Plane Wave expansion for Superconducting Domain Wall

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Abstract

Andreev Approximation Vs. Plane Wave Expansion

Bogoliubov-De Gennes Equations

We need to find the governing equations for the u's and v's which we can calculate self consistently along with the superconducting order parameter(De Gennes). Normalization of $\tilde{\phi}$ requires $\int dx(|u_k(x)|^2 + |v_k(x)|^2) = 1$. To proceed we start with the electronic superconducting Hamiltonian (without the presence of a magnetic field) in the mean field limit.

$$\mathcal{H} = \sum_\alpha \int dx \psi_\alpha^\dagger \left[\frac{p^2}{2m} + U(x)\right]\psi_\alpha - \frac{1}{2}\sum_{\alpha\beta}\int dx dx' \psi_\alpha^\dagger(x)\psi_\beta^\dagger(x')V(x,x')\psi_\beta(x')\psi_\alpha(x) = \mathcal{H}_0 + \mathcal{H}_1$$

From here we can rewrite $\mathcal{H}_1$ as an effective singlet interaction which acts on one particle at a time (ie contains only two operators).

$$\mathcal{H}_0 = \sum_\alpha \int dx \psi_\alpha^\dagger \Big[\mathcal{H}_e + U(x)\Big]\psi_\alpha$$

$$\mathcal{H}_1 = \int dx dx' [\Delta(x,x')\psi_1^\dagger(x)\psi_{-1}^\dagger(x') + \Delta(x,x')^*\psi_{-1}(x')\psi_1(x)]$$

Where we have introduced the superconducting order parameter $\Delta(x,x') = V(x,x') < \psi_{-1}(x')\psi_1(x) >$. Now we compute the commutator $[\mathcal{H}_{eff}, \psi]$ using the anticommutation relations for ψ.

$$[\psi_1(x), \mathcal{H}_{eff}] = (\mathcal{H}_e + U(x))\psi_1 + \int dx' \Delta(x,x')\psi_{-1}^\dagger(x')$$

$$[\psi_{-1}(x), \mathcal{H}_{eff}] = (\mathcal{H}_e + U(x))\psi_{-1} - \int dx' \Delta(x,x')\psi_1^\dagger(x')$$

Now we use the definition of $\psi_\alpha(x) = u(x)\gamma_\alpha + (i\sigma_2^{\alpha\beta})v(x)\gamma_\beta^\dagger$ which diagonalizes the Hamiltonian and separates the t and x variables. Thus, $\mathcal{H}_{eff}$ acting to find the right on a γ gives the energy ϵ

$$\epsilon\gamma_1(t)u(x) + \epsilon\gamma_{-1}^\dagger v^*(x) = (\mathcal{H}_e + U(x))(\gamma_1(t)u(x) - \gamma_{-1}^\dagger(t)v^*(x)) + \int dx' \Delta(x,x')(\gamma_{-1}^\dagger(t)u^*(x') + \gamma_1(t)v(x'))$$

$$\epsilon\gamma_{-1}(t)u(x) - \epsilon\gamma_1^\dagger v^*(x) = (\mathcal{H}_e + U(x))(\gamma_{-1}(t)u(x) + \gamma_1^\dagger(t)v^*(x)) - \int dx' \Delta(x,x')(\gamma_1^\dagger(t)u^*(x') - \gamma_{-1}(t)v(x))$$

Since γ and $\gamma^\dagger$ are linearly independent we can equate like terms to get two equations from each of the two previous expressions. They turn out to be equivalent:

$$\epsilon_k u_k(x) = (\mathcal{H}_e + U(x))u_k(x) + \int dx' \Delta(x,x')v_k(x')$$
$$\epsilon_k v_k(x) = -(\mathcal{H}_e^* + U(x))v_k(x) + \int dx' \Delta^*(x,x')u_k(x')$$

Here we note that $\mathcal{H}_e^* = \mathcal{H}_e$ as long as there is no oribtal field. These are the Bogoliubov-De Genne equations for an inhomogenious superconductor and an integral eigen-equation $\epsilon_k \begin{pmatrix} u_k \\ v_k \end{pmatrix} = \hat{\Omega} \begin{pmatrix} u_k \\ v_k \end{pmatrix}$.

