Documentation for BoltzPhlow and BTE Approach to QP-Phonon Transport

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Abstract

None.

1. Overview

This note is used as a study note for nonequilibrium quasiparticle and phonon dynamics in a general BCS superconductor. Based on the work of Fischer, Goldie, and Catelani [1, 2], our main subjects of study are the quasiparticle distribution function $f(E, t)$ and the phonon distribution function $n(\omega, t)$.

We will first introduce the basic constraint of the gap energy and some self-consistency relations. Then we will provide the kinetic equations and check for energy conservation.

1.1. Basic Constraints

In an ideal world (filled with spherical cows), we picture an infinite BCS superconductor. Its self consistency relation for the gap energy Δ is given by

$$\Delta = \frac{1}{2} \int_0^\infty dE \frac{\Delta}{\sqrt{E^2 + \Delta^2}} \tanh\left(\frac{\sqrt{E^2 + \Delta^2}}{2k_B T}\right) f(E, t) \tag{1}$$

Prove:

$$-\int_\Delta^\infty dE \int_0^\infty d\Omega (E + \Omega)\Omega^2 \rho(E + \Omega)\rho(E)K^-(E, E + \Omega)\{f(E)[1 - f(E + \Omega)]n(\Omega)\} \tag{2}$$

$$+\int_\Delta^\infty dE \int_0^{E-\Delta} d\Omega E\Omega^2 \rho(E - \Omega)\rho(E)K^-(E, E - \Omega)\{f(E - \Omega)[1 - f(E)]n(\Omega)\} = 0 \tag{3}$$

where:

$$K^-(E, E') = \left(1 - \frac{\Delta^2}{EE'}\right) \tag{4}$$

$$\rho(E) = \frac{E}{\sqrt{E^2 - \Delta^2}} \tag{5}$$

Proof: We can change the order of the double integral, followed by a change of variables. $\int_\Delta^\infty dE \int_0^{E-\Delta} d\Omega \rightarrow \int_0^\infty d\Omega \int_{\Delta+\Omega}^\infty dE$. Then we can change the variable $E \rightarrow E - \Omega$ in the second integral.

The power flow between the quasiparticle and phonon systems is given by:

$$P = 4N_0 \int_\Delta^\infty dE I_{qp-\phi}(E) E \rho(E) \tag{6}$$

And thus the coefficient in front the integrals is given by:

$$C_1 = \frac{4N_0}{\tau_0(k_B T_c)^3} = \frac{18 N_{\text{ion}}}{\pi \tau_0^\phi \Delta_0 \Omega_D^3} \tag{7}$$

Note that for recombination and pair-breaking term, we need to separate $4N_0 \rightarrow 2N_0 + 2N_0$ respectively, and change one of the variable $E \rightarrow (\Omega - E)$. In this way the integrals will be of forms:

$$2N_0 \int \dots (E + \Omega - E)\Omega^2 \dots \tag{8}$$

This gives the correct coefficient for the phonon system.

The total energy in the QP system is:

$$E_{qp} = 4N_0 \int_\Delta^\infty dE E \rho(E) f(E, t) \tag{9}$$

For the phonon system is:

$$E_\phi = 9\frac{N_{\text{ion}}}{\Omega_D^3} \int_0^\infty d\Omega \Omega^3 n(\Omega, t) \tag{10}$$

1.2. Extension to Bulk Superconductor

The heart of our theory is the Boltzmann Transport Equation (BTE). Simply put, the BTE assumes classical phase space and that the position and momentum of the quasiparticle and phonon excitations can be treated as separable variables.

The BTE is a differential equation for occupation function $f(\vec{x}, \vec{k}, t)$:

$$\frac{\partial f(\vec{x}, \vec{k}, t)}{\partial t} + \dot{\vec{x}} \cdot \vec{\nabla}_x f(\vec{x}, \vec{k}, t) + \dot{\vec{k}} \cdot \vec{\nabla}_k f(\vec{x}, \vec{k}, t) = I\{f\} \tag{11}$$

The collision integral $I\{f\}$ is a functional of f and describes the rate of change of the occupation function due to collisions.

In small perturbations from the equilibrium, instead of solving the entire BTE, we can expand in terms of the perturbation: $f = f_0 + \delta f$. In our assumption, the equilibrium distribution f_0 can be a function of position, instead of a global constant. Its functional form is also dependent on the particle type (Fermi-Dirac distribution for Fermions or Bose-Einstein distribution for Bosons).

The recipe is then to solve for δf and integrate over all momentum space to get the different current density observables we are interested in. For example, the energy current density is given by:

$$\vec{J}_E = \int \frac{d^3\vec{k}}{(2\pi)^3} E\vec{v}\delta f. \tag{12}$$

Note here that the velocity $\vec{v}$ follows the definition of $\vec{v} = \vec{\nabla}_k E/\hbar$.

The source for the small deviation δf comes from the *non-homogeneous* function f_0, such that $\vec{\nabla} f_0 \neq 0$. In general, even if the collision integral is highly non-linear, as long as it equilibriates locally fast enough, we can write out the simplified BTE as:

$$\vec{v} \cdot \vec{\nabla}_x f_0 + \frac{\vec{F}}{\hbar} \cdot \vec{\nabla}_k f_0 = I\{\delta f\}. \tag{13}$$

The reason for dropping f_0 in the collision integral is that the equilibrium distribution function is a solution to the BTE, and thus the collision integral is zero (known as detailed balance). Since f_0 is a function of energy, we can expand BTE in terms of initial derivatives of energy:

$$\vec{v} \cdot \vec{\nabla}_x f_0 + \frac{\vec{F}}{\hbar} \cdot \vec{\nabla}_k f_0 = \left(-\frac{\partial f_0}{\partial E}\right) \vec{v} \cdot \left(q\vec{\mathcal{E}} + \frac{E-\mu}{T}\vec{\nabla}T\right), \tag{14}$$

where $\vec{\mathcal{E}} = \vec{\nabla}(\phi + \mu/q)$ is the modified electrical potential.

Note that the collision integral can also be linearized in δf. If it is linearized, then we can see that the current densities are proportional to the gradients of the equilibrium distribution function. For example, we can apply linearization to elastic impurity scattering of quasiparticles. To start with, in normal metal the impurity scattering term is:

$$I_{\text{imp}} = \frac{2\pi}{\hbar} \sum_{\vec{k'}} \left|\sum_i U_i(\vec{k} - \vec{k'})\right|^2 \delta(E - E')[f'(1 - f) - f(1 - f')] \tag{15}$$

$$= \frac{2\pi n_{\text{imp}}}{\hbar} \int \frac{d^3 k'}{(2\pi)^3} |U(\vec{k} - \vec{k'})|^2 \delta(E - E')[\delta f' - \delta f + \mathcal{O}(\delta f^2)], \tag{16}$$

with the potential $U(\vec{k} - \vec{k'})$ being the Fourier transform of a single impurity potential $V(\vec{x})$. We also used the fact that for any f_0, the collision integral is zero to get the second line. For the quasiparticles in a BCS superconductor, under the Bogoliubov basis [3] we find an additional coherence factor within the collision integral:

$$I_{\text{imp}} = \frac{2\pi n_{\text{imp}}}{\hbar} \int \frac{d^3 k'}{(2\pi)^3} |U(\vec{k} - \vec{k'})|^2 \underbrace{\left(\frac{1}{2} + \frac{\epsilon\epsilon' - \Delta^2}{2EE'}\right)} \delta(E - E')[\delta f' - \delta f]. \tag{17}$$

Here, we have $\epsilon = \sqrt{E^2 - \Delta^2} = \hbar^2 k^2/(2m)$. At this point we will try to solve our δf by providing an ansatz:

$$\delta f = \tau(E)\left(\frac{\partial f_0}{\partial E}\right) \vec{v} \cdot \left(q\vec{\mathcal{E}} + \frac{E-\mu}{T}\vec{\nabla}T\right). \tag{18}$$

The only unknown is τ as a function of energy, and after some algebra we will find that:

$$\frac{1}{\tau_s} = \left(\frac{\epsilon}{E}\right)\frac{1}{\tau_n} = \left(\frac{\epsilon}{E}\right)\left(\frac{mkn_{\text{imp}}}{4\pi^2\hbar^3}\right) \int d\hat{k}' |U|^2 (1 - \hat{k} \cdot \hat{k}'). \tag{19}$$

Now we can backtrack and calculate our current densities by plugging in δf. We can reduce our work by defining the integral quantities (already taking into account of 2 spins polarizations):

$$\mathcal{I}_n = \frac{1}{12\pi^3\hbar} \int dE \tau(E - \mu)^n \left(-\frac{\partial f_0}{\partial E}\right) \int dS_E(\vec{k})|\vec{v}|, \tag{20}$$

and specifically the heat current density, when there is only a temperature gradient, is:

$$\vec{J}_q = -\frac{\mathcal{I}_2}{T}\vec{\nabla}T = -\kappa\vec{\nabla}T. \tag{21}$$

If we approximate the surface integral in $\mathcal{I}_n$ by the Fermi surface, and shift $\mu \to 0$, we can make the substitution:

$$k^2 dk \sim N_0\rho(E)dE. \tag{22}$$

In the end, we will arrive at κ_{es} being the same as the BRT result [3]:

$$|\kappa_{es}| = \frac{2N_0 v_F \ell}{3T}\int_\Delta^\infty dE E^2 \left|\frac{\partial f_0}{\partial E}\right|, \tag{23}$$

where v_F is the fermi velocity, N_0 is the electron density of state at the fermi energy, and $\ell = v\tau$ is the mean free path of the quasiparticles, which happens to be the same value as the mean free path of the normal electrons and independent of energy. The implication is important: if the normal electrons in the metal is diffusive in transport,, then the quasiparticles in the superconducting statearere also diffusive. The addition of phonon-mediated scattering will only shorten the mean free path: hence the diffusive characteristic is preserved. Finally, notice that we have an extra factor of 2 due to the fact that there are two branches of quasiparticles. The contributions of the two branches are the same.

