Bound states and impurity averaging in unconventional superconductors

Robert Joynt
Department of Physics
University of Wisconsin-Madison
1150 University Avenue
Madison, WI 53706
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Abstract

The question of anomalous transport due to a band of impurity states in unconventional superconductors is discussed. In general, the bound state energies are not in midgap, even in the unitarity limit. This implies that, generically, the states associated with impurities are broad resonances, not true bound states. There is no impurity band in the usual sense of the phrase. The wavefunctions of these resonances possess interesting anisotropies in real space, but this does not result in anomalous hopping between impurities. I conclude that the system of resonances produces no qualitative modifications to the T-matrix theory with impurity averaging which is normally used to treat the low-temperature transport of unconventional superconductors. However, users of this method often assume a density of states which is symmetric around the chemical potential. This is not normally the case. It is found that the non-crossing approximation is not valid in a strictly two-dimensional system.

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I. INTRODUCTION

Impurity scattering plays a dominant role in the transport and thermodynamic properties of unconventional superconductors, far larger than in conventional s-wave superconductors. This is a consequence of the gap nodes which prevent the complete freezing out of scattering processes, and the fact that an anisotropic order parameter is far more sensitive to disorder. The critical temperature for an anisotropic superconductor is suppressed even in lowest order by the disorder potential. This follows from the breakdown of one of the conditions for Anderson’s theorem [1], which is that the momentum dependence of the pair potential is weak. A breakdown of the theorem leads to bound states in the gap when there are magnetic impurities in s-wave materials. It also leads to the possibility of such bound states from nonmagnetic impurities in the gap of an unconventional superconductor. This paper is devoted to questions about these states: their energy levels, their wavefunctions, their lifetimes, and the role (if any) they play in observable properties at low temperatures.

This subject is topical because of the interest in high-temperature superconductors. Some of these systems appear to have gap nodes, implying the presence of an unconventional order parameter. No picture of these materials is complete without understanding the effects of dirt. Furthermore, experiments in the asymptotic low-temperature regime are special in that they probe the region of the Fermi surface near the nodes. It is in this region where the effects of impurities are most dramatic. The same considerations hold for the comparatively venerable heavy-fermion superconductors. Here we have solid grounds for supposing that some of these systems, particularly UPt$_3$ and UBe$_{13}$, are unconventional. Still, after more than a decade of investigation, the experimental details of the thermodynamic and transport properties of these systems at low temperatures are not fully reconciled with theory. In heavy fermion materials, however, it has become clear that strong impurity scattering, approaching the unitary limit, is the rule, not the exception. The Born approximation is inadequate. In high-$T_c$ systems, this is still under debate. In this paper, I will concentrate on this near-unitary limit.
The literature on impurity states in the superconducting gap begins with the papers of Yu [2] and Shiba [3] on magnetic impurities in s-wave systems. The two important ingredients are the pairbreaking nature of the disorder potential and the 'hard' energy gap - the density of states (DOS) is zero in some neighborhood of the chemical potential in the pure system. Bound states appear in the gap. Increasing the impurity concentration increases the number of bound states and decreases the gap, leading first to the gapless state and finally to the destruction of superconductivity [4].

In unconventional superconductors, the bound states arising from ordinary potential scattering were first considered by Buchholtz and Zwicknagl [5]. They concentrated on the Balian-Werthamer state, which has a hard energy gap, but the momentum-averaged gap vanishes: \( \sum \vec{k} \Delta(\vec{k}) = 0 \), where the sum is over the Fermi surface. For such a gap, the results are somewhat similar to the previous case as the disorder potential is likewise pairbreaking. Although time-reversal symmetry is not broken, the randomization of momentum in the eigenstates prevents pairing by a momentum-dependent potential. Bound states appear in the gap. These authors also state that, in the unitarity limit of very strong potentials on the impurities, the bound states are at midgap. This statement has been repeated many times in the literature. However, I will argue below that it is incorrect.

One important point about unconventional superconductors is that they cannot exist at very high impurity density. The critical temperature decreases as the impurity concentration is increased, and vanishes when \( \hbar/\tau \approx k_BT_c \), where \( T_c \) is the critical temperature in the absence of scattering. This implies that the regime of low impurity density is the only one of interest.

With the discovery in the 1980’s of the heavy fermion superconductors, there was an explosion of interest in the problem of disorder in unconventional superconductors. Many calculations of transport and thermodynamic properties at low temperatures have been published [6]. The standard method, explained most completely by Hirschfeld et al. [7], combines the T-matrix approximation with standard impurity averaging techniques. Generally speaking, scattering near or at the unitarity limit is required to explain experiments
in both the heavy-fermion \cite{6, 8} and perhaps also in the high-T\textsubscript{c} materials \cite{9, 10}. This suggestion that the unitary limit is the appropriate one for Kondo lattice systems is due to Pethick and Pines \cite{11}. While this model is certainly relevant to the weakly hybridizing \textit{f}-level electrons in heavy fermion materials, its applicability to high-T\textsubscript{c} systems is unclear.

The superconducting order parameters considered for both kinds of systems do satisfy the $\sum_{\vec{k}} \Delta(\vec{k}) = 0$ condition, but they do not have a hard energy gap. The DOS of the pure system is usually taken to vanish linearly or quadratically at the chemical potential $\mu$. The standard method of treating the disorder potential leads to a finite DOS at $\mu$ \cite{12}. The neighborhood of the chemical potential where the density of states is flat is sometimes referred to as the 'impurity band' \cite{10}.

The impurity averaging method for unconventional superconductors has been explicitly questioned by some recent work \cite{13}. The gap nodes lead to unusual wavefunctions for the bound states, with the possibility of anomalous overlaps between well-separated impurities. In compensated doped semiconductors, a high concentration of impurities can lead to a new conduction mechanism which predominates at low temperatures, conduction entirely through the impurity wavefunctions which form the impurity band \cite{14}. This possibility must be considered also in superconductors. The electrical conductivity of any such band would of course be shorted out by the conductivity of the condensate, but the opposite could well occur for the thermal conductivity. I will argue below that this does not occur.

A more radical criticism of impurity averaging for two-dimensional systems is contained in papers of Neresyan \textit{et al.} \cite{15}, who find that multisite processes restore the vanishing of the DOS at the chemical potential. A recent preprint of Ziegler \textit{et al.} \cite{16} shows that, for Lorentzian disorder, the finite DOS is not a consequence of impurity averaging.

While the aim of the current work is to clarify the theoretical situation for nonmagnetic impurities in unconventional superconductors, there has been considerable recent work on magnetic impurities in both conventional and unconventional superconductors, stimulated by experiments \cite{17}. Some of this work has reached conclusions similar to those presented here, particularly with regard to the importance of carefully considering the real part of the
Green’s function in T-matrix calculations [18], [19].

In order to build up the theory from the start, I begin in Sec. II with the question of bound states in the normal state of a semiconductor with a gap, in the limit of strong scattering. Since the semiconductor analogy is a powerful (but not omnipotent) one, this section provides much of the basis for the paper. The s-wave case is treated briefly in Sec. III, both to establish notation and to get a basis of comparison with unconventional superconductivity. This latter topic, the main subject of the paper, is begun with calculations of the wavefunctions and lifetimes for single impurities in d-wave-type systems in Sec. IV. Finally, in Sec. V the many-impurity case is discussed, along with the experimental implications for real systems.

II. BOUND STATES IN SEMICONDUCTORS

A. Introduction and formalism

I examine an imaginary semiconductor in this section. The goal is to understand the process of binding an electron to an impurity with a very strong short-range potential. The physics of this process is sufficiently different from the textbook cases that certain features are likely to be as unfamiliar to the reader as they were to the writer. These features are important for the superconducting model which is believed to be of most relevance for high-$T_c$ and heavy fermion superconductors.

Let us consider a semiconductor with a single impurity. The gap is the result of the lattice potential, a single-particle effect, and is not tied to the chemical potential, which lies in the gap. In the limit of weak scattering, this is essentially the familiar case of off-valence impurities in a Group IV material. This leads to impurity states very near the band edges. Our interest is in the opposite limit when the scattering is strong. The unperturbed Hamiltonian is

$$\hat{H}_0 = \sum_k \epsilon_{\vec{k}} n_{\vec{k}}.$$  

(1)
The energies are measured from the chemical potential. I have omitted band and spin indices for clarity. The sum over momentum is always taken to include a sum over bands. The potential for a single short-range impurity is

$$\hat{V} = V \sum_{\vec{k}, \vec{k}'} c_{\vec{k}}^\dagger c_{\vec{k}'}.$$

(2)

This is an s-wave potential. The phase shift is

$$\delta(\epsilon) = -\tan^{-1}(\pi N_0(\epsilon)V),$$

(3)

where $N_0(\epsilon)$ is the density of states of the unperturbed system. The phase shift normally quoted in papers on transport properties is for states at the Fermi surface:

$$\delta_0 = -\tan^{-1}[\pi N_0(\epsilon_F)V],$$

(4)

The unitarity limit $\delta \to \pi/2$ is reached when $V \to -\infty$.

The unperturbed Green’s function is

$$G_0(\vec{k}, i\omega) = \frac{1}{i\omega - \epsilon_{\vec{k}}}$$

(5)

The equation for the full Green’s function for the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ is

$$G(\vec{k}, \vec{k}', i\omega) = G_0(\vec{k}, i\omega)\delta_{\vec{k}, \vec{k}'} + G_0(\vec{k}, i\omega)V G_0(\vec{k}', i\omega) + G_0(\vec{k}, i\omega)V \sum_{\vec{k}_1} G_0(\vec{k}_1, i\omega)V G_0(\vec{k}', i\omega) + \ldots$$

$$= G_0(\vec{k}, i\omega)\delta_{\vec{k}, \vec{k}'} + G_0(\vec{k}, i\omega)T(i\omega)G_0(\vec{k}', i\omega).$$

(6)

Here

$$T(i\omega) = V + V^2 \sum_{\vec{k}} G_0(\vec{k}, i\omega) + V^3 [\sum_{\vec{k}} G_0(\vec{k}, i\omega)]^2 + \ldots$$

(7)

$$= \frac{V}{1 - V g_0(i\omega)}$$

(8)

and

$$g_0(i\omega) \equiv \sum_{\vec{k}} \frac{1}{i\omega - \epsilon_{\vec{k}}}. $$

(9)
Continuing this function to the real axis:

\[ g_0(\omega + i\delta) = \sum_k \frac{1}{\omega - \epsilon_k + i\delta} = \sum_k \frac{\mathcal{P}}{\omega - \epsilon_k} - i\pi \sum_k \delta(\omega - \epsilon_k). \]  

(10)

Thus

\[ \text{Im } g_0(\omega + i\delta) = -\pi \sum_k \delta(\omega - \epsilon_k) = -\pi N_0(\omega), \]

(11)

where \( N_0(\omega) \) is the density of states for one spin. Also

\[ \text{Re } g_0(\omega + i\delta) = \mathcal{P} \int \frac{N_0(\omega')}{\omega - \omega'} d\omega', \]

(12)

proportional to the Hilbert transform of the density of states.

The expression

\[ T(\omega) = \frac{V}{1 - Vg_0(\omega)} \]

(13)

shows that \( T \) has poles only when \( g_0 \) is purely real and

\[ \frac{1}{V} = \text{Re } g_0(\omega_b). \]

(14)

Let us agree that when real frequency arguments are used, a limit is implied where the real frequency axis is approached from above in the complex plane, corresponding to retarded functions. When Eq. 14 is satisfied but \( g_0 \) has an imaginary part, then \( T \) is a Lorentzian near \( \omega_b \), and we are dealing with a resonance. If there is a pole, it represents a bound (\( V < 0 \)) or an antibound (\( V > 0 \)) state. In these cases we may write

\[ T^{-1}(\omega \approx \omega_b) \approx \frac{1}{V} - g_0(\omega_b) - (\omega - \omega_b)g'_0(\omega_b) = -(\omega - \omega_b)g'_0(\omega_b), \]

(15)

where

\[ g'_0(\omega_b) = -\mathcal{P} \int \frac{N_0(\omega')d\omega'}{(\omega_b - \omega')^2} \equiv -Z. \]

(16)

The integral for \( Z \) always converges because \( N_0(\omega_b) = 0 \) for a true bound state. Therefore we find
\[ T(\omega \approx \omega_b) \approx \frac{Z^{-1}}{\omega - \omega_b}, \]  

(17)

in the neighborhood of the pole. The bound states are therefore characterized by poles in the T-matrix, and resonances by a sharp peak in the imaginary part of the T-matrix.

The T-matrix gives the exact solution for the one impurity problem. It is not an approximation.

**B. Case of symmetric bands**

Let us consider a semiconductor with an unperturbed density of states which has a gap of width \(2\Delta\), and satisfies the symmetry relation

\[ N_0(\omega) = N_0(-\omega). \]  

(18)

I will argue below that this is not likely to be realized in the cases of interest, but it is the simplest mathematically. The density of states is illustrated in Fig. [Fig.]. Now we have

\[ \text{Re} \ g_0(\omega) = \mathcal{P} \int \frac{N_0(\omega')d\omega'}{\omega - \omega'} \approx -\frac{2\omega}{\omega_g^2}, \]  

(19)

in the region \(|\omega| << \omega_g\), where

\[ \omega_g^{-2} \equiv \int \frac{N_0(\omega')d\omega'}{\omega'^2} > 0. \]  

(20)

\(\omega_g\) is of order \(\Delta\) if the bandwidth is smaller than the gap energy (characteristic of insulators) and is of order the geometric mean of bandwidth times the gap energy in the other limit where the bandwidth is much greater than the gap energy (characteristic of semiconductors). The bound state energy \(\omega_b\) satisfies

\[ \frac{1}{V} = -\frac{2\omega_b}{\Delta^2}, \]  

(21)

or

\[ \omega_b = -\frac{2\Delta^2}{V}. \]  

(22)
For large $|V|$, (the unitary limit) this is a midgap state. This limit is shown in Fig. [4]. For $V < 0$ the potential is attractive and the state sits just above the middle of the gap. This is an ordinary bound state. If $V > 0$, it sits just below the center of the band. It is an 'antibound' state, but the wavefunction is localized, just as for a bound state.