Free Energy

We can use these to calculate Δ and $U(x)$ self consistently. We first consider the pairing potential to be some average value $V(x,x') = V_0$ and minimize the free energy $F =< \mathcal{H} > -TS$. For the full Hamiltonian we have:

$$< \mathcal{H} >= \sum_\alpha \int dx < \psi_\alpha^\dagger \mathcal{H}_e \psi_\alpha > -\frac{V_0}{2} \sum_{\alpha\beta} \int dx dx' < \psi_\alpha^\dagger(x)\psi_\beta^\dagger(x')\psi_\beta(x')\psi_\alpha(x) >$$

The second term can be expanded via Wick contractions:

$$\begin{aligned} < \psi_\alpha^\dagger(x)\psi_\beta^\dagger(x')\psi_\beta(x')\psi_\alpha(x) > &=< \psi_\alpha^\dagger(x)\psi_\beta^\dagger(x') >< \psi_\beta(x')\psi_\alpha(x) > \\ &- < \psi_\alpha^\dagger(x)\psi_\beta(x') >< \psi_\beta^\dagger(x')\psi_\alpha(x) > \\ &+ < \psi_\alpha^\dagger(x)\psi_\alpha(x) >< \psi_\beta^\dagger(x')\psi_\beta(x') > \end{aligned}$$

Now we compute the variation in F:

$$\delta F = \sum_\alpha \int dx \delta[< \psi_\alpha^\dagger \mathcal{H}_e \psi_\alpha >] - V_0 \int dx dx' \Big[\delta[< \psi_1^\dagger(x)\psi_{-1}^\dagger(x') >] < \psi_{-1}(x')\psi_1(x) > + C.C. \Big]$$
$$- \sum_\alpha \delta[< \psi_\alpha^\dagger(x)\psi_\alpha(x') >] < \psi_\alpha^\dagger(x')\psi_\alpha(x) > + \sum_{\alpha\beta} \delta[< \psi_\alpha^\dagger(x)\psi_\alpha(x) >] < \psi_\beta^\dagger(x')\psi_\beta(x') > -T\delta S$$

Now we can compare this variation to the variation in F_{eff} noting that the Bogoliubov formulation diagnolizes $\mathcal{H}_{eff}$.

$$0 = \delta F_{eff} = \sum_\alpha \int dx \delta[< \psi_\alpha^\dagger(\mathcal{H}_e + U(x))\psi_\alpha >]$$
$$+ \int dx dx' \Big[\Delta(x,x')\delta[< \psi_1^\dagger(x)\psi_{-1}^\dagger(x') >] + \Delta^*(x,x')\delta[< \psi_{-1}(x')\psi_1(x) >] \Big] - T\delta S$$

Combining the previous two equations so that $\delta F = 0$ yields expressions for $U(x)$ and Δ. The equation for $U(x)$ is complicated and we will omit it here. The equation for Δ is:

$$\begin{aligned} \Delta(x,x') &= -V_0 < \psi_{-1}(x')\psi_1(x) >= V_0 < \psi_1(x)\psi_{-1}(x') > \\ &= V_0 \sum_k [u_k(x')v_k^*(x)(1 - f_{-1k}) - u_k(x)v_k^*(x')f_{1k}] \end{aligned}$$

Plane Wave Expansion

To solve the Bogoliubov equations we may employ numerical techniques. But first we write $\mathcal{H}_e + U(x) = \frac{\hbar^2 p^2}{2m} - \epsilon_f$.

$$\epsilon_k u_k(x) = (-\frac{\hbar^2 d^2}{2mdx^2} - \epsilon_f)u_k(x) + \int dx' \Delta(x,x')v_k(x')$$
$$\epsilon_k v_k(x) = -(-\frac{\hbar^2 d^2}{2mdx^2} - \epsilon_f)v_k(x) + \int dx' \Delta^*(x,x')u_k(x')$$