There is another interesting point: if we look at the heat capacity per unit volume of the superconductor, its "normal metal" part form will be:

$$c = \frac{\mathrm{d}E_{qp}}{\mathrm{d}T} \propto \int \frac{\partial f}{\partial T}E\rho(E)dE = \int \frac{\partial f}{\partial E}\frac{E^2}{T}\rho(E)dE. \tag{24}$$

But this is the same as κ_{es}, and we find out that the heat diffusion equation after the Kirkhoff-transform follows the standard heat equation form with a constant diffusivity. However, we will also need to include the change in Δ with temperature. The complete specific heat is then:

$$c = T\frac{\partial S}{\partial T} = T\frac{\partial}{\partial T}\left(-2k_B\sum_{\vec{k}}[f_k \ln f_k + (1-f_k)\ln(1-f_k)]\right) \tag{25}$$

$$= 2\beta k_B\sum -\frac{\partial f_k}{\partial E}\left(E^2 + \frac{1}{2}\beta\frac{\mathrm{d}\Delta^2}{\mathrm{d}\beta}\right). \tag{26}$$

The first term is the same as the normal metal, and the second term is the change in the gap energy with temperature.

Note:

$$\frac{\mathrm{d}}{\mathrm{d}\beta} \to \frac{\mathrm{d}}{\mathrm{d}T}\frac{\mathrm{d}T}{\mathrm{d}\beta} = -\frac{1}{k_B\beta^2}\frac{\mathrm{d}}{\mathrm{d}T}. \tag{27}$$

If we ignore the backscattering of the BTE (applying relaxation time approximation), we can write the thermal conductivity (of one branch of the QP) as:

$$\kappa_s = \frac{1}{2}\beta\frac{n}{m}\int_0^\infty d\epsilon_p \epsilon_p^2 \operatorname{sech}^2\left(\frac{1}{2}\beta E_p\right)\tau \tag{28}$$

With the identification of τ being decay time of the QP (i.e. *not* the transport time). Also note that $\frac{n}{m} = \frac{1}{3} N_0 v_F^2$, and also:

$$\frac{1}{2}\beta \operatorname{sech}^2\left(\frac{1}{2}\beta E_p\right) = -\frac{\partial f_0}{\partial E_p}. \tag{29}$$

Therefore, the only method to have ballistic transport is to have ballistic subgap phonons. However, the diffusion coefficient for the quasiparticles is on the order of a few 10^5 of $\mu m^2/\mu s$, while that for the above-gap phonons is on the order of a few hundreds of $\mu m^2/\mu s$.

2. Drafts

2.1. Zero Dimensional Dynamics

To simulate the simplest possible system, we start with the zero-dimensional dynamics. The following parts document the collision integrals used for this purpose. Note they are always proven to be energy-conserving.

2.1.1. Boltzmann Transport Equation for Quasi-Particles

The quasi-particle distribution function $f(E, \mathbf{x}, t)$ satisfies the Boltzmann transport equation:

$$\frac{\partial f}{\partial t} + \mathbf{v}_f \cdot \nabla f + \frac{\mathbf{F}}{\hbar} \cdot \frac{\partial f}{\partial \mathbf{k}} = S_{\text{coll}}^{\text{phon}}(f, n), \tag{30}$$

Note we here use $F = 0$ for quasiparticles. So the equation becomes:

$$\frac{\partial f}{\partial t} + \mathbf{v}_f \cdot \nabla f = S_{\text{coll}}^{\text{phon}}(f, n). \tag{31}$$

where the collision integral consists of four phonon-mediated terms:

$$S_{\text{coll}}^{\text{phon}}(f, n) = S_{\text{sc}}^{\text{phon}}(f) + S_{\text{r}}^{\text{phon}}(f, n) + S_{\text{pb}}^{\text{phon}}(f, n). \tag{32}$$

These terms explicitly take the form, with the following definitions:

$$U^{\pm}(E, E') = \left(1 \pm \frac{\Delta^2}{EE'}\right) \rho(E'), \tag{33}$$

The function $\rho(E)$ is the density of states, defined as (can be modified with Dynes broadening):

$$\rho(E) = \frac{E}{\sqrt{E^2 - \Delta^2}}. \tag{34}$$

Phonon Emission and Absorption (Scattering):

$$S_{\text{sc}}^{\text{phon}}(f, n) = \frac{1}{\tau_0 T_c^3} \left[\int_0^\infty d\omega \, \omega^2 \, U^-(E, E + \omega) \left[f(E + \omega)(1 - f(E))(1 + n(\omega)) \right] \right.$$
$$- \int_0^\infty d\omega \, \omega^2 \, U^-(E, E + \omega) \left[f(E)(1 - f(E + \omega))n(\omega) \right]$$
$$+ \int_0^{E-\Delta} d\omega \, \omega^2 \, U^-(E, E - \omega) \left[f(E - \omega)(1 - f(E))n(\omega) \right]$$
$$\left. - \int_0^{E-\Delta} d\omega \, \omega^2 \, U^-(E, E - \omega) \left[f(E)(1 - f(E - \omega))(1 + n(\omega)) \right] \right]. \tag{35}$$

Quasi-Particle Recombination:

$$S_{\text{r}}^{\text{phon}}(f, n) = -\frac{1}{\tau_0 T_c^3} \int_{E+\Delta}^\infty d\omega \, \omega^2 U^+(E, \omega - E) f(E) f(\omega - E)[1 + n(\omega)]. \tag{36}$$

Pair-Breaking by Phonons:

$$S_{\text{pb}}^{\text{phon}}(f, n) = \frac{1}{\tau_0 T_c^3} \int_{E+\Delta}^{\infty} d\omega\, \omega^2 U^+(E, \omega - E)[1 - f(E)][1 - f(\omega - E)]n(\omega). \qquad (37)$$

2.1.2. Boltzmann Transport Equation for Phonons

The phonon distribution function $n(\omega, \mathbf{x}, t)$ satisfies:

$$\frac{\partial n}{\partial t} + \mathbf{v}_p \cdot \nabla n = S_{\text{coll}}^{\text{qp}}(n, f). \qquad (38)$$

The collision integral $S_{\text{coll}}^{\text{qp}}(n, f)$ depends on whether ω is above or below 2Δ:

Sub-gap phonons cannot be generated via quasi-particle recombination, so the collision integral only includes phonon absorption and stimulated emission:

$$S_{\text{coll}}^{\text{qp}}(n, f) = \frac{2}{\pi \Delta_0 \tau_0^{\text{pb}}} \left[\int_{\Delta}^{\infty} dE \rho(E) U^-(E, E + \omega) f(E + \omega)(1 - f(E))(1 + n(\omega)) \right.$$

$$\left. - \int_{\Delta}^{\infty} dE \rho(E) U^-(E, E + \omega) f(E)(1 - f(E + \omega))n(\omega) \right]. \qquad (39)$$

When $\omega > 2\Delta$, phonons can also be created via quasi-particle recombination, introducing an additional term:

$$S_{\text{coll}}^{\text{qp}}(n, f) = \frac{2}{\pi \Delta_0 \tau_0^{\text{pb}}} \left[\int_{\Delta}^{\infty} dE \rho(E) U^-(E, E + \omega) f(E + \omega)(1 - f(E))(1 + n(\omega)) \right.$$

$$\left. - \int_{\Delta}^{\infty} dE \rho(E) U^-(E, E + \omega) f(E)(1 - f(E + \omega))n(\omega) \right]$$

$$+ \frac{1}{\pi \Delta_0 \tau_0^{\text{pb}}} \left[\int_{\Delta}^{\omega - \Delta} dE \rho(E) U^+(E, \omega - E) f(\omega - E) f(E)(1 + n(\omega)) \right.$$

$$\left. - \int_{\Delta}^{\omega - \Delta} dE \rho(E) U^+(E, \omega - E)(1 - f(\omega - E))(1 - f(E))n(\omega) \right]. \qquad (40)$$

This additional term accounts for phonon generation from quasi-particle recombination.

2.2. Explicit and Time-Relaxation Methods for Time Evolution

It is rather straightforward to implement the time evolution of the quasiparticle and phonon distribution functions given an initial condition: since we have the time derivative as a function of the distributions f and n at time t_n, we only need to calculate the collision integral with the same time value.

Generally this is an order N^2 operation, where N is the number of energy grids. However, we can use the fact that each collision integral is inherently either a convolution or correlation of the distribution functions to take advantage of the fast Fourier transform (FFT) algorithm.

Here's an example of the phonon emission integral:

$$S_{\text{sc}}^{\text{phon}}(f, n) \propto \int_0^\infty d\omega \, \omega^2 \, U^-(E, E + \omega) \left[f(E + \omega)(1 + n(\omega)) - f(E)f(E + \omega) - f(E)n(\omega) \right]$$

Taking the first of the three terms:

$$\begin{aligned}
\int_0^\infty d\omega \, \omega^2 \, U^-(E, E + \omega) f(E + \omega)(1 + n(\omega)) &= \int_0^\infty d\omega \, \omega^2 \rho(E + \omega) f(E + \omega) \left(1 + n(\omega) \right) \\
&\quad - \frac{\Delta^2}{E} \int_0^\infty d\omega \, \omega^2 \frac{\rho(E + \omega)}{E + \omega} f(E + \omega)(1 + n(\omega)) \\
&= (g_1 \star h_1)(E) - \frac{\Delta^2}{E} (g_2 \star h_2)(E), \quad (41)
\end{aligned}$$

where the $\star$ operation denotes cross-correlation between the two functions and we notice and define:

$$g_1(x) = \rho(x)f(x), \quad (42)$$
$$h_1(x) = x^2(1 + n(x)), \quad (43)$$
$$g_2(x) = \frac{\rho(x)}{x} f(x), \quad (44)$$
$$h_2(x) = h_1(x). \quad (45)$$

Now, one can rewrite each of the collision integrals to six correlation or convolution functions. Then we can use an explicit Runge-Kutta method or Euler method to step forward in time. Yet this time stepping method is not very efficient because it is only conditionally stable: if one time step is too large, the distribution function can become negative and thus unphysical.