C. Density of states

The density of states is

$$N(\omega) = -\frac{1}{\pi} \text{Im} \, T r \, G(\vec{k}, \vec{k'}, \omega + i\delta).$$  \hspace{1cm} (23)

Comparing this with the equation

$$G(\vec{k}, \vec{k'}, \omega) = G_0(\vec{k}, \omega) \delta_{\vec{k}, \vec{k'}} + G_0(\vec{k}, \omega) T(\omega) G_0(\vec{k'}, \omega),$$

we find in the gap region (when $\text{Im} \, G_0 = 0$):

$$N(\omega) = N_0(\omega) - \frac{1}{\pi} \sum_{\vec{k}} (\omega - \epsilon_{\vec{k}})^{-2} \text{Im} \, T(\omega),$$

which may be written in terms of the change in the density of states:

$$\Delta N(\omega) = N(\omega) - N_0(\omega) = -\frac{1}{\pi} \sum_{\vec{k}} (\omega - \epsilon_{\vec{k}})^{-2} \text{Im} \, T(\omega).$$

Near $\omega = \omega_b$ this expression yields

$$N_{imp} = -\frac{1}{\pi} \left[ \sum_{\vec{k}} (\omega - \epsilon_{\vec{k}})^{-2} \right] \text{Im} \frac{Z^{-1}}{\omega - \omega_b + i\delta} = \delta(\omega - \omega_b),$$

which is the impurity contribution to the density of states. To obtain the second equality, I have used Eq. [16]. In the region where $\text{Im} \, g_0(\omega) \neq 0$, we also have that $\text{Im} \, T(\omega) \neq 0$, and this represents a phase shift with an accompanying reduction of the density of states of the continuum such that

$$\int \Delta N(\omega) d\omega = 0.$$  \hspace{1cm} (28)

The reduction of the density of states of the continuum just cancels the additional bound state (Levinson’s theorem).
D. Local density of states

Near the bound state energy, the Green’s function in real space has the form

$$\frac{|\psi(\vec{r})|^2}{\omega - \epsilon_b + i\delta}. \quad (29)$$

Comparing with Eq. 6, we may extract the wavefunction $\psi(\vec{r})$ by taking the Fourier transform of $G_0(\omega + i\delta)$:

$$\psi(\vec{r}) \sim \int \frac{e^{i\vec{k} \cdot \vec{r}} d^3k}{\omega - \epsilon_k + i\delta}. \quad (30)$$

Consider a semiconductor with a bound state at $\omega_b$ and band edges at $\pm \Delta/2$. Let the bands be parabolic. Then the contribution from the upper band is:

$$\psi(\vec{r}) \sim \int \frac{e^{i\vec{k} \cdot \vec{r}} d^3k}{\omega_b - \epsilon_{k_0} + i\delta}. \quad (31)$$

$$= -2m \int \frac{e^{i\vec{k} \cdot \vec{r}} d^3k}{k^2 + k_0^2} \quad (32)$$

$$= -4\pi m \int_0^\infty k^2 dk \int_{-1}^1 dx \frac{e^{ikrx}}{k^2 + k_0^2} \quad (33)$$

$$= - \frac{4\pi m}{ir} \int_0^\infty kdk \frac{e^{ikr} - e^{-ikr}}{k^2 + k_0^2} \quad (34)$$

$$= - \frac{4\pi^2 m}{r} e^{-k_0 r}, \quad (35)$$

where $k_0^2 \equiv m\Delta - 2m\omega_b$. The contribution from the lower band is the same except that $k_0$ is replaced by $|m\Delta + 2m\omega_b|$. The wavefunction is very tightly bound, the decay length being short because the energy is far from the band edge.

In the limit of a very weak attractive potential ($V < 0$ and $VN_u << 1$), then we are interested in the form of $\text{Re} \ g_0(\omega)$ when $\omega \approx \Delta$. We find

$$\text{Re} \ g_0(\omega) \approx N_u \log \left( \frac{\Delta - \omega}{\epsilon_u} \right). \quad (36)$$

The bound state energy is:

$$\omega_b = \Delta - \epsilon_u e^{1/N_u V}. \quad (37)$$
This is a state just below the upper band. The lower band has no effect in this case. It is important to note that the exponential dependence for the bound state energy is due to the fact that there is a finite jump in the density of states at the band edge. If there is a square root singularity:

\[ N_0(\omega) \sim (\omega - \Delta)^{1/2} \]  

(38)

for \( \omega > \Delta \), as one would expect in three dimensions, then there is a threshold coupling strength below which there is no bound state.

The hydrogenic impurity case, of great practical importance, is different from all of these cases because of the long-range potential, which leads to an infinite number of bound states for all interaction strengths even in three dimensions.

E. Case of asymmetric bands

If the bands are asymmetric, \( N_0(\omega) \neq N_0(-\omega) \), then the bound state is not in the middle of the gap even when \(|V| \to \infty\). This result is illustrated in Fig. ?? . Consider an example where the lower band extends from \(-\epsilon_\ell\) to \(-\Delta\), and the upper band from \(\Delta\) to \(\epsilon_u\). Let the bands have constant density of states \(N_\ell\) and \(N_u\), respectively. Then

\[
Re \ g_0(\omega) = N_\ell \int_{-\epsilon_\ell}^{-\Delta} \frac{d\omega'}{\omega - \omega'} + N_u \int_{\Delta}^{\epsilon_u} \frac{d\omega'}{\omega - \omega'} \\
= -N_\ell \log \left| \frac{\omega + \Delta}{\epsilon_\ell} \right| + N_u \log \left| \frac{\omega - \Delta}{\epsilon_u} \right| .
\]  

(39)

(40)

If the energy is in the gap, \(|\omega| < \Delta\), then this may be written as

\[
Re \ g_0(\omega) = N_\ell \log \left| \frac{\epsilon_\ell}{\Delta} \right| - N_u \log \left| \frac{\epsilon_u}{\Delta} \right| - \frac{N_u + N_\ell}{\Delta} \omega.
\]  

(41)

The bound state equation \( Re \ g_0(\omega) = 1/V \) now has the solution:

\[
\omega_b = -\frac{\Delta}{N_u + N_\ell} \left[ \frac{1}{V} + N_u \log \left( \frac{\epsilon_u}{\Delta} \right) - N_\ell \log \left( \frac{\epsilon_\ell}{\Delta} \right) \right].
\]  

(42)

Even in the limit of very strong scattering, this is not a midgap state. The bound state energy is displaced away from the band with the higher density of states because of level
repulsion. The asymptotic behavior of the wavefunction (the radius of the bound state) is still determined by the distance to the nearest band edge and the effective mass of that band.

The effect of the asymmetry may be described as a renormalization of the potential in the following way. We may rewrite the eigenvalue equation as:

\[ \omega_b = -\frac{\Delta}{(N_u + N_\ell)V}, \tag{43} \]

if we define the renormalized potential strength as

\[ \tilde{V} = \frac{V}{1 + VN_u \log(e_u/\Delta) - VN_\ell \log(e_\ell/\Delta)} \equiv \frac{V}{1 + VN_A} . \tag{44} \]

This equation defines the asymmetry factor \( N_A \),

\[ N_A = N_u \log \left( \frac{e_u}{\Delta} \right) - N_\ell \log \left( \frac{e_\ell}{\Delta} \right) \tag{45} \]

which is of the same order of magnitude as the density of states at the Fermi energy. It is \( \tilde{V} \) not \( V \), that determines the energy of the bound state. It is important to note that, as \( V \to \infty \),

\[ \tilde{V} \to \frac{1}{N_A}. \tag{46} \]

If the upper band is dominant, \( N_A > 0 \), and the potential is repulsive, \( V > 0 \), then we have that \( \tilde{V} < V \) and the antibound state always stays below the center of the gap. This is simply a consequence of level repulsion. There is a similar effect for \( V < 0 \) and \( N_A < 0 \), with the bound state never reaching the center of the gap even if \( V \to \infty \). For the other combinations of signs, we will have a midgap state only in the 'accidental' case that \( V = -\frac{1}{N_A} \).

This issue of band symmetry is crucial for the understanding of the bound state problem. It is particularly important to distinguish band symmetry from particle-hole symmetry, which is a very useful approximation for many calculations in superconductivity theory. Particle-hole symmetry is the assumption, approximately true in most cases, that the density of states of the normal material does not vary appreciably in the neighborhood of the Fermi
energy, the neighborhood being here defined as the range of energies within the cutoff energy $\hbar \omega_c$ for the pairing interaction. The approximation may be stated as

$$\omega_c \frac{dN_0(\omega)}{d\omega}(\omega = \epsilon_F) << N_0(\epsilon_F)$$

(47)

This is used in many elementary calculations of superconducting properties because only this range of energies is important for many purposes. A good example is the calculation of the critical temperature in the weak-coupling theory. The validity of the approximation arises ultimately from the mismatch of electronic and phononic (or other bosonic) time scales.

Band symmetry is the assumption $N_0(\omega) = N_0(-\omega)$ which is essentially never valid. To give an idea of how far it fails, I have computed numerically the asymmetry factor for the following model semiconductor. It is a two-dimensional square lattice with a nearest-neighbor hopping matrix element $t$ and a filling of 0.8 electrons per unit cell. The dispersion is $\epsilon_{\mathbf{k}} = -2.0t[\cos(k_x) + \cos(k_y)]$. At the Fermi energy $\epsilon_F = -0.4t$, there is a gap, symmetric around $\epsilon_F$, of $0.02t$. The density of states is shown in Fig. [3]. Then $N_A$ is defined as

$$N_A = \langle \frac{1}{\epsilon_{\mathbf{k}} - \epsilon_F} \rangle,$$

(48)

where the brackets indicate an average over the band. The result is $N_A = 0.25/t$ per unit cell. Since the total band width is $W = 8t$, we see that the product $N_A W$ is of order unity. For any band, $N_A$ as a function of filling has one zero at some point. For this particular band, this occurs at half filling. In general, however, it is only for a special choice of $\epsilon_F$ that $N_A = 0$ and the band symmetry assumption is valid. The physical distinction between particle-hole and band symmetry is that there is no frequency mismatch for impurity scattering. The ionic potential which produces the band structure and the impurity potential are instantaneous. It is natural, but completely unjustifiable, to extend particle-hole symmetry to band symmetry. No conclusion which is based on such an extension is likely to apply to any real material.
F. Level occupation

In a semiconductor, the occupation of impurity levels is normally strongly dependent on
the valence of the impurity relative to the valence of the constituent atoms. Here, we have
been using a model in which the valence of the impurity and the background atoms is the
same. We explicitly do not introduce additional states, only a potential which moves the
old states around. This distinguishes the present work from Anderson magnetic impurity
models, which generally do introduce such new states.

The occupation at zero temperature is then as follows. If the potential is repulsive, the
impurity ‘peels off’ one state from the valence band. It is therefore full, regardless of its
position in the gap, and even if it is above midgap. If the potential is attractive, the impurity
peels off one state from the valence band. It is therefore empty, also regardless of its position
in the gap. In real semiconductors, it is normally true that the Coulomb repulsion prevents
double occupancy of impurity levels, an effect not considered here.

G. Many impurities

1. Impurity band formation

If there are $N_{\text{imp}}$ impurities at a finite density $n_{\text{imp}}$ in the system, we must consider the
possibility that the wavefunctions on different impurities overlap. We begin with the case
of two impurities. The Hamiltonian is then

$$\hat{H} = \hat{H}_0 + \hat{V}_1 + \hat{V}_2.$$  \hfill (49)

$\hat{H}_0$ is the Hamiltonian of the pure system, $\hat{V}_1$ is the potential of the impurity at site $\vec{r}$, and $\hat{V}_2$
is the potential of the impurity at the site $\vec{r} + \vec{R}$. Our interest is in the limit $Rk_0 \gg 1$, where
$k_0$ is the inverse of the bound state radius, as in Eq. [35]. The bound state wavefunctions
satisfy

$$(\hat{H}_0 + \hat{V}_1)\psi_1 = \omega_b \psi_1$$ \hfill (50)
and

\[(\hat{H}_0 + \hat{V}_0)\psi_2 = \omega_b \psi_2.\]  \hspace{1cm} (51)

The overlap matrix element is

\[M_{12} = \langle \psi_2 | \hat{H} | \psi_1 \rangle = \omega_b \langle \psi_2 | \psi_1 \rangle + \langle \psi_2 | \hat{H}_1 | \psi_1 \rangle.\]  \hspace{1cm} (52)

The two terms are generally of the same size and asymptotic behavior. Taking the first as representative, we find

\[M_{12} \sim \omega_b \langle \psi_2 | \psi_1 \rangle \sim \omega_b \int \psi^*(\vec{r}) \psi(\vec{r} + \vec{R}) d^3r,\]  \hspace{1cm} (53)

where \(\psi\) is the impurity wavefunction. Using Eq. 30, we find, for the symmetric case

\[M_{12}(\vec{R}) \sim \omega_b \int \frac{e^{i\vec{k} \cdot \vec{r}} d^3k}{\omega_b - \epsilon_\vec{k}} \int \frac{e^{i\vec{k} \cdot \vec{r} + \vec{k} \cdot \vec{R}} d^3k'}{\omega_b - \epsilon_\vec{k}'} d^3r \]

\[\sim \omega_b \int \frac{e^{i\vec{k} \cdot \vec{R}} d^3k}{\omega_b - \epsilon_\vec{k}} \int \frac{e^{-\vec{k} \cdot \vec{R}} d^3k'}{\omega_b - \epsilon_\vec{k}'} \]

\[= \frac{8\pi^2 m \omega_b}{k_0} e^{-k_0 R}.\]  \hspace{1cm} (54)

As in Eq. 35, we have the decay length \(k_0^2 \equiv m \Delta - 2m \omega_b\). We may now write a Hamiltonian for the many-impurity case in the basis of the bound state wavefunctions at different sites. The resulting impurity bandwidth is of order \(\omega_b \exp(-k_0 n_{imp}^{-1/3})\). \(\omega_b\) is less than the gap energy \(\Delta\) and \(1/k_0\) is of the order of the lattice spacing. We generally expect a very small bandwidth for this ‘deep impurity’ \((\omega_b \sim \Delta)\) case. There is therefore no metallic conduction when there is even a small amount of disorder in the impurity site energies. Interactions will also tend to localize the electrons and strengthen this conclusion.

