i + \psi_{i-1}\right] = \psi_0 \overbrace{\left[-v_{-i} + \frac{1}{l}(w_{1-i} - w_{-i})\right]}^{=:\, a_i} + \\ + \sum_{k=0}^{n-1} \psi_k \underbrace{\frac{1}{l}\left[w_{k+1-i} - 2w_{k-i} + w_{k-1-i}\right]}_{=:\, c_{ki}} + \psi_n \underbrace{\left[v_{n-i} - \frac{1}{l}(w_{n-i} - w_{n-1-i})\right]}_{=:\, b_i} \tag{17}$$

The boundary conditions translate into

$$\psi'(0) = \frac{1}{2l}\left[-3\psi_0 + 4\psi_1 - \psi_2\right] = 0 \tag{18}$$

$$\psi'(\Delta) = \frac{1}{2l}\left[-3\psi_n - 4\psi_{n-1} + \psi_{n-2}\right] = 1. \tag{19}$$

This equations can be written in matrix form

$$(D - C)\psi = d, \tag{20}$$

where

$$D = \frac{1}{\alpha l^2}\begin{bmatrix} 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & \dots & 0 \\ \vdots & & & & & & \vdots \\ 0 & 0 & \dots & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 \end{bmatrix} \tag{21}$$

$$C = \begin{bmatrix} -3/(2l) & 4/(2l) & -1/(2l) & 0 & \dots & 0 & 0 \\ a_1 & c_{11} & c_{21} & c_{31} & \dots & c_{n-1,1} & b_1 \\ a_2 & c_{12} & c_{22} & c_{32} & \dots & c_{n-1,2} & b_2 \\ \vdots & & & & & & \vdots \\ a_{n-1} & c_{1,n-1} & c_{2,n-1} & c_{3,n-1} & \dots & c_{n-1,n-1} & b_{n-1} \\ 0 & 0 & \dots & 0 & 1/(2l) & -4/(2l) & 3/(2l) \end{bmatrix} \tag{22}$$

$$d = \underbrace{\begin{bmatrix} 0 & 0 & 0 & \dots & 0 & 0 & 1 \end{bmatrix}}_{n+1 \text{ elements}} \tag{23}$$

The first ($k = 0$) and the last row ($k = n$) are due to the boundary conditions of Eqs.(18) and (19). The values for a_i, b_i, and c_{ki} are defined in Eq.(17).

Numerical Implementation

In order to solve the set of linear equations Eq.(20), I used the `nag` libraries [8]. For the incomplete gamma function, the routines `s14bac` and `s14aac` were used. In order to solve explicitly Eq.(20), the routines `f03afc` and `f04ajc` were used.
The fitting has been implemented in ROOT [9] using the TMinuit class.

References

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