Time Relaxation Method   Here we introduce an explicit, first-order time relaxation method to preserve the positivity of the distribution functions while stepping forward in time. This method [4] should allow for a larger time step, and we will see that at first order, it conserves the energy as well (this is not true to higher orders unfortunately).

The general idea is to consider the equation of the sort:

$$\frac{\partial f}{\partial t} = P(f, f) - \mu f. \quad (46)$$

If we make the transformation to $\tau = 1 - e^{-\mu t}$ and $F(\tau) = f(t)e^{\mu t}$, we can find that:

$$\frac{\partial F}{\partial \tau} = \frac{P(F, F)}{\mu}. \quad (47)$$

If P is always positive, then it is guaranteed that $F(\tau)$ is always positive, and in turn the positivity of $f(t)$ is preserved. For any operator $Q(f, f)$, one can write it as:

$$Q(f, f) = \underbrace{Q(f, f) + \mu f}_{P(f,f)} - \mu f, \quad (48)$$

for some sufficiently large $\mu > 0$.

Then we power expand the function $F(\tau)$ as a function of τ:

$$F(\tau) = \sum_{k=0}^{\infty} \tau^k \mathcal{F}_k. \tag{49}$$

Substituting this back to the differential equation for $F(\tau)$, we can find that:

$$\mathcal{F}_1 = \frac{1}{\mu} P(\mathcal{F}_0, \mathcal{F}_0)$$

$$\mathcal{F}_2 = \frac{1}{2\mu} \left[P(\mathcal{F}_0, \mathcal{F}_1) + P(\mathcal{F}_1, \mathcal{F}_0) \right]$$

$$\dots$$

$$\tag{50}$$

Finally, truncating the series F at some order n, we can obtain the next time step $f(t+\Delta t)$ as:

$$f(t + \Delta t) = e^{-\mu \Delta t} F(\tau). \tag{51}$$

Energy Conservation   We prove the energy conservation of the time relaxation method at first order here.

2.3.   Change in BTE when the Gap Energy has Dependence on Space and Time

In this section we will discuss the modifications on the BTE when the gap energy Δ has a dependence on space and time. There may be corrections actually from Kopnin's book [5], which could be added later. Starting from the BTE in continuity equation form (conservative form), and we will focus on the left hand side (and setting $\hbar = 1$):

$$\frac{\partial f}{\partial t} + \vec{\nabla} \cdot (\vec{u} f) = I\{f\}. \tag{52}$$

Here $\vec{u} = (\frac{d\vec{x}}{dt}, \frac{d\vec{k}}{dt})$ is the six-dimensional velocity vector in phase space. Notice the velocity in positonal space $\frac{d\vec{x}}{dt} = \vec{v} = \frac{\partial E}{\partial \vec{k}}$, which is a function of space and time if the gap is dynamic, and we can expand the left hand side of the BTE:

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \vec{\nabla}_x f + (\vec{\nabla}_x \cdot \vec{v}) f + \frac{d\vec{k}}{dt} \cdot \vec{\nabla}_k f + \left(\vec{\nabla}_k \cdot \frac{d\vec{k}}{dt} \right) f = I\{f\}. \tag{53}$$

Note here with the addition of spatial and temporal dependence of the gap, we are effectively adding an additional degree of freedom Δ, which needs to be constrained by the occupation function f itself through the gap self-consistency equation. This additional divergence of the velocity term $\vec{\nabla}_x \cdot \vec{v}$ represents the change of positional element dx^3 in phase space volume. Correspondingly, there is also a term that arises from the change of momentum phase space volume.

Interestingly, with the gap identity $E^2 = \xi(\vec{k})^2 + \Delta(\vec{x}, t)^2$, we will show that the phase space volume is still conserved, and so there's no dissipation. To see this, we can write the

velocity $\vec{v}$ as:

$$\vec{v} = \frac{\partial E}{\partial \vec{k}} = \frac{\xi}{E} \vec{\nabla}_k \xi \tag{54}$$

$$\Rightarrow \quad \vec{\nabla}_x \cdot \vec{v} = -\frac{\xi \Delta}{E^3} \vec{\nabla}_x \Delta \cdot \vec{\nabla}_k \xi. \tag{55}$$

Now the divergence of the momentum space velocity is:

$$\vec{\nabla}_k \cdot \frac{d\vec{k}}{dt} = \vec{\nabla}_k \cdot (-\vec{\nabla}_x E) = -\vec{\nabla}_k \cdot \left(\frac{\Delta}{E} \vec{\nabla}_x \Delta \right)$$

$$= \frac{\xi \Delta}{E^3} \vec{\nabla}_x \Delta \cdot \vec{\nabla}_k \xi. \tag{56}$$

Adding these two terms together we can see that the divergence of the velocities cancel out.

We want to integrate out the momentum space directions (angular variables) to get the boltzmann equation as only a function of space and quasiparticle energy E_k. To do this, let's integrate the function with (the $1/(2\pi)^3$ factor is set to normalize the phase space) $dk^3 \delta(E - E_k)/(2\pi)^3$:

$$\frac{1}{(2\pi)^3} \int d^3k \, \delta(E - E_k) \left(\frac{\partial f}{\partial t} + \vec{v} \cdot \vec{\nabla}_x f + \frac{d\vec{k}}{dt} \cdot \vec{\nabla}_k f \right). \tag{57}$$

We should emphasize that here our function $f(\vec{x}, \vec{k}, t)$ is still a function of position, momentum and time. After all the BTE is only guranteed to satisfy the continuitiy equation in the six dimensional phase space. So any change of variables to the energy space should come from here.

It should also be noted that we should recover the BCS density of states with just the integral over d^3k and the Dirac delta function as a sanity check. Another point to note is that our quasiparticle energy is given by the energy *shifted from the Fermi energy*:

$$E^2 = \underbrace{\left(\frac{\vec{k} \cdot \vec{k}}{2m} - E_F \right)^2}_{\xi(\vec{k})^2} + \Delta(\vec{x}, t)^2. \tag{58}$$

So let's do the sanity check first. From the following identities:

$$d^3k = mk d\xi \, d\Omega_k = m\sqrt{2m(\xi + E_F)} d\xi \, d\Omega_k \tag{59}$$

$$\Rightarrow \quad \frac{1}{(2\pi)^3} \int d^3k \, \delta(E - E_k)$$

$$= \frac{1}{(2\pi)^3} \int_{-E_F}^{\infty} d\xi \, d\Omega_k \, m\sqrt{2m(\xi + E_F)}$$

$$\xi \ll E_F \quad \Rightarrow \quad \approx \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} dE \underbrace{\left(\frac{|E|}{\sqrt{E^2 - \Delta^2}} \right)}_{\rho(E, \Delta)} 4\pi m \sqrt{2mE_F} \, \delta(E - E_k) \tag{60}$$

$$= \rho(E_k) \underbrace{\frac{1}{(2\pi)^3} 4\pi m \sqrt{2mE_F}}_{N_0} \tag{61}$$

Here N_0 is indeed the *single-spin* density of states at the Fermi level as usual, so this checks out.

2.4. Keldyish Formalism and Transport Equations for Variable-Gap Superconductors

In this section we aim to formulate the problem of non-equilirbium superconductivity with the Keldyish formalism, which is a set of self-consistent Green's function equations for superconductors driven far from equilibrium. We aim to make reasonable approximations to reduce the complexity and derive a BTE-like equation for the quasiparticles and phonons.

The Keldyish functions for superconductors are set up in Nambu-Gor'kov space. We follow the notations in [6, 7] and define:

$$\tilde{G} = \begin{pmatrix} \check{G}^R & \check{G}^K \\ 0 & \check{G}^A \end{pmatrix}. \tag{62}$$

This matrix in Keldyish space contains the retarded, advanced and Keldyish Green's functions. To get each one of these function, we start with a matrix defined as:

$$\tilde{G}'(1,1')_{\alpha\beta} \equiv -i \left\langle \mathcal{T}_c \Psi(1)\Psi^\dagger(1') \right\rangle_{\alpha\beta} = \begin{pmatrix} \check{G}_{11} & \check{G}_{12} \\ \check{G}_{21} & \check{G}_{22} \end{pmatrix}. \tag{63}$$

Here $\mathcal{T}_c$ is the time-ordering operator on the Keldyish contour which is taken to go from $t = -\infty$ to $t = +\infty$ and back to $t = -\infty$. The $\check{G}_{\alpha\beta}$ are the Green's functions defined on the two branches of the contour. To be explicit: $\check{G}_{11}$ is the time-ordered Green's function, $\check{G}_{12}$ is the lesser Green's function $\check{G}^<(1,1') = i \left\langle \Psi(1')^\dagger \Psi(1) \right\rangle$, $\check{G}^>(1,1') = -i \left\langle \Psi(1)\Psi(1')^\dagger \right\rangle$, and $\check{G}_{22}$ is the anti-time-ordered Green's function. Again we note that each $\check{G}_{\alpha\beta}$ is a 2×2 matrix. It is possible to perform a transformation [8] to get from the $\tilde{G}'$ representation to the $\tilde{G}$ representation, and thus we will work with the $\check{G}^R$, $\check{G}^A$ and $\check{G}^K$ functions from now on. For our convenience we also note the following identities:

$$\check{G}^R = \theta(1-1')(\check{G}^> - \check{G}^<) \tag{64}$$

$$\check{G}^A = -\theta(1'-1)(\check{G}^> - \check{G}^<), \tag{65}$$

$$\check{G}^K = \check{G}^> + \check{G}^<, \tag{66}$$

to transform between the two representations.