2. Impurity averaging

The Hamiltonian for the many-impurity case is

\[\hat{H} = \hat{H}_0 + \sum_i V(\vec{r} - \vec{R}_i).\]  \hspace{1cm} (55)
The impurities are located at the position $\vec{R}_i$. The standard method of calculation is to average over the positions $\vec{R}_i$ (impurity averaging) [20]. This method is valid for calculating the effects of impurities on the existing states if there are no correlations in the quantities $\psi_0^*(\vec{R}_i)\psi_0(\vec{R}_j)$, where $\psi_0^*(\vec{r})$ are the eigenfunctions of the Hamiltonian. This is a phase randomness assumption. The averaging process restores the translation invariance of the system on the average. The averaging method is clearly only appropriate when the number of impurities is an extensive quantity.

It is convenient to rewrite the Hamiltonian in Eq. 55 as

$$\hat{H} = \hat{H}_0 + \hat{V}_0 + \hat{V} - \hat{V}_0,$$  \hspace{1cm} (56)

where $\hat{V}_0$ is the spatial average of $\hat{V}$. We then define $G_0(\vec{k}, i\omega)$ as the unperturbed Green’s function belonging to the Hamiltonian $\hat{H}_0 + \hat{V}_0$. Both pieces of this Hamiltonian are diagonal in the momentum, and the second part gives only a rigid shift of the spectrum. The perturbation is then $\hat{V} - \hat{V}_0$, which scatters electrons from a state $\vec{k}$ to a state $\vec{k}'$. The scattering amplitude is zero if $\vec{k} = \vec{k}'$ because of the subtraction procedure. It is important to subtract the average potential explicitly, because the real part of the self-energy cannot be ignored in this problem, as it often can be in other contexts.

The equation for the Green’s function before averaging is

$$G(\vec{k}, \vec{k}', i\omega) = G_0(\vec{k}, i\omega)\delta_{\vec{k},\vec{k}'} + G_0(\vec{k}, i\omega)V_{\vec{k},\vec{k}'} G_0(\vec{k}', i\omega)$$

$$+ G_0(\vec{k}, i\omega) \sum_{\vec{k}''} V_{\vec{k},\vec{k}''} G_0(\vec{k}'', i\omega)V_{\vec{k}'',\vec{k}'} G_0(\vec{k}', i\omega) + \ldots$$

(57)

Here

$$V_{\vec{k},\vec{k}'} \equiv V \sum_i e^{i(\vec{k} - \vec{k}') \cdot \vec{R}_i} - N_{\text{imp}} V \delta_{\vec{k},\vec{k}'}.$$  \hspace{1cm} (58)

It is evident that in the extreme low density limit where the impurities have no influence on each other, this equation will reduce to the single impurity case. Quantities in Eq. 57 are averaged using the prescription:
\[ A = \frac{1}{L^{3N_{\text{imp}}}} \prod_i \int d^3 R_i A, \] (59)

where \( L \) is the linear dimension of the system (henceforth taken to be unity) and \( N_{\text{imp}} \) is the number of impurities. This leads to

\[ G(\vec{k}, \vec{k}', i\omega) = G_{\text{imp}}(\vec{k}, i\omega) \delta_{\vec{k}, \vec{k}'}. \] (60)

A Green’s function diagonal in the momentum \( G_{\text{imp}}(\vec{k}, i\omega) \) describes a state with uniform density. This shows that the averaging procedure washes out the density fluctuations which the impurities induce in the ground state (and other states) of the system. Bound states are an example of such density fluctuations. Thus, there is no possibility of bound states in this approximation.

Carrying out the averaging and neglecting diagrams with crossed lines (an approximation which will be discussed below) leads to the equation

\[ G_{\text{imp}}(\vec{k}, i\omega) = G_0(\vec{k}, i\omega) + G_0(\vec{k}, i\omega)n_{\text{imp}} V^2 \sum_{\vec{k}''} G_{\text{imp}}(\vec{k}''', i\omega) G_{\text{imp}}(\vec{k}, i\omega) \]
\[ + G_0(\vec{k}, i\omega)n_{\text{imp}} V^3 \sum_{\vec{k}'''} G_{\text{imp}}(\vec{k}''', i\omega) \sum_{\vec{k}''} G_{\text{imp}}(\vec{k}'', i\omega) G_{\text{imp}}(\vec{k}, i\omega) + \ldots \] (61)

The series is most conveniently summed by defining the self-energy

\[ \Sigma(\vec{k}, i\omega) = G_{\text{imp}}^{-1}(\vec{k}, i\omega) - G_0^{-1}(\vec{k}, i\omega), \] (62)

which leads to the equation

\[ \Sigma(\vec{k}, i\omega) = \frac{n_{\text{imp}} V^2 \sum_{\vec{k}''} [i\omega - \epsilon_{\vec{k}''} - \Sigma(\vec{k}, i\omega)]^{-1}}{1 - V \sum_{\vec{k}''} [i\omega - \epsilon_{\vec{k}''} - \Sigma(\vec{k}, i\omega)]^{-1}}. \] (63)

It is then seen that \( \Sigma \) is a function of frequency alone for the short-range scattering potential. For that reason, the equation is algebraic, not integral. In the Born approximation, the denominator in this expression would be absent:

\[ \Sigma(\vec{k}, i\omega) = n_{\text{imp}} V^2 \sum_{\vec{k}''} [i\omega - \epsilon_{\vec{k}''} - \Sigma(\vec{k}, i\omega)]^{-1} \] (64)

Eq. (63) contains two physical effects. The band edges are moved inwards because of level repulsion coming from the impurity potential. This directly affects the real part of the self-energy. The states are broadened because of the disorder which means that \( \vec{k} \)-states are no
longer eigenstates. This directly affects the imaginary part of the self-energy. Both of these
effects tend to close the gap.

To estimate the critical value of the potential strength at which this closure occurs, we
must first specify the model a bit more precisely. Let us take the symmetric model of Fig. 1.
Then we need only determine when, at midgap (ω = 0), the density of states first becomes
finite. At real frequencies, let us separate the real and imaginary parts of the self-energy:

\[ \Sigma(\omega) = \Sigma'(\omega) + i\Sigma''(\omega). \]  \hspace{1cm} (65)

Since we have

\[ N(\omega) = -Im \sum_{\vec{k}} \frac{\Sigma''}{(\omega - \epsilon_{\vec{k}} - \Sigma')^2 + \Sigma''^2}, \]  \hspace{1cm} (66)

we may simply increase the density \( n_{imp} \) and scattering strength \( V \) of the impurities, two
quantities which occur only in the combination \( n_{imp}V^2 \), and determine when \( \Sigma''(0) \neq 0 \).
First consider the Born approximation. Symmetry dictates that \( \Sigma'(0) = 0 \). The imaginary
part of Eq. 64 at zero frequency is then

\[ \Sigma''(0) = n_{imp}V^2 \Sigma''(0)f(0, \Sigma''(0)), \]  \hspace{1cm} (67)

where the function \( f \) is defined as

\[ f(\omega, \Sigma''(0)) \equiv N_0 \int \frac{d\epsilon}{(\omega - \epsilon)^2 + (\Sigma''(0))^2}, \]  \hspace{1cm} (68)

and the integral runs only over the energies for which the unperturbed density of states is
nonzero. Eq. 67 always has the solution \( \Sigma''(0) = 0 \). It develops a second solution when

\[ \frac{1}{n_{imp}V^2} = f(0, 0). \]  \hspace{1cm} (69)

\( f(0, \Sigma''(0)) \) is a positive, monotonically decreasing function of the nonnegative variable \( \Sigma''(0) \).
This implies that the critical value of the disorder is

\[ (n_{imp}V^2)_c = \frac{\Delta}{2N_0}. \]  \hspace{1cm} (70)
This is when the inverse relaxation time corresponds to the gap energy, as might be expected on physical grounds.

The consequences of band asymmetry are important for the density of states. Consideration of Eq. 64 shows that the real part of the self-energy is non-zero:

\[ \Sigma(\omega = 0) \approx \frac{1}{\pi \tau} \log(\frac{\epsilon_u}{\epsilon_\ell}), \]

and that the derivative of the derivative of the imaginary part also does not vanish at midgap. Eq. 66 then implies that the density of states also has a nonzero slope at midgap. I have computed numerically the solution of Eqs. 64 and 66 for the symmetric and asymmetric models. The results are shown in Fig. 4. It is seen that the minimum in the density of states shifts away from the middle of the gap. The chemical potential is given by a quite different equation than that for the gap minimum. It does not coincide with the minimum.

The calculation for the full T-matrix equation, Eq. 63, is only a little more complicated and will be omitted here. The result is that the threshold for complete closure of the gap is unchanged, but the spectral weight in the gap is larger for the same amount of disorder. The conclusions about the symmetry of the density of states in the gap are also unchanged.

H. Physical Picture

It should be evident that there are profound differences between the bound state calculations and the impurity-averaging calculations. The latter take into account only the potential fluctuations and even the sign of \( V \) is not very important. In the Born approximation, only \( V^2 \) enters the theory; even when the T-matrix is used, the main effect is to alter the extent of the phase randomization, not to create bound or antibound states. The scattering perturbs and broadens the extended states. The gap fills, but the states which are in the gap are extended states. There is no question of impurity band formation.

In the bound state calculation, the effect of the impurity potential on the extended states is to give them a phase shift. This does not move the band edges. The bound states are split off from the bands. The gap fills with localized states.
Very strong potential scattering in systems with a band gap does lead to deep impurity levels. There is no reason for the energy of these levels to be at midgap. This could only occur accidentally. The decay of the impurity wavefunctions is very fast, as they are well split from the band states. This prevents the formation of impurity bands in all except pathological cases.

How may we combine the results of both kinds of calculations, the bound state and the impurity averaging? Let us first consider the set of all diagrams for the single-particle Green’s function $G(\vec{k}, \vec{k}', \omega)$ associated with the perturbation Hamiltonian $\sum_i V(\vec{r} - \vec{R}_i)$. If the impurities are numbered from 1 up to $N_{\text{imp}}$, then a diagram of $n$-th order perturbation corresponds to an ordered sequence of these integers with $n$ members. A given integer may appear more than once (repeated scattering from a single impurity). Intermediate momenta must be integrated over. Each scattering contributes a phase factor associated with the position of the impurity. The T-matrix calculations correspond to keeping sequences in which the same integer is repeated in succession many times. If the impurities do not interact, then only sequences containing a single integer are considered. This allows the bound state pole to form. The impurity averaging calculations omit the phase factor and omit the momentum integration after the final appearance of any integer. This is impurity averaging. The neglect of phase information prevents the build-up of the bound-state pole. A further approximation is to discard sequences in which numbers are interleaved, (an example is 1,2,1,2). This is the noncrossing approximation. It will be defined and discussed more carefully in connection with calculations in the superconducting state.

In the dilute limit, the T-matrix approach is appropriate if $\omega$ lies in the gap (and the unperturbed Green’s function decays exponentially in real space), and impurity averaging is appropriate if $\omega$ lies in one of the bands. It is therefore reasonable to conclude that the DOS is properly given by superposing the DOS from the two types of calculations, with the proviso that there are $N - N_{\text{imp}}$ broadened band states and $N_{\text{imp}}$ gap states. Here $N$ is the total number of orbitals, proportional to the volume of the system. As the impurity density increases and the gap closes up, this energy separation argument no longer works. The
continuum states overlap in energy with the bound state. The phase information eventually becomes less important as the impurity states mix with the continuum states. The most likely scenario as the density is increased seems to be as follows.

For low concentrations, the bound states will form a very narrow band in the gap. The integrated spectral weight in this band proportional to $n_{\text{imp}}$. For subcritical disorder, there is no conduction associated with this band. There is some spectral weight in the gap because of the broadening of the band states. This weight is proportional to the total number of electrons, not the number of impurities. However, it does not overlap in energy with the bound state energy. If the disorder is above critical, then there is spectral weight everywhere in the gap, because of broadening and shifting of the band states. They overlap in energy with the bound state energy. This broadens the bound states, turning them into resonances. The qualitative behavior for $n_{\text{imp}}V^2 < (n_{\text{imp}}V^2)_c$ and $n_{\text{imp}}V^2 > (n_{\text{imp}}V^2)_c$ is shown in Figs. 5 and 6, for the asymmetric case.

The resonances can, in principle, play a role in conduction, since they are not necessarily localized. However, their density will normally be low compared to the band states, whose number is proportional to the total number of sites, not the number of impurities. This also means that if they do conduct, it is by hopping first into the continuum and perhaps later onto another impurity, not directly by impurity-impurity hopping as in an impurity band.