At this point it is nice to scale things by the Fermi energy and momentum: $x \to xk_f$, $\epsilon \to \epsilon/\epsilon_f$, $\Delta \to \Delta/\epsilon_f$ We now write the u's and v's as a sum over plane wave states $u(x) = \sum_q u_q e^{iqx}$, where q is scaled by k_f as well. After integrating to pick out a particular mode, these into the scaled BdG equations yield

$$\epsilon u_p = \xi_p u_p + \frac{1}{V}\sum_q \int dx' \int dx \Delta(x,x')v_q e^{iqx'}e^{-ipx}$$
$$\epsilon v_p = -\xi_p v_p + \frac{1}{V}\sum_q \int dx' \int dx \Delta^*(x,x')u_q e^{iqx'}e^{-ipx}$$

Where $\xi_p = p^2 - 1$.

Now the trick is the integral term which is more enlightening to write in terms of the relative (r=x-x') and center of mass coordinate (R=(x+x')/2). Then the integral term can be written as the Fourier transform of the order parameter in these new coordinates. The OP can also be written in separation of variable form $\Delta(r,R) = \Delta_0 g(r)f(R)$. The g(r) results in the OP symmetery (ie S-wave, D-wave etc) Δ_k, and f(R) gives a delta function for homogeneous solution, but in general we write it as $F(q-p) = \int dR \quad f(R)e^{i(q-p)R}$

$$\epsilon u_p = \xi_p u_p + \sum_q v_q \Delta_{(q+p)/2}F(q-p)$$
$$\epsilon v_p = -\xi_p v_p + \sum_q u_q \Delta_{(q+p)/2}F(q-p)$$

Andreev Approximation

The Bogoliubov equations can be simplified by making the Andreev Approximation and substituting the chemical potential times the number operator for $U(x)$. In the Andreev Approximation we assume that the functions u and v take the form $u_(x) = \tilde{u}(x)e^{ix}$ ($e^{ix} = e^{ip_f x}$ in unscaled variables) . This approximation assumes that the envelope function $\tilde{u}(x)$ is slow varying on the same scale as $\Delta(R)$. The function $\tilde{u}$ is assumed to be slowly varying while the exponential is fast varying. The Bogoliubov equations then become:

$$\epsilon\tilde{u}(x)e^{ix} = e^{ix}\left(\tilde{u}(x) - i\frac{d}{dx}\tilde{u}(x) - \frac{d^2}{dx^2}\tilde{u}(x) - \tilde{u}(x)\right) + \int dx' \Delta(x,x')\tilde{v}(x')e^{ix'}$$
$$\epsilon\tilde{v}(x)e^{ix} = -e^{ix}\left(\tilde{v}(x) - i\frac{d}{dx}\tilde{v}(x) - \frac{d^2}{dx^2}\tilde{v}(x) - \tilde{v}(x)\right) + \int dx' \Delta^*(x,x')\tilde{u}(x')e^{ix'}$$

Now we say that $i\frac{d}{dx}\tilde{u}(x) >> \frac{d^2}{dx^2}\tilde{u}(x)$.

$$\epsilon\tilde{u}(x)e^{ix} = -ie^{ix}\frac{d}{dx}\tilde{u}(x) + \int dx'\Delta(x,x')\tilde{v}(x')e^{ix'}$$
$$\epsilon\tilde{v}(x)e^{ix} = ie^{ix}\frac{d}{dx}\tilde{v}(x) + \int dx'\Delta^*(x,x')\tilde{u}(x')e^{ix'}$$

Here we assume the "contact" potential $\Delta(x,x') = \Delta_0\delta(x-x')$ for S-wave. We also make a plane wave expansion of $\tilde{v}(x) = \sum_q \tilde{v}_q e^{iqx}$

$$\epsilon\tilde{u}_p = p\tilde{u}_p + \Delta_0\sum_q \tilde{v}_q F(q-p)$$
$$\epsilon\tilde{v}_p = -p\tilde{v}_p + \Delta_0\sum_q \tilde{u}_q F(q-p)$$

Where $F(q-p)$ is the same as the previous section.