The Green's functions satisfy the Dyson equation:

$$(\tilde{G}_0^{-1} - \tilde{\Sigma}) \circ \tilde{G} = \tilde{1}, \tag{67}$$

where $\circ$ is the convolution operator in space and time and $\tilde{\Sigma}$ is the self-energy matrix, where we could include the electron-phonon interaction, impurity scattering, etc. It is denoted as:

$$\tilde{\Sigma} = \begin{pmatrix} \check{\Sigma}^R & \check{\Sigma}^K \\ 0 & \check{\Sigma}^A \end{pmatrix}. \tag{68}$$

We will define the self-energy matrix later. Note that we implicitly have excluded the local gap parameter from the self-energy matrix. This convolution in space and time can be

transformed to be a convolution in momentum and energy space. We parametrize by the center-of-mass coordinates $\vec{r} = (\vec{r}_1 + \vec{r}_2)/2$ and $t = (t_1 + t_2)/2$, and the relative coordinates $\vec{\rho} = \vec{r}_1 - \vec{r}_2$ and $\tau = t_1 - t_2$. Then we present the Green's function as a function of Fourier-transformed variables ($\vec{r} \to \vec{p}$, $t \to \epsilon$, $\vec{\rho} \to \vec{k}$ and $\tau \to \omega$): $\check{G}(\vec{r}_1, t_1; \vec{r}_2, t_2) \to \check{G}(\epsilon^+, \vec{p}^+; \epsilon^-, \vec{p}^-)$, where $\epsilon^\pm = \epsilon \pm \omega/2$ and $\vec{p}^\pm = \vec{p} \pm \vec{k}/2$. Then the Dyson equation becomes:

$$\left[\left(\check{G}_0^{-1} - \check{\Sigma}\right)\check{G}\right]_{\epsilon^+, \epsilon^-} = \check{1} \cdot (2\pi)^4 \delta(\omega)\delta(\vec{k}). \tag{69}$$

The bracket $[\cdots]_{\epsilon^+, \epsilon^-}$ denotes convolution within intermediate energies and momentum:

$$[\check{A}\check{B}]_{\epsilon^+, \epsilon^-} = \int \frac{d\epsilon'}{2\pi} \frac{d^3 p'}{(2\pi)^3} \check{A}(\epsilon^+, \vec{p}^+; \epsilon', \vec{p}')\check{B}(\epsilon', \vec{p}'; \epsilon^-, \vec{p}^-). \tag{70}$$

We further parametrize the intermediate energy and momentum as: $\epsilon' = \epsilon^+ - \omega'$ and $\vec{p}' = \vec{p}^+ - \vec{k}'$. The inverse of the free Green's function is given by:

$$\check{G}_0^{-1}(\epsilon^+, \vec{p}^+; \epsilon', \vec{p}') = \check{G}_0^{-1}(\epsilon^+, \vec{p}^+; \omega', \vec{k}') \tag{71}$$

$$= \left[\tau_0 \epsilon^+ - \tau_3 \xi(\vec{p}^+)\right](2\pi)^4 \delta(\omega')\delta(\vec{k}') + \check{\mathcal{H}}(\omega', \vec{k}'), \tag{72}$$

where $\xi(\vec{p}) = \frac{\vec{p}^2}{2m} - E_F$ is the normal-state electron energy, and τ_i are the Pauli matrices (i.e. τ_0 is the identity matrix, $\tau_1 = \sigma_x$, $\tau_2 = \sigma_y$, $\tau_3 = \sigma_z$). If we keep only linear order in external electromagnetic field drive, we have:

$$\check{\mathcal{H}}(\omega', \vec{k}') = \begin{pmatrix} \frac{e}{c}\vec{v}_F \cdot \vec{A}(\vec{k}') - e\varphi & -\Delta(\omega', \vec{k}') \\ -\Delta^*(\omega', \vec{k}') & +\frac{e}{c}\vec{v}_F \cdot \vec{A}(\vec{k}') + e\varphi \end{pmatrix}. \tag{73}$$

The reason for the linearization is that usually the external electromagnetic field momentum is small compared to the Fermi momentum. In our case of superconducting calorimeters, we set $\vec{A} = 0$ and $\varphi = 0$, and thus $\check{\mathcal{H}}$ is only off-diagonal.

We can expand the Green's function in small ω and $\vec{k}$, which in turn gives us the mixed-coordinate representation $\check{G}(\epsilon, \vec{p}; \vec{r}, t)$. The coordinate $\vec{r}$ and t are the center-of-mass coordinates. This approximation is valid when the relative momentum change $\vec{k}$ and energy change ω are small compared to the Fermi momentum and Fermi energy. With the estimated wave-length of a typical 10Δ phonon in Sn being $f \sim 1.3\,\text{THz}$, and thus $\lambda = v_s/f \sim 2\,\text{nm}$, we can see that even for phonon distributions peaking well above 2Δ, the wavelength is still much larger than the Fermi wave-length. However, when the phonon energy gets close to the Debye energy, the phonon wavelength becomes comparable to the Fermi wave-length. If we use a grid size larger than the typical $\vec{r}$, we may operate in the "diffusive" regime: where we cannot assume local translational invariance.

Another observation is that the phonons propagate much slower than the quasiparticles. So for each time step we can assume that the local phonon distribution is "frozen" in time, and we update the local gap parameter and renormalization function with the knowledge of local quasiparticle and phonon distributions for each space grid and time step. Our final goal is to write out a set of differential equations suitable for calculating the energy and thermal transport in clean, bulk superconductors, but also straight-forward to implement. To achieve this, we will make the following approximations:

- *Local translational and time invariance*: we will try to solve the local retarded and advanced Green's functions assuming that the local gap parameter and renormalization function are constant in space and time. This is a reasonable approximation if the spatial variation of the gap is small within the spatial grid size, and the time variation of the gap is small compared to typical gap dynamics.

- *Quasi-classical approximation*: we work near the Fermi surface and use reasonable Fermi Surface Averages (FSA) to determine for example the gap parameter.

- *Particle-hole symmetry*: we assume that the distribution function is symmetric about the Fermi energy so no charge imbalance is considered.

- *Spherical symmetry*: Because the initial electron or phonon energy is very high compared to the Debye energy, we assume the formation of a phonon bubble, which randomizes the momentum directions. This leads to the assumption that we have spherically isotropic distribution functions and Green's functions. Locally, though, the Green's functions are still assumed to be translationally invariant.

To solve for retarded and advanced Green's functions, we start with the Dyson equation:

$$(\check{G}_0^{-1} - \check{\Sigma}^{R(A)}) \circ \check{G}^{R(A)} \equiv \check{\Lambda}^{R(A)} \circ \check{G}^{R(A)} = \check{1}. \tag{74}$$

We then parametrize with the following variables:

$$\check{\Lambda}^{R(A)} = H \mp \frac{i}{2}\Gamma, \tag{75}$$

$$H = \tau_0 \epsilon Z_1(\epsilon) - \tau_3 \xi_{\vec{p}} - \tau_1 \phi_1(\epsilon), \tag{76}$$

$$\Gamma = 2(\epsilon Z_2(\epsilon)\tau_0 - \phi_2(\epsilon)), \tag{77}$$

$$Z(\epsilon) = Z_1(\epsilon) + iZ_2(\epsilon), \tag{78}$$

$$\phi(\epsilon) = \phi_1(\epsilon) + i\phi_2(\epsilon). \tag{79}$$

So far, we have not made any attempt to solve for the complex components Z and $\phi = \Delta Z$. At this point we need to remind ourselves that we do not have the luxury of assuming that the system is in equilibrium, so we need to solve for the green's functions with the local distribution functions.

Let's begin with *normal metal*'s case and we will see that the superconducting case can be treated similarly. We follow the treatment in [8] closely. To start with, we define the self-energy matrix for both the non-paramagnetic impurity scattering and the electron-phonon interaction:

$$\tilde{\Sigma}_{\text{imp}} = n_i \int \frac{d^3p'}{(2\pi)^3} |u(\vec{p} - \vec{p}')|^2 \tilde{G}(\epsilon, \vec{p}'; \vec{r}, t), \tag{80}$$

$$\Sigma^R_{\text{e-ph}} = \frac{ig^2}{2} \left(D^K \circ G^R + D^R \circ G^K \right), \tag{81}$$

$$\Sigma^A_{\text{e-ph}} = \frac{ig^2}{2} \left(D^A \circ G^K + D^K \circ G^A \right), \tag{82}$$

$$\Sigma^K_{\text{e-ph}} = \frac{ig^2}{2} \left(D^R \circ G^R + D^A \circ G^A + D^K \circ G^K \right). \tag{83}$$

Here n_i is the impurity density, $u(\vec{p} - \vec{p}')$ is the impurity scattering potential, and g is the electron-phonon coupling constant. The circle $\circ$ denotes convolution in space and time or energy and momentum. We also define the spectrum functions and the distribution functions.

$$A(\epsilon, \vec{p}) = i(G^R - G^A) = i(G^> - G^<),\tag{84}$$

$$B(\omega, \vec{q}) = i(D^R - D^A) = i(D^> - D^<),\tag{85}$$

$$G^K(\epsilon, \vec{p}; \vec{r}, t) = -iA(\epsilon, \vec{p})F_e(\epsilon, \vec{p}; \vec{r}, t),\tag{86}$$

$$D^K(\omega, \vec{q}; \vec{r}, t) = -iB(\omega, \vec{q})F_b(\omega, \vec{q}; \vec{r}, t).\tag{87}$$