The question of localization of all these states is subtle. In the impurity-averaging method, the single-particle Green’s function is independent of position, seemingly indicating extended states. However, when transport properties are calculated using this method, localization may appear in spite of this. Thus the states in the gap whose number of states is proportional to the total volume may or may not be Anderson-localized by the disorder - the impurity-averaging calculation of the single-particle Green’s function as carried out here gives no useful information about this. Conventional wisdom tells us that, in the low impurity concentration regime considered here, states near the chemical potential should be extended in three dimensions and localized, but with extremely long localization lengths, in two dimensions.
III. S-WAVE SUPERCONDUCTORS

The calculations of the effects of impurities in superconductors are very analogous to the calculations in semiconductors. This analogy is most easily exploited if we introduce the Nambu operators. The defining equation is

$$\Psi^\dagger_k = (c^\dagger_{k\uparrow}, c^\dagger_{k\downarrow}).$$  \hspace{1cm} (72)

The Pauli matrices $\tau_1, \tau_2, \tau_3$ and the identity matrix $\tau_0$ (omitted when clarity requires), act in this two-dimensional space. The unperturbed mean-field Hamiltonian for a superconductor with a constant gap $\Delta$ is:

$$\hat{H}_0 = \sum_k \Psi^\dagger_k \epsilon_k \tau_3 \Psi_k + \sum_k \Psi^\dagger_k \Delta \tau_1 \Psi_k,$$  \hspace{1cm} (73)

and the impurity potential is:

$$\hat{V} = V \sum_{k,k'} \Psi^\dagger_{k'} \tau_3 \Psi_k.$$  \hspace{1cm} (74)

The matrix Green’s function is defined as

$$\mathcal{G}(\vec{k}, i\omega) = - < T \tau \Psi_{\vec{k}}(\tau) \Psi^\dagger_{\vec{k}}(0) >.$$  \hspace{1cm} (75)

In comparison to ordinary notation we find

$$\mathcal{G}_{11}(\vec{k}, i\omega) = \mathcal{G}_{\uparrow\uparrow}(\vec{k}, i\omega)$$  \hspace{1cm} (76)

$$\mathcal{G}_{22}(\vec{k}, i\omega) = - \mathcal{G}_{\downarrow\downarrow}(\vec{k}, -i\omega)$$  \hspace{1cm} (77)

$$\mathcal{G}_{12}(\vec{k}, i\omega) = \mathcal{F}(\vec{k}, i\omega).$$  \hspace{1cm} (78)

Since the density of states is independent of the spin direction in singlet superconductors, we have that

$$N(\omega) = - \frac{1}{\pi} \text{Im} \text{ Tr } \mathcal{G}_{11}(\vec{k}, \omega + i\delta).$$  \hspace{1cm} (79)

We may now easily calculate the unperturbed Green's function:
\[ G_0(\vec{k}, i\omega) = \frac{1}{i\omega - \epsilon_\vec{k}\tau_3 - \Delta\tau_1} = \frac{i\omega + \epsilon_\vec{k}\tau_3 + \Delta\tau_1}{\omega^2 + \epsilon_\vec{k}^2 + \Delta^2}. \]  

(80)

The T-matrix is again defined by:

\[ G(\vec{k}, \vec{k}', i\omega) = G_0(\vec{k}, i\omega)\delta_{\vec{k},\vec{k}'} + G_0(\vec{k}, i\omega)T(i\omega)G_0(\vec{k}', i\omega), \]  

(81)

which leads to:

\[ T(i\omega) = V\tau_3 + V^2\tau_3g_0(i\omega)\tau_3 + V^3\tau_3g_0(i\omega)\tau_3g_0(i\omega)\tau_3 + \ldots, \]  

(82)

where

\[ g_0(i\omega) = \sum_\vec{k} G_0(\vec{k}, i\omega) = -\sum_\vec{k} \frac{i\omega\tau_0 + \epsilon_\vec{k}\tau_3 + \Delta\tau_1}{\omega^2 + \epsilon_\vec{k}^2 + \Delta^2}. \]  

(83)

We shall assume particle-hole symmetry so that

\[ \int_{-\omega_c}^{\omega_c} \epsilon_\vec{k} = 0, \]  

(84)

where \(\omega_c\) is the cutoff frequency of the interaction, which is much smaller than the bandwidth.

We also recall that in weak coupling \(\Delta = 0\) for \(|\epsilon_\vec{k}| > \omega_c\). Then:

\[ g_0(i\omega) = -(i\omega\tau_0 + \Delta\tau_1)N_0(\epsilon_F) \int_{-\omega_c}^{\omega_c} \frac{d\epsilon}{\omega^2 + \epsilon^2 + \Delta^2} \]  

\[ - \int_{|\epsilon| > \omega_c} \frac{(i\omega\tau_0 + \epsilon\tau_3)N(\epsilon)d\epsilon}{\omega^2 + \epsilon^2} \]  

(85)

\[ = -(i\omega\tau_0 + \Delta\tau_1)N_0(\epsilon_F) \int_{-\omega_c}^{\omega_c} \frac{d\epsilon}{\omega^2 + \epsilon^2 + \Delta^2} + A_s \]  

(86)

\[ = -(i\omega\tau_0 + \Delta\tau_1) \frac{\pi N_0(\epsilon_F)}{\sqrt{\omega^2 + \Delta^2}} + A_s. \]  

(87)

The asymmetry factor is defined as

\[ A_s \equiv \tau_3 N_A = \tau_3 \left[ \sum_k \frac{\epsilon_\vec{k}}{\omega^2 + \epsilon_\vec{k}^2} \right], \]  

(88)

where the sum runs over wavevectors whose energies are farther from the Fermi surface than the cutoff frequency \(\omega_c\). We find

\[ N_A = N_u \log\left(\frac{\epsilon_u}{\omega_c}\right) - N_f \log\left(\frac{\epsilon_f}{\omega_c}\right), \]  

(89)
in the model of constant density of states beyond $\omega_c$. $A_s$ also has an imaginary part, but it is smaller by a factor of $\omega/\omega_c$.

We may now compute the T-matrix:

$$T(i\omega) = V\tau_3 + V^2\tau_3(a\tau_0 + b\tau_1 + N_A\tau_3)\tau_3 + V^3\tau_3(a\tau_0 + b\tau_1 + N_A\tau_3)\tau_3(a\tau_0 + b\tau_1 + N_A\tau_3)\tau_3 + \ldots,$$

(90)

where the definitions $a(i\omega) = -i\pi N_0(\epsilon_F)\omega/\sqrt{\omega^2 + \Delta^2}$, and $b(i\omega) = -\pi N_0(\epsilon_F)\Delta/\sqrt{\omega^2 + \Delta^2}$ have been made. It remains to sum the geometric series and invert the resulting matrix:

$$T(i\omega) = V\tau_3 \sum_{n=0}^{\infty} [V(a\tau_0 + b\tau_1 + N_A\tau_3)\tau_3]^n$$

$$= V\tau_3[\tau_0 - Va\tau_3 - Vb\tau_1\tau_3 - VN_A\tau_0]^{-1}$$

$$= \tilde{V}\tau_3[\tau_0 - \tilde{V}a\tau_3 - \tilde{V}b\tau_1\tau_3]^{-1}$$

$$= \frac{a\tilde{V}^2\tau_0 - b\tilde{V}^2\tau_1 + \tau_3\tilde{V}}{1 - a\tilde{V}^2 + b^2\tilde{V}^2}.$$  

(91)

In these equations, we have made the definition, as before:

$$\tilde{V} = \frac{V}{1 + N_AV}.$$  

(92)

This shows that the binding potential is renormalized by the band asymmetry just as in the semiconductor case. This limits its strength to something on the order of the bandwidth.

Continuing to the real axis, we find

$$T(\omega) = \frac{a(\omega)\tilde{V}^2\tau_0 - b(\omega)\tilde{V}^2\tau_1 + \tau_3\tilde{V}}{1 - a(\omega)^2\tilde{V}^2 + b(\omega)^2\tilde{V}^2}$$

$$= \frac{a(\omega)\tilde{V}^2\tau_0 - b(\omega)\tilde{V}^2\tau_1 + \tau_3\tilde{V}}{1 + (\pi N_0(\epsilon_F)\tilde{V})^2}.$$  

(93)

This function is nonsingular, indicating that there are no bound states in the gap. This arises from a cancellation of the frequency dependence in the denominator, essentially that of Anderson’s theorem.

The asymptotic dependence of the Green’s functions at large distances is of interest for later considerations. The computational method is very similar for all cases, so it is given in some detail here and abbreviated later. In three dimensions, we have:
\[ G(\vec{r}, i\omega) = \int e^{i\vec{k} \cdot \vec{r}} G(\vec{k}, i\omega) d^3k \]
\[ = -\frac{N_0}{4\pi} \int de \int_{-1}^{1} dx \int_{0}^{2\pi} d\phi \frac{i\omega \tau_0 + \epsilon_F \tau_3 + \Delta F \tau_1}{\omega^2 + \epsilon_F^2 + \Delta_F^2} e^{ikrx}. \]

The x-integral is performed by choosing a contour which runs from \( z = -1 + i\infty \) to \(-1\), then from \(-1\) to \(+1\), then from \(+1\) to \(+1 + i\infty\). Since we will use this contour several times, it is shown in Fig. 7 for reference. Let \( u \equiv (k_F + \epsilon/v_F)r \). This variable must be treated carefully as the approximation of linear dispersion is a very limited one. We may extend the limits of integration over \( u \) only if the integral is rapidly convergent. This usually means that \( u \) must be integrated last. Bearing this in mind we have:
\[ \int dz e^{iuz} = \int_{-1}^{1} dx e^{iux} + i \int_{0}^{\infty} dy e^{iu(1+iy)} - i \int_{0}^{\infty} dy e^{iu(-1+iy)}, \]

as long as \( u > 0 \). The contour integral vanishes because the function is analytic, so we find
\[ \int_{-1}^{1} dx e^{iux} = -i e^{iu} \int_{0}^{\infty} e^{-uy} dy + i \int_{0}^{\infty} e^{-uy} dy \]
\[ = -\frac{i}{u} (e^{iu} - e^{-iu}) \approx -\frac{i}{k_F r} (e^{iu} - e^{-iu}). \]

Substituting yields
\[ \frac{iN_0}{2k_F r} \int de [e^{ir(k_F + \epsilon/v_F)} - e^{-ir(k_F + \epsilon/v_F)}] \frac{i\omega \tau_0 + \epsilon \tau_3 + \Delta \tau_1}{\omega^2 + \epsilon^2 + \Delta^2} \]
\[ = \frac{i\pi N_0 e^{-dr/v_F}}{2k_F r d} \left[ (i\omega \tau_0 + id \tau_3 + \Delta \tau_1) e^{ikrF} - (i\omega \tau_0 - id \tau_3 + \Delta \tau_1) e^{-ikrF} \right]. \]

Here \( d \equiv \sqrt{\omega^2 + \Delta^2} \). As \( \Delta \to 0 \), this becomes
\[ \frac{G(\vec{r}, i\omega, \Delta = 0)}{-\frac{\pi N_0}{2k_F r} e^{-|\omega|r/v_F} [(sgn(\omega)\tau_0 + \tau_3)e^{ikrF} - (sgn(\omega)\tau_0 - \tau_3)e^{-ikrF}].} \]

This is the normal state Green’s function. The off-diagonal components are zero, and the diagonal one may be written as:
\[ \frac{G_{11}(\vec{r}, i\omega, \Delta = 0)}{-\frac{\pi N_0}{k_F r} e^{-|\omega|r/v_F} sgn(\omega)\tau_0.} \]

For future reference, the corresponding result in two dimensions is
\[ \frac{G_{11}(\vec{r}, i\omega, \Delta = 0)}{-\frac{N_0}{\sqrt{2\pi k_F r}} e^{-|\omega|r/v_F} sgn(\omega).} \]
At low frequencies, $\omega << \Delta$, we find
\[ \mathcal{G}(\vec{r}, i\omega, \omega < \Delta) = -\frac{\pi N_0}{2k_F^r} e^{-\Delta r/v_F} [(sgn(\omega)\tau_1 + \tau_3)e^{ik_F r} - (sgn(\omega)\tau_1 - \tau_3)e^{-ik_F r}]. \quad (103) \]

The particle-hole part in the low frequency limit is
\[ \mathcal{G}_{11}(\vec{r}, \omega, \omega < \Delta) = -\pi N_0 e^{-\Delta r/v_F} \frac{\cos(k_F r)}{k_F r}. \quad (104) \]

The density of states is zero in the gap, so the Green's function is purely real. The exponential damping in real space is also due to this fact, the pole of the function
\[ \frac{1}{\epsilon^2 + \omega^2 + \Delta^2} \quad (105) \]
being off the real axis. The decay length is the coherence length $v_F/\Delta$.

\section*{IV. UNCONVENTIONAL SUPERCONDUCTORS}

\subsection*{A. Bound state energies}

I will restrict the discussion to the singlet case. The new feature in the equations is that the gap function is now $\vec{k}$-dependent, and satisfies:
\[ \sum_{\vec{k}} \Delta_{\vec{k}} = 0. \quad (106) \]

The Green's function is the same as above, and the T-matrix is still given by
\[ \mathcal{T}(i\omega) = \tilde{V}\tau_3 + \tilde{V}^2\tau_3 g_0(i\omega)\tau_3 + \tilde{V}^3\tau_3 g_0(i\omega)\tau_3 g_0(i\omega)\tau_3 + \ldots, \quad (107) \]

where
\[ g_0(i\omega) = \sum_{\vec{k}} \mathcal{G}_0(\vec{k}, i\omega) \]
\[ = -i\omega N_0 \tau_0 \frac{1}{4\pi} \int d\Omega_{\vec{k}} \left[ \frac{d\epsilon}{\omega^2 + \epsilon^2 + \Delta^2_{\vec{k}}} + \int_{|\epsilon|>\omega_c} \frac{d\epsilon}{\omega^2 + \epsilon^2} \right] \quad (108) \]
\[ = -i\omega \tau_0 \pi N_0 \frac{1}{4\pi} \left[ \int \frac{d\Omega_{\vec{k}}}{\sqrt{\omega^2 + \Delta^2_{\vec{k}}} + A_s} \right]. \quad (109) \]
Here $\Omega_{\vec{k}}$ is the solid angle on the sphere. The band asymmetry is represented by the second term in the equation, and comes from the integral over energies far from the Fermi surface. Its effect is the same as above, i.e. , it results in the replacement of the bare potential $V$ by $\tilde{V} = V/(1 + N_A V)$.

The equations for the unconventional case are, to this point, actually somewhat simpler than the $s$-wave case. The $T$-matrix is obtained from Eq. 91 by setting $b = 0$ and $a = g_0(i \omega)$:

$$T(i \omega) = \frac{g_0(i \omega) \tilde{V}^2 \tau_0 + \tau_3 \tilde{V}}{1 - g_0(i \omega)^2 \tilde{V}^2}.$$  \hfill (110)

Component by component, we find

$$T_{11}(\omega) = \frac{g_0(\omega) \tilde{V}^2 + \tilde{V}}{1 - g_0(\omega)^2 \tilde{V}^2} = \tilde{V} \frac{1 + \tilde{V} g_0(\omega)}{1 - V^2 g_0(\omega)} = \tilde{V} \frac{1}{1 - V g_0(\omega)},$$  \hfill (111)

for the up-spin electrons, and

$$T_{22}(-\omega) = \frac{-\tilde{V}}{1 + \tilde{V} g_0(-\omega)},$$  \hfill (112)

for the down spins. The corresponding equations for the binding energies are:

$$\text{Re} \ g_0(\omega_b) = \frac{1}{V},$$  \hfill (113)

and

$$\text{Re} \ g_0(-\omega_b) = -\frac{1}{V}.$$  \hfill (114)

Since, from Eq. 108, $\text{Re} \ g_0(\omega)$ is odd (if we exclude the asymmetry term), these equations have the same solution for the bound state energy $\omega_b$, as indeed they must.

To get some insight into the equations, we compute the $T$-matrix for the ‘polar’ case, which has a line of nodes on the equatorial plane of the Fermi surface: $\Delta_{\vec{k}} = \Delta_0 \cos(\theta_{\vec{k}})$. We have

$$\text{Im} \ g_0(\omega) = -\pi \frac{N_0}{4 \pi} \int_{-\infty}^{\infty} d\epsilon \int d\Omega_{\vec{k}} [\delta(\omega - E_{\vec{k}}) + \delta(\omega + E_{\vec{k}})]$$  \hfill (115)

$$= -\pi N_0 \int_{-\infty}^{\infty} d\epsilon \int_0^1 dx \delta(|\epsilon| - \sqrt{\epsilon^2 + \Delta_0^2 x^2}),$$  \hfill (116)
which gives

\[
Im \, g_0(\omega) = \frac{-|\omega|N_0\pi^2}{2\Delta_0}, \quad |\omega| < \Delta_0 \\
= \frac{-|\omega|N_0\pi}{\Delta_0} \sin^{-1}\left(\frac{\Delta_0}{\omega}\right), \quad |\omega| > \Delta_0.
\] (117)

Computing the real part:

\[
Re \, g_0(\omega) = -\frac{1}{\pi} \int \frac{Im \, g_0(\omega')}{\omega - \omega'} d\omega' \\
\approx \frac{N_0\pi}{2\Delta_0} \int_{-\Delta_0}^{\Delta_0} \frac{\omega'}{\omega - \omega'} d\omega' + \frac{N_0\pi}{2} \left[ \int_{-\omega_c}^{\omega_c} \frac{d\omega'}{\omega - \omega'} + \int_{-\omega_c}^{-\Delta_0} \frac{d\omega'}{\omega - \omega'} \right] \\
= \frac{N_0\pi\omega}{2\Delta_0} \log|\omega^2| - \frac{N_0\pi}{2} \log\left|\frac{(\omega_c - \omega)(\Delta_0 + \omega)}{(\omega_c + \omega)(\Delta_0 - \omega)}\right| \\
\approx -\frac{N_0\pi\omega}{\Delta_0} \left(1 - \frac{1}{2} \log\left|\frac{\omega^2}{\Delta_0^2 - \omega^2}\right|\right),
\] (119)

at small \(\omega\). The asymmetry term \(A_s\) has not been explicitly included in this expression, since we may more conveniently include it in the potential strength. \([A_s = -N_0 \log(\varepsilon_u/\varepsilon_\ell)\) in the simplest model density of states.] For other gap functions which give an even smaller density of states at low energies, the slope of the real part is completely dominated by the first term, and gives a generic result:

\[
Re \, g_0(\omega) \sim -\beta \frac{N_0\omega}{\Delta_0},
\] (123)

where \(\beta\) is a number of order one. The bound state energy is:

\[
\omega_b = -\frac{\Delta_0}{\beta N_0\tilde{V}},
\] (124)

as long as \(N_0\tilde{V} > > 1\). This is the more generic result from Eq. [123], which we will also use below. The logarithmic corrections in the polar case are only important if, for accidental reasons, \(1 + N A \tilde{V}\) is exponentially small.

Once again, in this case, the bound state energy does not go to zero even in the unitarity limit. This is very important for the properties of the bound state wavefunctions, to which we turn next.
B. Asymptotic Spatial Dependence

At large distances from the impurity, the wavefunctions for bound states are determined by the asymptotics of the diagonal elements of the real-space Green’s functions evaluated at \( \omega_b \). The off-diagonal elements are also of interest, as they represent the suppression of the gap in the neighborhood of the impurity. Their asymptotic spatial dependence is always the same as that of the diagonal elements, so I do not give expressions for them separately.

In three dimensions I shall concentrate on the polar case. The gap takes the form \( \Delta(\vec{k}) = \Delta_0 \cos \theta_{\vec{k}} \). We shall take a spherical Fermi surface; for this situation the gap has a line of nodes around the equator. As in the previous section, we assume that the pair wavefunction is a singlet in spin space. This total pair wavefunction does not satisfy the Pauli principle. However, it is the simplest example of an unconventional state with a line of nodes in three dimensions and the calculations for it are already complicated.

Now take the direction \( \hat{r} \) from the impurity to be in the z-direction. I will work out the Green’s function in the main text for this case. For other cases, the intermediate steps are relegated to the appendix.

Then
\[
G(r\hat{z}, i\omega_b) = -\frac{N_0}{2} \int \int_{-1}^{1} e^{iux} \frac{i\omega_b + \epsilon \sigma_3 + \Delta_0 x \sigma_1}{\omega_b^2 + \epsilon^2 + \Delta_0^2 x^2} dx.
\]

The important integral (because it expresses the angular dependence) is the x integral.
This is:
\[
I(\epsilon, i\omega_b) = \int_{-1}^{1} e^{iux} \frac{i\omega_b + \epsilon \tau_3 + \Delta_0 x \tau_1}{\omega_b^2 + \epsilon^2 + \Delta_0^2 x^2} dx
\]
\[
= \frac{1}{\Delta_0} \int_{-1}^{1} e^{iux} \frac{i\Omega + s \tau_3 + x \tau_1}{\Omega^2 + s^2 + x^2} dx
\]
\[
= \frac{1}{\Delta_0} \int e^{iux} \frac{i\Omega + s \tau_3 + z \tau_1}{\Omega^2 + s^2 + z^2} dz
\]
\[
- ie^{iu} \frac{1}{\Delta_0} \int_{0}^{\infty} e^{-uy} \frac{i\Omega + s \tau_3 + (1 + iy) \tau_1}{\Omega^2 + s^2 + (1 + iy)^2} dy
\]
\[
+ ie^{-iu} \frac{1}{\Delta_0} \int_{0}^{\infty} e^{-uy} \frac{i\Omega + s \tau_3 + (-1 + iy) \tau_1}{\Omega^2 + s^2 + (-1 + iy)^2} dy.
\] (126)

The method is the same as in the s-wave case, and we use the same contour, as shown in Fig. 7. The scaled variables \( s = \epsilon/\Delta_0, \Omega = \omega_b/\Delta_0, \) have been used, and again \( u = (k_F + \epsilon/v_F)r. \)

We are interested in the limits \( \Omega << 1, \) and \( k_F r >> 1. \) The contour integral is easily performed by the residue theorem, and the strongly peaked function \( e^{-uy} \) allows us to do the other two integrals. Thus,
\[
I(\epsilon, i\omega_b) = \pi \frac{e^{-u\sqrt{\Omega^2 + s^2} i\Omega + s \tau_3 + i\sqrt{\Omega^2 + s^2} \tau_1}}{\Delta_0 \sqrt{\Omega^2 + s^2}} - \frac{e^{iu}}{u \Delta_0} \frac{s \tau_3 + \tau_1}{1 + s^2 + \Omega^2} + \frac{e^{-iu}}{u \Delta_0} \frac{s \tau_3 - \tau_1}{1 + s^2 + \Omega^2}. \] (127)

For \( u >> 1, \) we have the useful integrals:
\[
I_1 \equiv \int_{-\infty}^{\infty} e^{-u(\Omega^2 + s^2)^{1/2}} ds \approx \left( \frac{2\pi}{u|\Omega|} \right)^{1/2} e^{-u|\Omega|}, \] (128)
\[
I_2 \equiv \int_{-\infty}^{\infty} e^{-u(\Omega^2 + s^2)^{1/2}} ds \approx \left( \frac{2\pi |\Omega|}{u} \right)^{1/2} e^{-u|\Omega|}. \] (129)

This yields
\[
\int_{-\infty}^{\infty} ds I(\epsilon, \omega_b) = \pi \frac{e^{-u|\Omega|}}{\Delta_0} \left[ i\Omega \left( \frac{2\pi}{u|\Omega|} \right)^{1/2} + i\tau_1 \left( \frac{2\pi |\Omega|}{u} \right)^{1/2} \right]
\]
\[
+ \frac{\pi (\Omega + \sqrt{1 + \Omega^2} \tau_3 - i \tau_1)}{\Delta_0 k_F r \sqrt{1 + \Omega^2}} \exp[ik_F r - \sqrt{1 + \Omega^2 \Delta_0 r/v_F}]
\]
\[
+ \frac{\pi (-\Omega + \sqrt{1 + \Omega^2} \tau_3 - i \tau_1)}{\Delta_0 k_F r \sqrt{1 + \Omega^2}} \exp[-ik_F r - \sqrt{1 + \Omega^2 \Delta_0 r/v_F}]. \] (130)

The Green’s function at large distances is therefore
\[ G(\hat{r}, i\omega_b) = -\frac{N_0\Delta_0}{2} \int_{-\infty}^{\infty} ds I(\epsilon, \omega_b) \]

\[ = -i\pi \frac{N_0}{2} \left( \frac{2\pi|\omega_b|}{\Delta_0k_F} \right)^{1/2} e^{-k_Fr|\omega_b|/\Delta_0} (sgn (\omega_b) + \tau_1) \]

\[ - \frac{\pi N_0 e^{-(\omega_b^2 + \Delta_0^2)^{1/2}r/v_F}}{2(\omega_b^2 + \Delta_0^2)^{1/2}} \times \]

\[ [\omega_b + (\omega_b^2 + \Delta_0^2)^{1/2}\tau_3 - i\tau_1] e^{ik_Fr} + (-\omega_b + (\omega_b^2 + \Delta_0^2)^{1/2}\tau_3 - i\tau_1) e^{-ik_Fr}]. \quad (131) \]

The component of most interest is the particle-hole part at real frequencies:

\[ G_{11}(\hat{r},\omega) = -\frac{\pi N_0}{2} \left( \frac{2\pi|\omega_b|}{\Delta_0k_F} \right)^{1/2} e^{-k_Fr|\omega_b|/\Delta_0} sgn (\omega_b) \]

\[ + \frac{i\pi N_0}{2} e^{-(\omega_b^2 + \Delta_0^2)^{1/2}r/v_F} \times \]

\[ \left\{ \frac{\omega_b + (\omega_b^2 - \Delta_0^2)^{1/2}}{(\Delta_0^2 - \omega_b^2)^{1/2}} e^{ik_Fr} - \frac{\omega_b - (\omega_b^2 - \Delta_0^2)^{1/2}}{(\Delta_0^2 - \omega_b^2)^{1/2}} e^{-ik_Fr} \right\}. \quad (132) \]

The first term is the pole contribution, which arises from interference of the low energy states near the line of nodes. If the state is precisely at the chemical potential, then these states interfere to give a power law decay. There is no oscillatory component because the states on the nodal line have \( \vec{k} \cdot \vec{r} = 0 \) for this direction of \( \vec{r} \). The length scale of this decay is \( \Delta_0/|\omega_b|k_F \), which is the interatomic spacing unless the binding energy happens to be very small.

The second term is the stationary-phase contribution which is due to the states near the north and south poles of the Fermi surface. Since these are gapped, we get an exponential falloff which reflects the energy gap at these points. There is an oscillatory behavior because \( \vec{k} \cdot \vec{r} = \pm k_Fr \) at these points. The length scale of the decay is the 'local' coherence length (coherence length at the pole) \( \Delta(\vec{k}\hat{z})/v_F \) if the binding energy is small.