For phonons, we assume that their propagators are not affected by any quasiparticle distributions, and thus we can use the bare phonon propagators:

$$D^R(\omega, \vec{q}) = \frac{1}{\omega - \omega_{\vec{q}} + i0^+} - \frac{1}{\omega + \omega_{\vec{q}} + i0^+},\tag{88}$$

$$D^A(\omega, \vec{q}) = \frac{1}{\omega - \omega_{\vec{q}} - i0^+} - \frac{1}{\omega + \omega_{\vec{q}} - i0^+},\tag{89}$$

$$B(\omega, \vec{q}) = 2\pi[\delta(\omega - \omega_{\vec{q}}) - \delta(\omega + \omega_{\vec{q}})],\tag{90}$$

$$\tag{91}$$

and $\omega_{\vec{q}} = \sqrt{\kappa_{\vec{q}}/M}$ are the possible phonon energies. The generalized distribution functions are related to the usual distribution functions with:

$$F_e(\epsilon, \vec{p}; \vec{r}, t) = 1 - 2f(\epsilon, \vec{p}; \vec{r}, t),\tag{92}$$

$$F_b(\omega, \vec{q}; \vec{r}, t) = 1 + 2n(\omega, \vec{q}; \vec{r}, t).\tag{93}$$

Now define:

$$\Sigma^R = \Sigma_1 - i\Gamma/2,\tag{94}$$

$$\Sigma^A = \Sigma_1 + i\Gamma/2.\tag{95}$$

$$\implies \quad \Gamma = i(\Sigma^R - \Sigma^A).\tag{96}$$

We also define the quasi-classical Green's function for later use:

$$\mathcal{G}(\epsilon, \hat{p}; \vec{r}, t) = \frac{i}{\pi} \int d\xi_{\vec{p}} G(\epsilon, \vec{p}; \vec{r}, t).\tag{97}$$

Then we can find that:

$$\Gamma(\epsilon, \vec{p}) = i\left(\Sigma^R - \Sigma^A\right)\tag{98}$$

$$= \frac{g^2}{2}\left[(B\,F_b)\circ A \; + \; B\circ(A\,F_e)\right]\tag{99}$$

$$= \frac{g^2}{2}\int\frac{d\omega\,d^d q}{(2\pi)^{d+1}}\,B(\omega, \vec{q})\,A(\epsilon - \omega, \vec{p} - \vec{q})\left[F_b(\omega, \vec{q}) + F_e(\epsilon - \omega, \vec{p} - \vec{q})\right]\tag{100}$$

$$= g^2\int\frac{d\omega\,d^d q}{(2\pi)^{d+1}}\,B(\omega, \vec{q})\,A(\epsilon - \omega, \vec{p} - \vec{q})\left[1 + n_b(\omega, \vec{q}) - f_e(\epsilon - \omega, \vec{p} - \vec{q})\right],\tag{101}$$

Now we can use analytical continuation to find the retarded self-energy real part, and the actual transformation is equivalent to a Hilbert transform:

$$\Sigma_1(\epsilon, \vec{p}) = \frac{1}{2\pi} \mathcal{P} \int d\epsilon' \frac{\Gamma(\epsilon', \vec{p})}{\epsilon - \epsilon'} \tag{102}$$

$$\equiv \frac{1}{2} \mathcal{H}[\Gamma](\epsilon, \vec{p}) \tag{103}$$

Then the retarded Green's function is given by:

$$G^R(\epsilon, \vec{p}) = \frac{1}{\epsilon - \xi_{\vec{p}} - \Sigma_1(\epsilon, \vec{p}) + \frac{i}{2}\Gamma(\epsilon, \vec{p})}. \tag{104}$$

The advanced Green's function is just the complex conjugate of the retarded one. The spectrum function is given by:

$$A(\epsilon, \vec{p}) = \frac{\Gamma(\epsilon, \vec{p})}{\left[\epsilon - \xi_{\vec{p}} - \Sigma_1(\epsilon, \vec{p})\right]^2 + \left[\Gamma(\epsilon, \vec{p})/2\right]^2}. \tag{105}$$

If we approximate the self energy Σ_1 and Γ as independent of energy and momentum, then this is just a Lorentzian function peaked at $\tilde{\epsilon} = \xi_{\vec{p}} + \Sigma_1$ with a full-width-half-maximum of Γ.

Extending the normal metal to the superconductor only involves using the Nambu matrix space instead of just a single-valued Green's function. Due to the way our Green's function is defined, we need to add τ_3 matrices before and after each $\check{G}^R, \check{G}^A, \check{G}^K$ in the self-energies. We also list the self-energy with the quasi-classical approximation here:

$$\check{\Sigma}_{\text{imp}}^{R,K,A} = n_i \int \frac{d^3 p'}{(2\pi)^3} |u(\vec{p} - \vec{p}')|^2 \tau_3 \check{G}^{R,K,A}(\epsilon, \vec{p}'; \vec{r}, t)\tau_3, \tag{106}$$

$$= -i\pi n_i N_0 \int \frac{d\hat{p}'}{4\pi} |u(\hat{p} \cdot \hat{p}')|^2 \tau_3 \check{\mathcal{G}}^{R,K,A} \tau_3, \tag{107}$$

$$\check{\Sigma}_{\text{mag}}^{R,K,A} = -i\pi \tilde{n}_i N_0 \int \frac{d\hat{p}'}{4\pi} |\tilde{u}(\hat{p} \cdot \hat{p}')|^2 \check{\mathcal{G}}^{R,K,A}, \tag{108}$$

$$\check{\Sigma}_{\text{e-ph}}^{R(A)} = \frac{ig^2}{2} \tau_3 \Big(D^K \circ G^{R(A)} + D^{R(A)} \circ G^K \Big)\tau_3 \tag{109}$$

$$= \frac{g^2 \pi N_0}{2} \int \frac{d\omega}{2\pi} \int \frac{d\hat{p}'}{4\pi} \tau_3 \Big(D^K \circ \check{\mathcal{G}}^{R(A)} + D^{R(A)} \circ \check{\mathcal{G}}^K \Big)\tau_3, \tag{110}$$

$$\check{\Sigma}_{\text{e-ph}}^{K} = \frac{g^2 \pi N_0}{2} \int \frac{d\omega}{2\pi} \int \frac{d\hat{p}'}{4\pi} \tau_3 \Big(D^R \circ \check{\mathcal{G}}^R + D^A \circ \check{\mathcal{G}}^A + \check{D}^K \circ \check{\mathcal{G}}^K \Big)\tau_3. \tag{111}$$

The inverse of the bare propagator is defined as in Eqn.(71):

$$\check{G}_0^{-1}(\epsilon, \vec{p}) = \tau_0 \epsilon - \tau_3 \xi_{\vec{p}}. \tag{112}$$

We further parametrize the electron-phonon self-energy as:

$$\check{\Sigma}^R = (\epsilon - \epsilon Z)\tau_0 + \phi\tau_1. \tag{113}$$

After inverting then we have:

$$\check{G}^R(\epsilon, \vec{p}) = \frac{1}{(\epsilon Z)^2 - \xi_{\vec{p}}^2 - (\phi)^2} \begin{pmatrix} \epsilon Z + \xi_{\vec{p}} & \phi \\ \phi & \epsilon Z - \xi_{\vec{p}} \end{pmatrix}. \tag{114}$$

We apply the quasi-classical approximation and integrate out the ξ_p dependence, assuming that Z and ϕ are independent of ξ_p:

$$\check{\mathcal{G}}^R(\epsilon, \hat{p}) = \frac{i}{\pi} \int d\xi_{\vec{p}} \check{G}(\epsilon, \vec{p}) \tag{115}$$

$$= \frac{i}{\pi} \left(\epsilon Z \tau_0 \int \frac{d\xi}{\Omega^2 - \xi^2 + i0} + \tau_3 \underbrace{\int \frac{\xi d\xi}{\Omega^2 - \xi^2 + i0}}_{= 0 \,(\text{odd integrand})} \right.$$

$$\left. + \phi \tau_1 \int \frac{d\xi}{\Omega^2 - \xi^2 + i0} \right) \tag{116}$$

$$= \frac{i}{\pi} \left(\epsilon Z \tau_0 + \phi \tau_1 \right) \left(-\frac{\pi i}{\Omega} \right) \tag{117}$$

$$= \frac{1}{\sqrt{(\epsilon Z)^2 - \phi^2}} \left[(\epsilon Z)\tau_0 + \phi \tau_1 \right] \tag{118}$$

$$Z \to Z \in \Re \quad = \frac{1}{\sqrt{\epsilon^2 - \Delta^2}} \left(\epsilon \tau_0 + \Delta \tau_1 \right). \tag{119}$$

We can check that indeed the normalization condition is satisfied:

$$(\tau_3 \check{\mathcal{G}}^R)^2 = \check{1}. \tag{120}$$

Note that the advanced quasi-classical function here is also defined with the same prefactor i/π so we have:

$$\check{\mathcal{G}}^A(\epsilon, \hat{p}) = -\check{\mathcal{G}}^R(\epsilon, \hat{p})^\dagger \tag{121}$$

Next we parametrize the spectrum function and distribution function of the quasiparticles in the quasi-classical limit as:

$$\check{a}(\epsilon, \hat{p}) = \frac{1}{2}(\check{\mathcal{G}}^R - \check{\mathcal{G}}^A) = \Re\left[\mathcal{G}^R\right] = \frac{1}{2\pi} \int d\xi_p \check{A}, \tag{122}$$

$$\check{\mathcal{G}}^K(\epsilon, \hat{p}) = 2\check{a}(\epsilon, \hat{p}) F_e(\epsilon, \hat{p}). \tag{123}$$