A second special case of interest is when the direction of \( \vec{r} \) is on the plane of nodes. Then we have

\[ G(\hat{r}, i\omega_b) = -\frac{N_0}{4\pi} \int d\phi \int ds \int_{-1}^{1} e^{iux} i\omega_b + s\tau_3 + \cos \phi(1 - x^2)^{1/2}\tau_1 dx. \quad (133) \]

The details of the integration are given in the appendix. The result is:

\[ G(\hat{r}, i\omega_b) = -\frac{\pi N_0}{2k_F} e^{-|\omega_b| r/v_F} \left[ e^{ik_Fr}(sgn (\omega_b) \tau_0 + \tau_3) - e^{-ik_Fr}(sgn (\omega_b) \tau_0 - \tau_3) \right]. \quad (134) \]
The particle-hole part is
\[ G_{11}(r\hat{x},\omega_b) = \frac{-\pi N_0}{2k_F r} e^{-|\omega_b|r/v_F} e^{ik_F r} \text{sgn} (\omega_b). \] (135)

These are essentially the normal state results. The point here is that the stationary phase points at \( \vec{k} = \pm k_F \hat{x} \) have no gap and the behavior is therefore entirely normal.

The general case is rather complicated. Let the direction from the impurity be inclined at an angle \( \psi \) to the z-axis. Let us define
\[ G(r, \psi, i\omega_b) \equiv G(r (\sin \psi \hat{x} + \cos \psi \hat{z}, i\omega_b)) \] (136)

We have that
\[ G(r, \psi, i\omega_b) = -\frac{N_0}{4\pi} \int_0^{2\pi} d\phi \int d\epsilon \int_{-1}^1 dx e^{iux} i\omega_b + \epsilon \tau_3 + \Delta_0 \tau_1 (ax - b\sqrt{1-x^2}) \frac{\omega_b}{\omega_b^2 + \epsilon^2 + \Delta_0^2 (ax - b\sqrt{1-x^2})^2}, \] (137)
where \( a \equiv \cos \psi, b = \cos \phi \sin \psi, \) and \( u \equiv (k_F + \epsilon/v_F)r. \) The coordinates for the integration have been rotated so that the polar axis defined by \( x = \pm 1 \) is along \( \vec{r}. \) The particle-hole part of the Green’s function is found in the appendix to be:
\[ G_{11}(r, \psi, \omega_b) = \frac{\pi N_0 \text{sgn} (\omega_b)}{k_F r} \left( \frac{2|\omega_b|}{\Delta_0 \cos^2 \psi \sin^2 \psi} \right)^{1/2} \sin(k_F r \sin \psi) e^{ik_F r |\omega_b| |\cos \psi|/\Delta_0} \]
\[ \times e^{-\sqrt{\Delta_0^2 \cos^2 \psi - \omega_b^2} - \frac{\omega_b}{\Delta_0^2 \cos^2 \psi - \omega_b^2}} \times e^{-\sqrt{\Delta_0^2 \cos^2 \psi - \omega_b^2} - \frac{\omega_b}{\Delta_0^2 \cos^2 \psi - \omega_b^2}}. \] (138)

This general form does not reduce to Eq. [135] when \( \psi = \pi/2 \) or to Eq. [132] when \( \psi = 0. \) It is only valid in the intermediate regime of angles. The result does, however, show that the two distinct decay behaviors noted above are both present in the generic case.

C. Two dimensions

We now turn to the case most relevant to high-\( T_c, \) which is two dimensions with a singlet \( d \)-wave gap, (which is consistent with the Pauli principle). The Fermi surface is a circle and the gap will be taken as
\[ \Delta(\vec{k}) = \Delta_0 \cos 2\phi_{\vec{k}}. \quad (139) \]

This d-wave gap has nodes at the intersection of the lines \( k_x = \pm k_y \) with the Fermi surface.

Let us first determine the Green’s function for the direction along one of the axes. We have

\[ G(r \hat{x}, i \omega_b) = -\frac{2N_0}{\pi} \int dv \int_{-1}^1 dv \frac{i \omega_b + \epsilon \tau_3 + \Delta_0 \tau_1 (2v^2 - 1)}{\sqrt{1 - v^2}} e^{iuv}. \quad (140) \]

Here we have defined \( v = \cos \phi_{\vec{k}} \) so that \( \Delta = \Delta_0(2v^2 - 1) \). Also \( u = (k_F + \epsilon/v_F)r \). The integrations are performed in the appendix. The particle-hole part is

\[
G_{11}(r \hat{x}, \omega_b) = -\frac{2iN_0}{\pi} \times \frac{1}{\sqrt{\Delta_0}} \left\{ \begin{array}{c}
1/2 \\
\frac{1}{\sqrt{\Delta_0}} \left[ (\sqrt{\Delta_0^2 - \omega_b^2} - \Delta_0)^{1/4} \Delta_0^{1/4} (\frac{\pi}{k_F r})(\frac{8\pi}{2\sqrt{\Delta_0}}) e^{i \frac{k_F r}{\sqrt{\Delta_0}} \sqrt{\Delta_0^2 - \omega_b^2}} \right] \cos \left( \frac{k_F r}{2\sqrt{\Delta_0}} \sqrt{\Delta_0^2 - \omega_b^2} + \Delta_0 \right) \\
\frac{1}{\sqrt{\Delta_0}} \left[ \frac{(1 - i)\pi}{2} e^{i k_F r} e^{-\sqrt{\Delta_0^2 - \omega_b^2}/v_F} i \Omega \right] + \frac{1}{\sqrt{\Delta_0}} \left[ \frac{(1 - i)\pi}{2} e^{-i k_F r} e^{-\sqrt{\Delta_0^2 - \omega_b^2}/v_F} i \Omega \right]
\end{array} \right\}. \quad (141) \]

The peculiar phase factors reflect the orientation of the nodal directions relative to the crystal axes. The overall behavior is very similar to the three-dimensional case, Eq. 132.

The direction along the node is more easily computed.

\[ G(r \hat{x} + \hat{y}/\sqrt{2}, i \omega_b) = -\frac{2N_0}{\pi} \int dv \int_{-1}^1 dv \frac{i \omega_b + \epsilon \tau_3 + \Delta_0 \tau_1 v \sqrt{1 - v^2}}{\sqrt{1 - v^2}} e^{iuv}, \quad (142) \]

where the part proportional to \( \tau_1 \) vanishes by symmetry. The integrations are performed in the appendix, with the result that:

\[
G_{11}(r \hat{x} + \hat{y}/\sqrt{2}, \omega_b) = -\frac{2iN_0}{\pi} \times \left[ \begin{array}{c}
\frac{4\pi^3 \sqrt{2}}{k_F r} \frac{\text{sgn} \ (\omega_b)}{(\Delta_0^2 - \omega_b^2)^{1/4}} (\sqrt{\Delta_0^2 - \omega_b^2} - \Delta_0)^{1/4} \Delta_0^{1/4} e^{-k_F r(\sqrt{\Delta_0^2 - \omega_b^2} - \Delta_0)^{1/2}} \sqrt{2\Delta_0} \\
\frac{1 - i\pi}{2} e^{i k_F r} (\text{sgn} \ (\omega_b) + 1)e^{-|\omega_b|r/v_F} \\
\frac{1 + i\pi}{2} e^{-i k_F r} (\text{sgn} \ (\omega_b) - 1)e^{-|\omega_b|r/v_F}
\end{array} \right]. \quad (143) \]
This is essentially the two-dimensional normal state result.

Now consider the general case, where the direction is inclined at an angle \( \psi \) from the diagonal and define:

\[
G(r, \psi, i\omega_b) \equiv G(i\omega_b, r \cos(\frac{\pi}{4} - \psi)\hat{x} + \sin(\frac{\pi}{4} - \psi)\hat{y}).
\]  

The result, derived in the appendix, is:

\[
G_{11}(r, \psi, \omega_b) = -\frac{2iN_0}{\pi} \times \left\{ \left(\frac{8\pi^3\sqrt{2}}{|k_{F}\rho| \cos \psi}\right)^{1/2} \left(\frac{\text{sgn } \omega_b}{\Delta^2_b - \omega^2_b - \Delta_0}\right)^{1/4} \times \right. \\
\times e^{-k_{F}r \cos \psi} \left(\sqrt{\Delta^2_b - \omega^2_b - \Delta_0}\right)^{1/2} / \sqrt{2\Delta_0} \\
+ \frac{(1 - i)\pi}{2} \left( e^{i\Delta_b \cos \psi} \right) \left( \text{sgn } \omega_b + 1 \right) e^{-|\omega_b \cos \psi|r/v_F} e^{-k_{F}r \cos \psi} \left(\sqrt{\Delta^2_b - \omega^2_b - \Delta_0}\right)^{1/2} / \sqrt{2\Delta_0} \\
+ \frac{(1 + i)\pi}{2} \left( e^{-i\Delta_b \cos \psi} \right) \left( \text{sgn } \omega_b - 1 \right) e^{-|\omega_b \cos \psi|r/v_F} \right\}.  
\]  

\[ (145) \]

D. Discussion

As compared with the semiconductor, there are several interesting differences in the bound state wavefunctions of the unconventional superconductor. The most important is the fact that the decay length may become longer, not shorter, as the bound state energy approaches midgap. In both cases, however, there is nothing special about the middle of the gap in a real system, so exponential decay is still the norm.

In the superconductor, the wavefunctions have two components when viewed in real space. The two components correspond to two different exponential decay lengths. One of these lengths is determined by the gap along the direction of propagation. This length is \( v_F / \sqrt{\Delta(\hat{k})^2 - \omega^2_b} \). This is similar to the s-wave case except for the anisotropy. Indeed, this contribution comes from the fully gapped region of the Fermi surface. The second length is \( v_F / |\omega_b \cos \psi| \), where \( \psi \) is the angle away from the nodal plane. This contribution is peculiar to the unconventional case, arising from the gap nodes. These lengths are anisotropic, so
the wavefunctions are also anisotropic, with ‘arms’ in the directions of the gap nodes. Some very nice pictures of these wavefunctions may be found in Ref. [18].

The decay is always exponential in all directions unless, for accidental reasons, the bound state energy is zero.

V. MANY IMPURITIES IN SUPERCONDUCTORS

A. Introduction

The discussion of many impurities in the metal and the superconductor are usually considered to be parallel, and the same equations, with only the generalization to the Nambu formalism, are used for both [20]. In particular, the method of impurity averaging is not modified. Hence, in this section we shall not repeat the calculations of Sec. II G.

For unconventional superconductors, without a hard gap, this is fundamentally reasonable. We have seen that impurity averaging becomes valid when the continuum states overlap the bound state energy. The constructive buildup of phase required to make the bound state is destroyed when there is overlap with the continuum states, themselves possessing a random shift. This is always the case, as the bound state energy is not in midgap. Accordingly, the pole found in the T-matrix calculations should immediately broaden into a resonance. This being said, one should address four basic issues which arise in practical calculations. These are: symmetry of the DOS around the chemical potential, the nature of the states at the chemical potential, the validity of the noncrossing approximation, and impurity band formation.

The first two are relatively easily dealt with. The third and fourth are treated in the next two sections.

The density of states is not symmetric about the chemical potential, even when particle-hole symmetry is valid. This has already been pointed recently by other authors in the magnetic impurity case [18, 19]. This arises from the same source as in the semiconductor.
Symmetry of the DOS requires that the bands themselves be symmetric over their whole energy range, not just over the neighborhood of the chemical potential. It appears that this fact is often not taken into account in practical calculations. The classic reference [20] advises us to neglect the real part of the energy shift. This is indeed safe for the neighborhood of the Fermi energy in a metal, and for weak scattering in s-wave superconductors, the cases discussed in Ref. [20]. It is not valid in unconventional superconductors with a soft gap.

The states at the chemical potential are sometimes termed 'bound states', and their heritage as the descendants of the T-matrix poles is emphasized. It should be clear from the discussion that this is not correct. These states are the broadened and shifted continuum states. The number of such states in any range of energies is proportional to the total number of orbitals in the system. The daughters of the bound states will generally live in a resonance away from the chemical potential. Their number is proportional to the number of impurities.

B. Noncrossing approximation

One approximation used in nearly all calculations of superconducting properties is the noncrossing approximation. This has been questioned in recent work, [15], and I reproduce and expand this criticism here. This approximation is defined diagramatically by representing each impurity as a cross through which momentum flows and is conserved. Let us restrict the discussion in this section to the Born approximation for simplicity. Then two typical diagrams for the normal state are shown in Fig. 8. We take a circular Fermi curve in a two-dimensional system. Diagram (a) in Fig. 8 has no crossed lines, whereas diagram (b) does. The same processes are shown in momentum space in the diagrams in Fig. 9. Diagram (a) describes a retraceable path, while diagram (b) contains a circuit. Therefore, the second diagram must satisfy one additional momentum conservation condition. It is therefore smaller in magnitude than the first. Explicit calculation shows that the small parameter involved is $(1/k_F \ell)$, where $\ell$ is the mean free path.
In a two-dimensional d-wave superconducting state at low temperatures, this argument must be reconsidered. All diagrams must effectively satisfy additional momentum constraints, as only scattering between gap nodes, situated at \((\pm k_F/\sqrt{2}, \pm k_F/\sqrt{2})\) is important. The two diagrams in Fig. 10 again correspond to the processes of Fig. 8. The two diagrams are of roughly equal weight, even though the second one is crossed. There are no additional constraints which must be satisfied by the second diagram.

The noncrossing approximation is therefore very questionable in unconventional superconductors with point nodes. The authors of Ref. 15 attempt to go beyond this approximation in a not very realistic model. No calculations of transport properties have been carried out except using the noncrossing approximation. It certainly is difficult to justify for the d-wave states considered in the context of high-temperature superconductivity, if these materials are taken to be two-dimensional.

C. Impurity band formation

Does there exist the possibility of the formation of an impurity band? Does conduction in this band influence, or even dominate, the transport properties in the limit of low temperatures?

We begin, as in Sec. II G, by considering two impurities. The overlap now depends, to some extent, on the direction of the vector connecting the two impurities, with the direction of minimum gap being the direction of maximum overlap. If we take the two-dimensional example summarized in Eq. 145 the overlap proceeds according to \(\exp(-k_F r \cos \psi)\) or \(\exp(-|\omega_b \cos \psi|r/v_F)\).

The introduction of many impurities always brings one new number to the problem: the average distance between impurities, which shall be denoted by \(\ell_{\text{imp}} \approx n_{\text{imp}}^{-1/d}\), where \(n_{\text{imp}}\) is the number of impurities per unit volume. If the impurities are not identical, we have a disorder parameter \(W\), defined as the width of the distribution of the potential strength, previously the single number \(V\), of the impurities. The usual model of impurities is that they
are all identical: \( W = 0 \), but we will consider also \( W \neq 0 \). If interactions on the impurities are important, we may introduce a Hubbard-type parameter to describe the interaction strength. We shall not discuss this possibility, but only note that this also introduces a breaking of the band symmetry which can move the bound state away from midgap. This situation is treated in Ref. [18].

The first question for band formation is the following: given a wavepacket located at an impurity site, is it more likely to hop to a neighboring impurity, or to leak into a continuum state? If the latter, then the impurities merely form a system of resonances and averaging procedures should be approximately valid. In this case, we may make arguments similar to those for the semiconductor to argue that the results of the two types of calculations may be combined.

If \( W = 0 \), then the bound state energy \( \omega_b \) is fixed at some position relative to the chemical potential \( \mu \). In the general case \( \omega_b \neq \mu \), even in the unitary limit, as we have seen above. This means that there is a finite density of states at \( \omega_b \). The lifetime of the wavepacket for decay into the continuum \( \tau_c \) is given by

\[
\frac{1}{\tau_c} = \pi N(\omega_b)|V|^2.
\] (146)

Near the unitary limit, we have \( |V| > 1/N_0 \). Using Eq. [123], we then find

\[
\frac{1}{\tau_c} > \frac{\omega_b}{\Delta N_0}.
\] (147)

This may be anomalous only if \( |\omega_b| \ll \Delta_0 \). The rate for interimpurity hopping \( 1/\tau_i \), is of order

\[
\frac{1}{\tau_i} \sim \frac{e^{-\ell_{imp}/\xi_d}}{N_0},
\] (148)

where \( \xi_d \) is the minimum decay length. As shown above, we have that \( \xi_d = v_F/|\omega_b| \).

The criterion for band formation is then

\[
e^{-\ell_{imp}/\xi_d} \geq \frac{\pi \beta \omega_b}{\Delta}.
\] (149)
Unless $\omega_b$ is accidentally very small, this means that we must have $\ell_{\text{imp}} \sim \xi_d$. However, this is the dirty limit. This limit does not exist for unconventional superconductors because the critical temperature $T_c$ is a sensitive function of impurity concentration and the situation $\ell_{\text{imp}} \sim \xi_d$ corresponds to $T_c \to 0$. Hence band formation does not occur in the $W = 0$ case. The only possible exception would be if, by some accident, $|\omega_b| << \Delta$. This is an intriguing possibility. However, it is not related to the unitary limit.

Now consider the case of finite $W$. There will be a distribution of bound state energies. If this distribution does not include the chemical potential, then the previous conclusion that no impurity band forms remains valid, as no quasi-bound states have low enough energy to be anything but broad resonances. The interesting case is when the distribution is broad enough that some of the bound states have very small $|\omega_b|$, $(|\omega_b| << \Delta)$.

We may build up the state by considering pairs of impurities. Almost all such pairs which involve a low-energy impurity state (energy $|\omega_{b1}|$) will then involve as the second member a state for which $|\omega_{b2}| \sim \Delta$. These states will mix, with overlap matrix element $M_{12}$. Under the influence of the mixing, state 1 then has probability amplitude on site 2 of $M_{12}^2/(\omega_{b1} - \omega_{b2})^2$, when $|M_{12}| << |(\omega_{b1} - \omega_{b2})|$. The transition rate to the continuum for this state is then

$$\frac{1}{\tau_c} \sim \frac{M_{12}^2 \pi \beta}{|\omega_{b2}| \Delta N_0}.$$

(150)

If site 1 has many such neighbors, then the transition rate to the continuum is multiplied by the number of neighbors. What happens is that the state leaks first through an impurity and then into the continuum. Rare transitions from one low energy impurity state to another will therefore not lead to the formation of a well-defined band, and transport occurs through the extended states.

The result is a collection of resonances together with a set of broadened continuum levels. As in the semiconductor case, the total number of continuum states is equal to the number of atomic orbitals in the sample; the number of resonances is equal to the number of impurities. The resulting total density of states is shown in Fig. [1]. We must conclude that
the low temperature behavior in this system is never dominated by interimpurity hopping. As a result, calculations using impurity averaging methods should lead to correct results. However, the noncrossing approximation may be dangerous in two dimensions, and the use of a symmetric density of states is not justified.

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VI. APPENDIX

In this appendix I give details of the more lengthy integrations. Eq. (151) is

\[ G(i\omega, \hat{r}\hat{x}) = -\frac{N_0}{4\pi} \int d\phi \int ds \int_{-1}^{1} e^{iux} \frac{i\Omega + s\tau_3 + \cos(\phi)(1 - x^2)^{1/2}\tau_1}{\Omega^2 + s^2 + \cos^2(\phi)(1 - x^2)} dx. \] (151)

The last term in the numerator gives zero on integration over $\phi$. We again write the $x$ integral as

\[
\begin{align*}
I &= \int_{-1}^{1} dx e^{iux} \\
&= \int dz e^{iuz} \\
&= \int_{0}^{\infty} dy e^{iu(1+iy)} \\
&+ \int_{0}^{\infty} dy e^{iu(-1+iy)}
\end{align*}
\] (152)

The poles lie on the real axis outside the contour, so the contour integral is zero. Thus we obtain a very simple result:

\[
I = -\frac{i(i\Omega + s\tau_3) e^{iu} - e^{-iu}}{\Omega^2 + s^2} u,
\] (153)

again because $u >> 1$. Then

\[
G(i\omega, \hat{r}\hat{x}) = \frac{iN_0}{4\pi k_F r} \int d\phi \int ds \frac{(i\Omega + s\tau_3) ds}{\Omega^2 + s^2} (e^{i(k_F + s\Delta_0/v_F)r} - e^{-i(k_F + s\Delta_0/v_F)r})
\]

\[
= -\frac{\pi N_0}{2k_F r} \left[ e^{ik_F r} (sgn (\omega)\tau_0 + \tau_3) - e^{-ik_F r} (sgn (\omega)\tau_0 - \tau_3) \right].
\] (154)
This is Eq. 134.

Let us now carry out the integration for a polar gap in the general case. The Green’s function is given by Eq. 137:

$$G(r, \sin \psi \hat{x} + \cos \psi \hat{z}, i\omega) = -\frac{N_0}{4\pi} \int_0^{2\pi} d\phi \int_{-1}^{1} dx e^{iux} \frac{i\omega + \epsilon \tau_3 + \Delta_0 \tau_1(ax - b\sqrt{1-x^2})}{\omega^2 + \epsilon^2 + \Delta_0^2(ax - b\sqrt{1-x^2})^2},$$

(155)

where $a \equiv \cos \psi, b = \cos \phi \sin \psi$, and $u \equiv (k_F + \epsilon/v_F)r$. The coordinates for the integration have been rotated so that the polar axis defined by $x = \pm 1$ is along $\hat{r}$. This is rewritten as:

$$G(r, \sin \psi \hat{x} + \cos \psi \hat{z}, i\omega) = -\frac{N_0}{4\pi \Delta_0} \int_0^{2\pi} d\phi \int ds I(\Omega, a, b),$$

(156)

where

$$I(\Omega, a, b) = \int_{-1}^{1} dx e^{iux} \frac{i\Omega + s\tau_3 + \tau_1(ax - b\sqrt{1-x^2})}{\Omega^2 + s^2 + (ax - b\sqrt{1-x^2})^2}. $$

(157)

which may again be evaluated using the same contour as above. This procedure yields

$$I(\Omega, a, b) = \oint dz e^{iuz} \frac{i\Omega + s\tau_3 + \tau_1(ax - b\sqrt{1-z^2})}{\Omega^2 + s^2 + (az - b\sqrt{1-z^2})^2} - i \int_0^\infty dy e^{i(1+iy)} \frac{i\Omega + s\tau_3 + \tau_1([a + iy] - b\sqrt{1-(1+iy)^2})}{\Omega^2 + s^2 + [a(1+iy) - b\sqrt{1-(1+iy)^2}]^2} + i \int_0^\infty dy e^{i(1-iy)} \frac{i\Omega + s\tau_3 + \tau_1([a - iy] - b\sqrt{1-(-1+iy)^2})}{\Omega^2 + s^2 + [a(-1+iy) - b\sqrt{1-(-1+iy)^2}]^2}. $$

(158)

The poles lie at points determined by the equation

$$ax - b\sqrt{1-x^2} = \pm i(\Omega^2 + s^2)^{1/2}. $$

(159)

There are four such roots:

$$x_{\pm, \pm} = \pm \frac{b(a^2 + b^2 + s^2 + \Omega^2)^{1/2}}{(a^2 + b^2)} \pm \frac{ia(\Omega^2 + s^2)^{1/2}}{a^2 + b^2}. $$

(160)

Only the two with positive imaginary parts ($x_{++}$ and $x_{-+}$) may lie in the contour, and then only if $|Re x| < 1$. This is the case if $|s| < (a^4/b^2 + a^2 - \Omega^2)^{1/2} \equiv s_0$. The cuts produced
by the square roots can be chosen to be along \((-\infty, -1)\) and \((1, \infty)\). They lie outside the contour. Performing the integrations leads to

\[
I(\Omega, a, b) = \Theta(s_0 - |s|)\pi e^{iu\pi} \frac{i\Omega + s\tau_3 + i\sqrt{\Omega^2 + s^2}\tau_1}{\sqrt{\Omega^2 + s^2}} + \Theta(s_0 - |s|)\pi e^{iu\pi} \frac{i\Omega + s\tau_3 + i\sqrt{\Omega^2 + s^2}\tau_1}{\sqrt{\Omega^2 + s^2}}
\]

\[
- \frac{e^{ik_Fr}}{k_Fr} \frac{i\Omega + s\tau_3 + a\tau_1}{\sqrt{\Omega^2 + s^2 + a^2}} e^{is\Delta_0r/v_F}
\]

\[
+ \frac{e^{-ik_Fr}}{k_Fr} \frac{i\Omega + s\tau_3 - a\tau_1}{\sqrt{\Omega^2 + s^2 + a^2}} e^{-is\Delta_0r/v_F}.
\]

(161)

This must next be integrated over \(s\). The first two integrals can be performed by the stationary phase approximation, taking \(u\) as a large parameter and expanding the argument of the exponential about its maximum. These expansions are valid if \(k_Fr\sin\psi >> 1\) and \(k_Fr\cos\psi >> 1\). Thus, the result is not valid near the equator or the poles. Fortunately, we already have results in these regions. The second two integrals are standard contour integrations. This leads to the expression

\[
\int_{-\infty}^{\infty} I(\Omega, a, b) = 2\pi i(sgn (\omega) + \tau_1) \left[ \frac{2\pi|\Omega|(a^2 + b^2)}{au} \right]^{1/2} \exp \left[ \frac{iub\sqrt{a^2 + b^2 + \Omega^2 - au|\Omega|}}{a^2 + b^2} \right]
\]

\[
+ 2\pi i(sgn (\omega) + \tau_1) \left[ \frac{2\pi|\Omega|(a^2 + b^2)}{au} \right]^{1/2} \exp \left[ -iub\sqrt{a^2 + b^2 + \Omega^2 - au|\Omega|} \right]
\]

\[
+ \frac{\pi e^{ik_Fr}}{k_Fr} \left[ \frac{\Omega}{\sqrt{\Omega^2 + a^2}} - i\frac{a\tau_1}{\sqrt{\Omega^2 + a^2}} + \tau_3 \right] e^{-\sqrt{\Omega^2 + a^2}\Delta_0r/v_F}
\]

\[
- \frac{\pi e^{-ik_Fr}}{k_Fr} \left[ \frac{\Omega}{\sqrt{\Omega^2 + a^2}} + i\frac{a\tau_1}{\sqrt{\Omega^2 + a^2}} - \tau_3 \right] e^{-\sqrt{\Omega^2 + a^2}\Delta_0r/v_F}.
\]

(162)

The final integration over the azimuthal angle is also simplified by the fact that \(u >> 1\), and the same method may be used.
\[ G(r \sin \psi \hat{x} + \cos \psi \hat{z}, i\omega) = -\frac{N_0 \Delta_0}{4\pi} \int_0^{2\pi} d\phi \int dI(\Omega, a, b) \]

\[ = -\frac{iN_0 \Delta_0}{2} (\text{sgn}(\Omega) + \tau_1) \int_0^{2\pi} \left[ \frac{2|\Omega|}{u \cos \psi} \right]^{1/2} \times \]

\[ \exp[-i u \sin \psi \cos \phi - u|\Omega| \cos \psi \cos^2 \phi + u|\Omega| \cos \psi \sin^2 \psi \cos^2 \phi] d\phi \]

\[ -\frac{iN_0 \Delta_0}{2} (\text{sgn}(\Omega) + \tau_1) \int_0^{2\pi} \left[ \frac{2|\Omega|}{u \cos \psi} \right]^{1/2} \times \]

\[ \exp[-i u \sin \psi \cos \phi - u|\Omega| \cos \psi \cos^2 \phi + u|\Omega| \cos \psi \sin^2 \psi \cos^2 \phi] d\phi \]

\[ + \frac{iN_0 \pi e^{ik_{FR}}}{2k_{FR}} \left[ \frac{\omega}{\sqrt{\omega^2 + \Delta_0^2 \cos^2 \psi}} - i \frac{\cos \psi \tau_1}{\sqrt{\omega^2 + \Delta_0^2 \cos^2 \psi}} + \tau_3 \right] \times \]

\[ e^{-\sqrt{\omega^2 + \Delta_0^2 \cos^2 \psi} / v_F} \]

\[ + \frac{iN_0 \pi e^{ik_{FR}}}{2k_{FR}} \left[ \frac{\omega}{\sqrt{\omega^2 + \Delta_0^2 \cos^2 \psi}} + i \frac{\cos \psi \tau_1}{\sqrt{\omega^2 + \Delta_0^2 \cos^2 \psi}} - \tau_3 \right] \times \]

\[ e^{-\sqrt{\omega^2 + \Delta_0^2 \cos^2 \psi} / v_F} . \] (163)