With these then the imaginary part of the self-energy is given by:

$$\check{\Gamma}_{\text{e-ph}}(\epsilon, \hat{p}) = i(\check{\Sigma}_{\text{e-ph}}^R - \check{\Sigma}_{\text{e-ph}}^A) = -2\Im\left(\check{\Sigma}^R\right) \tag{124}$$

$$= \pi N_0 \int \frac{d\omega}{2\pi} \left\langle |g_{\vec{q}}|^2 B(\omega, \vec{q}) \tau_3 \check{a}(\epsilon - \omega, \hat{p}') \tau_3 \left[F_b(\omega, \vec{q}) + F_e(\epsilon - \omega, \hat{p}') \right] \right\rangle_{\hat{p}'} \tag{125}$$

$$= 2\pi N_0 \int \frac{d\omega}{2\pi} \left\langle |g_{\vec{q}}|^2 B(\omega, \vec{q}) \tau_3 \check{a}(\epsilon - \omega, \hat{p}') \tau_3 \left[1 + n_b(\omega, \vec{q}) - f_e(\epsilon - \omega, \hat{p}') \right] \right\rangle_{\hat{p}'} \tag{126}$$

We use the notation $\langle \cdots \rangle_{\hat{p}'} = \int d\hat{p}'/4\pi$ to denote the average over all angles $\hat{p}' = \hat{p} - \vec{q}$. If we further assume that our distribution functions are isotropic in momentum space, then we can see that:

$$\check{\Gamma}_{\text{e-ph}}(\epsilon)_{12} = \langle \check{\Gamma}_{\text{e-ph}}(\epsilon, \hat{p})_{12} \rangle_{\hat{p}} \tag{127}$$

$$= -2\pi \int d\omega \, N_0 \sum_{\vec{q}} |g_{\vec{q}}|^2 \left[\delta(\omega - \omega_{\vec{q}}) - \delta(\omega + \omega_{\vec{q}}) \right]$$

$$\times \check{a}_{12}(\epsilon - \omega)\left[1 + n(\omega) - f(\epsilon - \omega) \right] \tag{128}$$

$$= -2\pi \int_0^{\Omega_D} d\omega \alpha^2 F(\omega) \Big\{ \check{a}_{12}(\epsilon - \omega)\left[1 + n(\omega) - f(\epsilon - \omega) \right]$$

$$+ \check{a}_{12}(\epsilon + \omega)\left[n(\omega) + f(\epsilon + \omega) \right] \Big\}. \tag{129}$$

This is indeed the Eliashberg equation for the imaginary part of the off-diagonal self-energy, if we define $\alpha^2 F(\omega) \equiv N_0 \sum_{\vec{q}} |g_{\vec{q}}|^2 \delta(\omega - \omega_{\vec{q}})$. We will retain directional dependence, and write out the rules for the full closed set of equations here:

$$-2\Im\left[\Delta Z\right](\epsilon, \hat{p}) = \check{\Gamma}_{\text{e-ph}}(\epsilon, \hat{p})_{12}$$

$$= -N_0 \int d\omega \left\langle |g_{\vec{q}}|^2 B(\omega, \vec{q}) \, \check{a}_{12}(\epsilon - \omega, \hat{p}')\left[1 + n_b(\omega, \vec{q}) - f_e(\epsilon - \omega, \hat{p}') \right] \right\rangle_{\hat{p}'} \tag{130}$$

$$-2\Im\left[\epsilon - \epsilon Z\right](\epsilon, \hat{p}) = \check{\Gamma}_{\text{e-ph}}(\epsilon, \hat{p})_{11}$$

$$= N_0 \int d\omega \left\langle |g_{\vec{q}}|^2 B(\omega, \vec{q}) \, \check{a}_{11}(\epsilon - \omega, \hat{p}')\left[1 + n_b(\omega, \vec{q}) - f_e(\epsilon - \omega, \hat{p}') \right] \right\rangle_{\hat{p}'} \tag{131}$$

At this point we are ready to close the loop and solve for both the Green's functions and the self-energies consistently.

The kinetic equation for the Keldysh Green's function incorporate the time and spatial evolution of the distribution functions. We will start with the Keldysh Green's function:

$$\check{G}^K = \check{G}^R \circ \check{\Sigma}^K \circ \check{G}^A. \tag{132}$$

If we parametrize it with a diagonal distribution function:

$$\check{G}^K = \check{G}^R \circ F_e - F_e \circ \check{G}^A, \tag{133}$$

we will obtain a kinetic equation for F_e. Before we proceed, we will transform to the mixed representation and substitute the convolution with the Moyal product:

$$A \circ B \to A \star B = AB + \frac{i}{2}\{A, B\}, \tag{134}$$

where $\{A, B\}_{\text{PB}} = \partial_\epsilon A \partial_t B - \partial_t A \partial_\epsilon B - \vec{\nabla}_p A \cdot \vec{\nabla}_r B + \vec{\nabla}_r A \cdot \vec{\nabla}_p B$ is the Poisson bracket. We define our convention of the Poisson bracket according to [8]. It is important to note that to first order, the retarded and advanced Green's functions can be solved by promoting the self-energy to be space and time dependent. In other words,

$$\check{G}^R(\epsilon, \vec{p}; \vec{r}, t) = \left[(\epsilon Z)(\epsilon, \vec{p}; \vec{r}, t)\tau_0 - \xi_{\vec{p}}\tau_3 - \phi(\epsilon, \vec{p}; \vec{r}, t)\tau_1 \right]^{-1} \tag{135}$$

satisfies to first order:

$$\check{\Lambda}^R(\epsilon, \vec{p}; \vec{r}, t) \star \check{G}^R(\epsilon, \vec{p}; \vec{r}, t) \equiv \left[\check{G}_0^{-1}(\epsilon, \vec{p}) - \check{\Sigma}^R(\epsilon, \vec{p}; \vec{r}, t) \right] \star \check{G}^R(\epsilon, \vec{p}; \vec{r}, t) = \check{1}. \tag{136}$$

Utilizing this identity, we get from Eqn.(132):

$$\check{\Lambda}^R \star F_e - F_e \star \check{\Lambda}^A = -\check{\Sigma}^K. \tag{137}$$

Remember that $\check{\Lambda}^R = \check{G}_0^{-1} - \check{\Sigma}^R = \left(\check{G}_0^{-1} - \Re\left[\check{\Sigma}^R\right] \right) - i\Im\left[\check{\Sigma}^R\right] \equiv \check{H} + \frac{i}{2}\check{\Gamma}$ (note the sign for $\check{\Gamma}$, as this is fixed by its relation to the $\check{\Sigma}^R$ matrix), and the left-hand side can be expanded as:

$$\check{\Lambda}^R \star F_e - F_e \star \check{\Lambda}^A = i\check{\Gamma}F_e + i\{\check{H}, F_e\}_{\text{PB}} = -\check{\Sigma}^K \tag{138}$$

$$\implies \quad \{F_e, \check{H}\}_{\text{PB}} = -i\check{\Sigma}^K + \check{\Gamma}F_e \tag{139}$$

$$= -\partial_t F_e \partial_\epsilon \check{H} + \partial_\epsilon F_e \partial_t \check{H}$$

$$+ \vec{\nabla}_r F_e \cdot \vec{\nabla}_p \check{H} - \vec{\nabla}_p F_e \cdot \vec{\nabla}_r \check{H}. \tag{140}$$

We evaluate each derivative term now: recall $\check{H} = (\epsilon Z_1)\tau_0 - \xi_{\vec{p}}\tau_3 - \phi_1\tau_1$, and that $Z = Z_1 + iZ_2$ and $\phi = \phi_1 + i\phi_2$.

$$\partial_\epsilon \check{H} = (Z_1 + \epsilon\partial_\epsilon Z_1)\,\tau_0 - \partial_\epsilon \phi_1 \tau_1, \tag{141}$$

$$\partial_t \check{H} = (\epsilon\partial_t Z_1)\tau_0 - (\partial_t \phi_1)\tau_1, \tag{142}$$

$$\vec{\nabla}_p \check{H} = (\epsilon\vec{\nabla}_p Z_1)\tau_0 - \vec{v}_F \tau_3 - (\vec{\nabla}_p \phi_1)\tau_1, \tag{143}$$

$$\vec{\nabla}_r \check{H} = (\epsilon\vec{\nabla}_r Z_1)\tau_0 - (\vec{\nabla}_r \phi_1)\tau_1. \tag{144}$$

Combining these results, we have:

$$\boxed{\begin{aligned} \{F_e, \check{H}\}_{\text{PB}} &= -\partial_t F_e\left[(Z_1 + \epsilon\partial_\epsilon Z_1)\tau_0 - (\partial_\epsilon \phi_1)\tau_1\right] \\ &\quad + \partial_\epsilon F_e\left[(\epsilon\partial_t Z_1)\tau_0 - (\partial_t \phi_1)\tau_1\right] \\ &\quad - \vec{\nabla}_r F_e \cdot \vec{v}_F \tau_3 + \vec{\nabla}_r F_e \cdot \left[(\epsilon\vec{\nabla}_p Z_1)\tau_0 - (\vec{\nabla}_p \phi_1)\tau_1\right] \\ &\quad - \vec{\nabla}_p F_e \cdot \left[(\epsilon\vec{\nabla}_r Z_1)\tau_0 - (\vec{\nabla}_r \phi_1)\tau_1\right] \\ &= -i\check{\Sigma}^K + \check{\Gamma}F_e. \end{aligned}} \tag{145}$$

This is the quantum kinetic equation for the distribution function $F_e(\epsilon, \vec{p}; \vec{r}, t) = 1 - 2f$. It can be seen that this equation is indeed the same as Eqn.(3.85) in [8]. The right-hand side of the equation can be written out explicitly after some algebra:

$$(-i\check{\Sigma}^K + \check{\Gamma}F_e)(\epsilon, \vec{p}) = 2g^2\tau_3\left[\check{A}(\epsilon - \Omega, \vec{p} - \vec{q}) \circ B(\Omega, \vec{q})\right]\tau_3\left[Nf'(1 - f) - (N+1)(1 - f')f\right]. \tag{146}$$

The reader can verify with the following definitions:

$$A = i(G^R - G^A) = i(G^> - G^<), \tag{147}$$

$$B = i(D^R - D^A) = i(D^> - D^<), \tag{148}$$

$$G^K = -iAF_e = -iA(1 - 2f), \tag{149}$$

$$D^K = -iBF_b = -iB(1 + 2N), \tag{150}$$

$$G^< = iAf, \tag{151}$$

$$G^> = -iA(1 - f), \tag{152}$$

$$D^< = -iBN, \tag{153}$$

$$D^> = -iB(1 + N), \tag{154}$$

$$f = f(\epsilon, \vec{p}; \vec{r}, t), \quad f' = f(\epsilon - \Omega, \vec{p} - \vec{q}; \vec{r}, t). \tag{155}$$

Now to get the above matrix equation Eqn.(145) into a more and familiar form, we can check the quasi-classical limit and take projections with the spectrum function matrix. Let's multiply both sides of the equation with $\check{A}(\epsilon, \vec{p})$, take the trace and average over the momentum magnitude $\xi_{\vec{p}}$. Before we begin, we note the following projection identities for $\check{A}$, in the "infinite" lifetime limit, i.e. $\check{\Gamma} \to 0$. Starting from the retarded and advanced Green's functions:

$$\check{G}^R(\epsilon, \xi) = \frac{1}{\epsilon Z \, \tau_0 - \xi \, \tau_3 - \phi \, \tau_1 + i0}, \qquad \check{G}^A(\epsilon, \xi) = \frac{1}{\epsilon Z \, \tau_0 - \xi \, \tau_3 - \phi \, \tau_1 - i0}, \tag{156}$$

where $E = \sqrt{\xi^2 + \phi^2}$, and Z, ϕ are real functions. Introduce the "direction" matrix

$$\check{h} \equiv \frac{\xi}{E} \, \tau_3 + \frac{\phi}{E} \, \tau_1, \tag{157}$$

which satisfies $\check{h}^2 = \tau_0$. The projectors onto the Bogoliubov branches are

$$\check{P}_\pm = \frac{1}{2} \left(\tau_0 \pm \check{h} \right), \qquad \check{P}_+ + \check{P}_- = \tau_0, \qquad \check{h} \, \check{P}_\pm = \pm \check{P}_\pm. \tag{158}$$

Using

$$(\epsilon Z + E) \, \check{P}_+ + (\epsilon Z - E) \, \check{P}_- = \epsilon Z \, \tau_0 - \xi \, \tau_3 - \phi \, \tau_1, \tag{159}$$

we can decompose

$$\check{G}^R = \frac{\check{P}_+}{\epsilon Z - E + i0} + \frac{\check{P}_-}{\epsilon Z + E + i0}, \qquad \check{G}^A = \frac{\check{P}_+}{\epsilon Z - E - i0} + \frac{\check{P}_-}{\epsilon Z + E - i0}. \tag{160}$$

Therefore, the spectral function is

$$\check{A}(\epsilon, \xi) = i\left(\check{G}^R - \check{G}^A \right) = 2\pi \left[\check{P}_+ \, \delta(\epsilon Z - E) + \check{P}_- \, \delta(\epsilon Z + E) \right]. \tag{161}$$

The delta functions can be rewritten as

$$\delta(\epsilon Z \pm E) = \frac{|\epsilon Z|}{\sqrt{(\epsilon Z)^2 - \phi^2}} \left[\delta(\xi - \xi_0) + \delta(\xi + \xi_0) \right], \qquad \xi_0 = \sqrt{(\epsilon Z)^2 - \phi^2}. \tag{162}$$

It is nice to see that the relative density of state factor $\rho(\epsilon) \equiv |\epsilon Z|/\sqrt{(\epsilon Z)^2 - \phi^2}$ emerges naturally from the spectral function. Next, we define the energy–shell average

$$\langle X \rangle_{\check{A}} \equiv \frac{1}{4\pi} \int d\xi_{\mathbf{p}} \; \text{Tr}\Big[\check{A}(\epsilon, \xi_{\mathbf{p}}) \, X\Big]. \tag{163}$$

To find the average, we first calculate the integration over ξ for $\check{A}$:

$$\int d\xi \, \check{A} = 2\pi \frac{|\epsilon Z|}{\sqrt{(\epsilon Z)^2 - \phi^2}} \left[\tau_0 + \frac{\phi}{\epsilon Z} \, \tau_1 \right]. \tag{164}$$

Depending on the sign of ϵZ, only one of the two delta functions will contribute. The odd function proportional to $\xi \tau_3$ vanishes after integration. We can also verify that this form of $\check{A}$ satisfies our previous result of Eqn.(122) in the limit where Z and ϕ becomes real functions. The sign function comes from analytical continuation of the retarded Green's function in the upper half plane. In general when we cannot ignore the imaginary part of the self-energy, we have:

$$\frac{1}{2\pi} \int d\xi_{\vec{p}} \check{A}(\epsilon, \vec{p}) = \Re \left[\frac{\epsilon Z}{\sqrt{(\epsilon Z)^2 - \phi^2}} \right] \tau_0 + \Re \left[\frac{\phi}{\sqrt{(\epsilon Z)^2 - \phi^2}} \right] \tau_1. \tag{165}$$

Using $\text{Tr} \, \tau_0 = 2$ and $\text{Tr} \, \tau_{1,2,3} = 0$, the ξ–averaged traces are

$$\langle \tau_0 \rangle_{\check{A}} = \rho(\epsilon) = \Re \left[\frac{\epsilon Z}{\sqrt{(\epsilon Z)^2 - \phi^2}} \right], \tag{166}$$

$$\langle \tau_1 \rangle_{\check{A}} = \varphi(\epsilon) = \Re \left[\frac{\phi}{\sqrt{(\epsilon Z)^2 - \phi^2}} \right], \tag{167}$$

$$\langle \tau_3 \rangle_{\check{A}} = 0. \tag{168}$$

Now if we apply the following operation to both sides of Eqn.(145):

$$\langle \cdots \rangle_{\check{Q}\check{A}} = \frac{1}{4\pi} \int d\xi_{\vec{p}} \text{Tr} \left[\check{Q} \check{A}(\epsilon, \vec{p})(\cdots) \right], \tag{169}$$

where $\check{Q} = \tau_3 + \tau_0$: we see for the left-hand side divided by 2 (to get an equation for f), there is:

$$\boxed{\begin{aligned} \text{LHS}[f] = \rho(\epsilon)\Big\{ &\partial_t f \left(Z_1 + \epsilon \partial_\epsilon Z_1 \right) - \partial_\epsilon f \left(\epsilon \partial_t Z_1 \right) + \vec{\nabla}_r f \cdot (\vec{v}_F - \epsilon \vec{\nabla}_p Z_1) + \vec{\nabla}_p f \cdot (\epsilon \vec{\nabla}_r Z_1) \Big\} \\ + \varphi(\epsilon)\Big\{ &- \partial_t f \, \partial_\epsilon \phi_1 + \partial_\epsilon f \left(\partial_t \phi_1 \right) + \vec{\nabla}_r f \cdot (\vec{\nabla}_p \phi_1) - \vec{\nabla}_p f \cdot (\vec{\nabla}_r \phi_1) \Big\}. \end{aligned}}$$

$$\tag{170}$$

It is clear that in the homogeneous BCS limit where $Z_1 \to 1$ and $\phi_1 \to \Delta$, we recover the usual Boltzmann equation multiplied by $\rho(\epsilon)$:

$$\text{LHS}[f] = \rho(\epsilon) \left(\partial_t f + \vec{v}_F \cdot \vec{\nabla}_r f \right). \tag{171}$$

On the right-hand side, we obtain something proportional to the collision kernel:

$$\mathcal{K} \equiv \int d\xi_{\vec{p}} \int d\xi_{\vec{p}'} \, \text{Tr} \left[\check{Q} \check{A} \tau_3 \check{A}' \tau_3 \right] \tag{172}$$

where we use $\vec{p}' = \vec{p} - \vec{q}$ and changed the momentum convolution to be an integral over $\vec{p}'$. To evaluate the collision kernel, we first observe that the trace of $\check{A} \tau_3 \check{A}' \tau_3$ is proportional to 4 sums of $\check{P}_{\pm} \tau_3 \check{P}'_{\pm} \tau_3$ projectors. We can write them out explicitly, for example:

$$\check{P}_+ \tau_3 \check{P}'_+ \tau_3 = \frac{1}{4} \left[\left(1 + \frac{\xi \xi'}{EE'} - \frac{\phi \phi'}{EE'} \right) \tau_0 + \dots \right] \tag{173}$$

$$\check{P}_+ \tau_3 \check{P}'_- \tau_3 = \frac{1}{4} \left[\left(1 - \frac{\xi \xi'}{EE'} + \frac{\phi \phi'}{EE'} \right) \tau_0 + \dots \right], \tag{174}$$

Adding all four terms together and taking note of the sign of $\epsilon Z = sE$, $s = \pm 1$, we can see that after the integration over ξ and ξ' and taking the trace,

$$\int d\xi_{\vec{p}} \int d\xi_{\vec{p}'} \, \text{Tr} \left[\check{Q} \check{A} \tau_3 \check{A}' \tau_3 \right] = \sum_{s,s'=\pm 1} (2\pi)^2 \left(1 - ss' \frac{\phi \phi'}{EE'} \right) \rho \rho'. \tag{175}$$

Putting everything together for the right-hand side, we have:

$$\text{RHS}[f] = \pi N_0 \int \frac{d\omega}{2\pi} \int \frac{d\hat{p}'}{4\pi} |g_{\vec{q}}|^2 B(\omega, \vec{q}) \sum_{s,s'=\pm 1} \left(1 - ss' \frac{\phi \phi'}{EE'} \right) \rho(\epsilon) \rho(\epsilon')$$
$$\times \left[N f'(1-f) - (N+1)(1-f')f \right] \tag{176}$$

$$= (2\pi) N_0 \int \frac{d\omega}{2\pi} \int \frac{d\hat{p}'}{4\pi} |g_{\vec{q}}|^2 B(\omega, \vec{q})$$
$$\times \left\{ (\rho \rho' - \varphi \varphi') \left[N f'(1-f) - (N+1)(1-f')f \right] \right.$$
$$\left. + (\rho \rho' + \varphi \varphi') \left[N(1-f')(1-f) - (N+1)f'f \right] \right\}. \tag{177}$$

Both single-quasiparticle scattering, and pairing and recombination processes emerge with the correct coherence factors. We used the identity $f(-\epsilon) = 1 - f(\epsilon)$ in the second term of the curly bracket to transform to the more familiar gain and loss functions, so that we ensure our energies ϵ, ϵ' are always positive.

In summary of this section, we have derived the quantum kinetic equation for the distribution function of quasiparticles in a superconductor, which needs to be solved self-consistently with the Eliashberg equations for the self-energies to obtain Z and ϕ. We have also shown that after applying the quasi-classical approximation and projecting with the spectral function, we recover a Boltzmann-like equation with the correct coherence factors for both scattering and recombination processes.

We lay out in the following paragraph some observations that take advantage of the spherical symmetry of the problem:

- Because of spherical symmetry, on spatial coordinates Δ and Z are both only a function of r for all times. There is no reason to believe that they will vary spatially except in the radial direction.

- However, in the momentum space, because of the directional dependence of the distribution function $f(\epsilon, \hat{p}; r, t)$, the self-energies $\Delta(\epsilon, \hat{p}; r, t)$ and $Z(\epsilon, \hat{p}; r, t)$ will also depend on the direction $\hat{p}$.

- Combining both of above, we see that in Eqn.(170), the spatial gradient $\vec{\nabla}_r Z_1$ and $\vec{\nabla}_r \phi_1$ will only have a radial component, while the momentum gradient $\vec{\nabla}_p f$ will only have angular components. Therefore, the terms like $\vec{\nabla}_p f \cdot (\epsilon \vec{\nabla}_r Z_1)$, $\vec{\nabla}_p f \cdot (\vec{\nabla}_r \phi_1)$, $\vec{\nabla}_r f \cdot (\epsilon \vec{\nabla}_p Z_1)$, $\vec{\nabla}_r f \cdot (\vec{\nabla}_p \phi_1)$ will be zero.

- One may wonder the origin of the directional dependence in f if the BTE does not explicitly has any angular dependence terms: the actual angular dependence comes from the streaming term $\vec{v}_F \cdot \vec{\nabla}_r f = v_F \cos\theta \partial_r f$, where θ is the angle between $\hat{p}$ and $\hat{r}$. This term couples the radial spatial gradient to the angular momentum gradient, and therefore induces angular dependence in f.

- In general, all the directional "smearing" effects will come from the right-hand side of the equation, and if the phonon momentum $\vec{q}$ is small, it has a weak effect on the direction of our quasi-particle momentum.

In the simplest case, we can just use two dimensions, r and ϵ, to parametrize our distribution function $f(\epsilon, r; t)$, and assume that the angular dependence is weak. We can assume that the angular dependence of f is only induced by the streaming term, which in the low-energy limit will be minimal and can be neglected. This assumption restores the isotropy of Z and ϕ, and the only important corrections to the traditional BTE are the presence of energy- and time-dependent Z and ϕ factors in the left-hand side. We will also ignore the time-derivative terms of Z and ϕ.

The full set of simplified equations are:

$$\text{LHS}[f] = \partial_t f \left(Z_1 + \epsilon \partial_\epsilon Z_1 - \frac{\varphi}{\rho} \partial_\epsilon \phi_1 \right) + \vec{v}_F \cdot \vec{\nabla}_r f \tag{178}$$

$$= (2\pi) N_0 \int \frac{d\omega}{2\pi} \int \frac{d\hat{p}'}{4\pi} |g_{\vec{q}}|^2 B(\omega, \vec{q})$$

$$\times \left\{ \left(1 - \frac{\varphi\varphi'}{\rho\rho'} \right) \rho' \left[N f'(1-f) - (N+1)(1-f')f \right] \right.$$

$$\left. + \left(1 + \frac{\varphi\varphi'}{\rho\rho'} \right) \rho' \left[N(1-f')(1-f) - (N+1)f'f \right] \right\}, \tag{179}$$

$$2\Im[\phi](\epsilon, \hat{p}) = N_0 \int d\omega \, \langle |g_{\vec{q}}|^2 B(\omega, q) \breve{a}_{12}(\epsilon - \omega, \hat{p}')[1 + n_b(\omega, q) - f_e(\epsilon - \omega, \hat{p}')] \rangle_{\hat{p}'}, \tag{180}$$

$$2\Im[\epsilon Z](\epsilon, \hat{p}) = N_0 \int d\omega \, \langle |g_{\vec{q}}|^2 B(\omega, q) \breve{a}_{11}(\epsilon - \omega, \hat{p}')[1 + n_b(\omega, q) - f_e(\epsilon - \omega, \hat{p}')] \rangle_{\hat{p}'}. \tag{181}$$

Note that the parametrization of $(\epsilon, \hat{p})$ can be changed to (ϵ, θ), where θ is the angle between $\hat{p}$ and $\hat{r}$ under spherical symmetry. The boundary conditions for the coordinates are:

- $r = 0$: $\partial_r f = 0$ (spherical symmetry);

- $r = R$: Extrapolation boundary condition where the energy flows freely out of the system, and f and $\partial_r f$ are continuous;

- $\epsilon = 0$: $f = \frac{1}{2}$ (fixed to the value at the Fermi surface);

- $\epsilon = \infty$: $f = 0$.

- $\theta = 0, \pi$: $\partial_\theta f = 0$ (spherical symmetry).

- Z, and ϕ are pre-computed as a function of ϵ.

The initial condition for f is just a Gaussian packet centered at some energy ϵ_0 and $r = 0$, with a uniform excitation among all direction $\hat{p}$.

3. Numerical Implementation

In this section we will document the implementation details and charts for our numerical simulation.

3.1. Evaluation of the Self-consistent Eliashberg Equations

To 0th order, let's solve the eliashberg equations without momentum directional dependence. We will then use the imaginary part of the self energy to solve for the real part.

First, solve $\Im[\epsilon Z]$ and $\Im[\phi]$:

$$
\begin{aligned}
\Im[\epsilon Z] &= \frac{N_0}{2} \int d\omega \langle |g_{\vec{q}}|^2 B(\omega, \vec{q}) \breve{a}_{11}(\epsilon - \omega)[1 + n_b(\omega, \vec{q}) - f_e(\epsilon - \omega, \hat{p}')]\rangle_{\hat{p}'} \\
&= \pi N_0 \int_{-\infty}^{\infty} d\omega \langle |g_{\vec{q}}|^2 [\delta(\omega - \omega_{\vec{q}}) - \delta(\omega + \omega_{\vec{q}})]\rho(\epsilon - \omega) \\
&\qquad\qquad\qquad \times [1 + n_b(\omega, \vec{q}) - f_e(\epsilon - \omega)]\rangle_{\hat{p}'} \\
&\approx \pi N_0 \sum_{\vec{q}} |g_{\vec{q}}|^2 \delta(\omega - \omega_{\vec{q}})\rho(\epsilon - \omega_{\vec{q}})\left[1 - f_e(\epsilon - \omega_{\vec{q}})\right] \\
\omega_{\vec{q}} \to \Omega \quad &= \pi \int_0^\epsilon d\Omega \alpha^2 F(\Omega)\rho(\epsilon - \Omega).
\end{aligned}
\tag{182}
$$

and:

$$
\begin{aligned}
\Im[\phi] &= \frac{N_0}{2} \int d\omega \langle |g_{\vec{q}}|^2 B(\omega, \vec{q}) \breve{a}_{12}(\epsilon - \omega)[1 + n_b(\omega, \vec{q}) - f_e(\epsilon - \omega, \hat{p}')]\rangle_{\hat{p}'} \\
&\approx \pi \int_0^\epsilon d\Omega\, \alpha^2 F(\Omega)\varphi(\epsilon - \Omega).
\end{aligned}
\tag{183}
$$

We then use the Kramers-Kronig relation to solve for the real part. Note as expected physically, the imaginary part of the Z function is an odd function. Then for the Z function:

$$
\Re[Z](\epsilon) = 1 + \frac{2}{\pi}\mathcal{P}\int_0^\infty d\epsilon' \frac{\epsilon' \Im[Z]}{\epsilon'^2 - \epsilon^2}
\tag{184}
$$

$$
\tag{185}
$$

and for the ϕ function:

$$\Re[\phi](\epsilon) = \frac{2}{\pi}\mathcal{P}\int_0^\infty d\epsilon' \frac{\epsilon'\Im[\phi]}{\epsilon'^2 - \epsilon^2}. \tag{186}$$

We can start with the BCS solution for $\Delta = \phi/Z$ as the initial guess, and $Z = 1$. Also note that the upper limit of the Ω integral is actually bounded by $\min(\epsilon, \Omega_D)$.

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