The integrations then give

\[ G(r \sin \psi \hat{x} + \cos \psi \hat{z}, i\omega) = -\frac{i\pi N_0}{2k_{FR}} \left[ \text{sgn}(\omega) + \tau_1 \right] \left[ \frac{2|\omega|}{\Delta_0^2 \cos^2 \psi} \right]^{1/2} \times \]

\[ e^{ik_{FR} \sin \psi - k_{FR}|\omega| \cos \psi / \Delta_0} \]

\[ -\frac{i\pi N_0}{2k_{FR}} \left[ \text{sgn}(\omega) + \tau_1 \right] \left[ \frac{2|\omega|}{\Delta_0^2 \cos^2 \psi} \right]^{1/2} \times \]

\[ e^{-ik_{FR} \sin \psi - k_{FR}|\omega| \cos \psi / \Delta_0} \]

\[ + \frac{-iN_0 \pi e^{ik_{FR}}}{2k_{FR}} \left[ \frac{\omega}{\sqrt{\omega^2 + \Delta_0^2 \cos^2 \psi}} - i \frac{\cos \psi \tau_1}{\sqrt{\omega^2 + \Delta_0^2 \cos^2 \psi}} + \tau_3 \right] \times \]

\[ e^{-\sqrt{\omega^2 + \Delta_0^2 \cos^2 \psi} / v_F} \]

\[ + \frac{iN_0 \pi e^{ik_{FR}}}{2k_{FR}} \left[ \frac{\omega}{\sqrt{\omega^2 + \Delta_0^2 \cos^2 \psi}} + i \frac{\cos \psi \tau_1}{\sqrt{\omega^2 + \Delta_0^2 \cos^2 \psi}} - \tau_3 \right] \times \]

\[ e^{-\sqrt{\omega^2 + \Delta_0^2 \cos^2 \psi} / v_F} . \] (164)

This leads immediately to Eq. 138.

The Green’s function for motion away from the impurity along the x-axis in two dimensions is given by Eq. 140:

\[ G(i\omega, r \hat{x}) = -\frac{2N_0}{\pi} \int_{-1}^{1} dv \int_{-1}^{1} \frac{dv}{\sqrt{1 - v^2}} \omega^2 + \epsilon^2 + \Delta_0^2(2v^2 - 1)^2 \exp{iuv} . \] (165)
Here \( v = \cos(\varphi) \), \( \Delta = \Delta_0(2v^2 - 1) \) and \( u = (k_F + \epsilon/v_F)r \). We may also write

\[
G(i\omega, \hat{x}) = -\frac{2N_0}{\pi} \int ds I(\Omega, s),
\]

(166)

where

\[
I(\Omega, s) \equiv \int_{-1}^{1} \frac{du}{\sqrt{1 - u^2}} \frac{i\Omega + s\tau_3 + \tau_1(2u^2 - 1)}{t^2 + (2u^2 - 1)^2} e^{iu},
\]

(167)

and \( \Omega = \omega/\Delta_0 \), \( s = \epsilon/\Delta_0 \), and \( t = \sqrt{\Omega^2 + s^2} \). As usual, we split the integral into three parts:

\[
I(\Omega, s) = I_1(\Omega, s) + I_2(\Omega, s) + I_3(\Omega, s),
\]

(168)

with

\[
I_1(\Omega, s) = \int \frac{dz}{\sqrt{1 - z^2}} \frac{i\Omega + s\tau_3 + \tau_1(2z^2 - 1)}{t^2 + (2z^2 - 1)^2} e^{iz},
\]

(169)

\[
I_2(\Omega, s) = -i \int_0^{\infty} \frac{dy}{\sqrt{1 - (1 + iy)^2}} \frac{i\Omega + s\tau_3 + \tau_1[2(1 + iy)^2 - 1]}{t^2 + [2(1 + iy)^2 - 1]^2} e^{iu(1+iy)},
\]

(170)

and

\[
I_3(\Omega, s) = i \int_0^{\infty} \frac{dy}{\sqrt{1 - (-1 + iy)^2}} \frac{i\Omega + s\tau_3 + \tau_1[2(-1 + iy)^2 - 1]}{t^2 + [2(-1 + iy)^2 - 1]^2} e^{iu(-1+iy)}.
\]

(171)

Turning first to \( I_1 \), we locate the poles of the integrand at

\[
t^2 + (2z^2 - 1)^2 = 0
\]

(172)

or

\[
z^2 = \frac{1}{2}(1 \pm it).
\]

(173)

There are four poles, only two of which have positive imaginary parts and thus may lie in the contour. Let us call them \( z_1 \) and \( z_2 \). They satisfy

\[
|z_1| = |z_2| = |z| \frac{1}{\sqrt{2}}(1 + t^2)^{1/4}
\]

(174)
and \( z_1 = -|z|e^{-i\theta}, z_2 = |z|e^{i\theta} \), with \( \theta = \frac{1}{2} \tan^{-1}(t) \). If the real parts of these quantities are less than unity in absolute magnitude, then they lie in the contour. A bit of trigonometry shows that this occurs only if \( t < 2\sqrt{2} \). This condition will normally be fulfilled in our problem. The other two roots lie at \( z_3 = -|z|e^{i\theta} \) and \( z_4 = |z|e^{-i\theta} \).

The contour integral is now written as:

\[
I_1(\Omega, s) = \frac{1}{4} \oint dz \frac{i\Omega + s\tau_3 + \tau_1(2z^2 - 1)}{\sqrt{1 - z^2} (z - z_1)(z - z_2)(z - z_3)(z - z_4)} e^{iuz},
\]

and the residue theorem gives

\[
I_1(\Omega, s) = \frac{1}{4} 2\pi i \Theta(\sqrt{8} - t) \times \begin{bmatrix} i\Omega + s\tau_3 + \tau_1(2z_1^2 - 1) \quad e^{iuz_1} \\ \sqrt{1 - z_1^2}(z_1 - z_2)(z_1 - z_3)(z_1 - z_4) \end{bmatrix} + \begin{bmatrix} i\Omega + s\tau_3 + \tau_1(2z_2^2 - 1) \quad e^{iuz_2} \\ \sqrt{1 - z_2^2}(z_2 - z_1)(z_2 - z_3)(z_2 - z_4) \end{bmatrix}. \]

Using

\[
\sqrt{1 - z_1^2} = \frac{1}{\sqrt{2}} (1 + t^2)^{1/4} e^{i\theta} = |z|e^{i\theta},
\]

\[
\sqrt{1 - z_2^2} = \frac{1}{\sqrt{2}} (1 + t^2)^{1/4} e^{-i\theta} = |z|e^{-i\theta},
\]

\[
2z_1^2 - 1 = -it,
\]

\[
2z_2^2 - 1 = it,
\]

this may be rewritten as

\[
I_1(\Omega, s) = \frac{i\pi}{2} \Theta(\sqrt{8} - t)|z|^{-4} \times \begin{bmatrix} (i\Omega + s\tau_3 - it\tau_1)e^{iuz_1} \\ e^{i\theta}(-e^{-i\theta} - e^{i\theta})(-e^{-i\theta} + e^{i\theta})(-e^{-i\theta} - e^{i\theta}) \end{bmatrix} + \begin{bmatrix} (i\Omega + s\tau_3 + it\tau_1)e^{iuz_2} \\ e^{i\theta}(e^{i\theta} + e^{-i\theta})(e^{i\theta} + e^{-i\theta})(e^{i\theta} - e^{-i\theta}) \end{bmatrix}
\]

\[
= \frac{i\pi}{2} \Theta(\sqrt{8} - t)(\frac{4}{1 + t^2}) \times \begin{bmatrix} (i\Omega + s\tau_3 - it\tau_1)e^{iuz_1} \\ (-2\cos\theta)(2i\sin\theta)(-2) \end{bmatrix} + \begin{bmatrix} (i\Omega + s\tau_3 + it\tau_1)e^{iuz_2} \\ (2\cos\theta)(2)(2i\sin\theta) \end{bmatrix}.
\]

Since \( \frac{1}{2} \sin\theta \cos\theta \sin 2\theta = \sin \tan^{-1}(t) = t/\sqrt{1 + t^2} \), this becomes
\[ I_1(\Omega, s) = \frac{\pi}{2} \Theta(\sqrt{8} - t)\left(\frac{1}{t\sqrt{1 + t^2}}\right) \times \]
\[ [(i\Omega + s\tau_3 - it\tau_1)e^{iu_1} + (i\Omega + s\tau_3 + it\tau_1)e^{iu_2}]. \quad (179) \]

Integrating this:
\[
\int ds I_1(\Omega, s) = \frac{\pi}{2} \int_{-\infty}^{\infty} ds \Theta(\sqrt{8} - \sqrt{\Omega^2 + s^2})\left(\frac{1}{\sqrt{\Omega^2 + s^2}\sqrt{1 + \Omega^2 + s^2}}\right) \times 
\]
\[ [(i\Omega + s\tau_3 - i\sqrt{\Omega^2 + s^2}\tau_1) \exp\left(\frac{-iu}{2\sqrt{1 + \Omega^2 + s^2 + 1}}\right) \times 
\]
\[ \exp\left(\frac{-u}{2\sqrt{1 + \Omega^2 + s^2 - 1}}\right) + (i\Omega + s\tau_3 + i\sqrt{\Omega^2 + s^2}\tau_1) \exp\left(\frac{iu}{2\sqrt{1 + \Omega^2 + s^2 + 1}}\right) \times 
\]
\[ \exp\left(\left(\frac{-u}{2\sqrt{1 + \Omega^2 + s^2 - 1}}\right\right) \right]. \quad (180) \]

Since \( u \gg 1 \), we expand the argument of the exponential around its maximum at \( s = 0 \):
\[
\exp\left(\frac{-u}{2\sqrt{1 + \Omega^2 + s^2 - 1}}\right) \approx \exp\left(\frac{-u}{2\sqrt{1 + \Omega^2 - 1}}\right) \times 
\]
\[ \exp\left[\frac{-us^2}{8}(\sqrt{1 + \Omega^2 - 1})^{-1/2}(1 + \Omega^2)^{-1/2}\right], \quad (181) \]
and evaluate the rest of the integrand at \( s = 0 \), so that \( t \to \Omega \). This yields
\[
\int ds I_1(\Omega, s) = \frac{\pi}{2}\left(\frac{\sqrt{1 + \Omega^2 - 1}^{1/4}}{(1 + \Omega^2)^{1/4}}\right)\left(\frac{8\pi}{k_{Fr}}\right)^{1/2} \exp\left(\frac{-u}{2\sqrt{1 + \Omega^2 - 1}}\right) \times 
\]
\[ [(i\sgn \Omega - i\tau_1) \exp\left(\frac{-iu}{2\sqrt{1 + \Omega^2 + 1}}\right) + (is\sgn \Omega + i\tau_1) \exp\left(\frac{iu}{2\sqrt{1 + \Omega^2 + 1}}\right)]. \quad (182) \]

The other integrals are simpler:
\[
I_2(\Omega, s) = -ie^{iu} \int \frac{dy}{\sqrt{y^2 - 2iy}} \frac{i\Omega + s\tau_3 + \tau_1[2(1 + iy)^2 - 1]}{t^2 + [2(1 + iy)^2 - 1]^2} e^{-uy} 
\]
\[ \approx -i(-2i)^{-1/2}e^{iu} \frac{i\Omega + s\tau_3 + \tau_1}{t^2 + 1} \int_0^{\infty} \frac{dy}{\sqrt{y}} e^{-uy} 
\]
\[ = \frac{1 - i}{2}\sqrt{\frac{\pi}{k_{Fr}}} e^{i k_{Fr}e^{is\Delta_0 + \nu_F}} \frac{i\Omega + s\tau_3 + \tau_1}{s^2 + \Omega^2 + 1}, \quad (183) \]
and similarly
\[
I_3(\Omega, s) = \frac{1 + i}{2}\sqrt{\frac{\pi}{k_{Fr}}} e^{-ik_{Fr}e^{-is\Delta_0 + \nu_F}} \frac{i\Omega + s\tau_3 + \tau_1}{s^2 + \Omega^2 + 1}. \quad (184) \]
These expressions are easily integrated over energy:

$$\int_{-\infty}^{\infty} ds I_2(\Omega, s) = \frac{(1 - i)\pi}{2} \sqrt{\frac{1 + \Omega^2}{\sqrt{1 + \Omega^2}}} \frac{e^{ik_F r} e^{-\sqrt{1 + \Omega^2} \Delta \tau/v_F i\Omega + i\sqrt{1 + \Omega^2} r_3 + \tau_1}}{\sqrt{1 + \Omega^2}}$$

(185)

and

$$\int_{-\infty}^{\infty} ds I_3(\Omega, s) = \frac{(1 + i)\pi}{2} \sqrt{\frac{1 + \Omega^2}{\sqrt{1 + \Omega^2}}} \frac{e^{-ik_F r} e^{-\sqrt{1 + \Omega^2} \Delta \tau/v_F i\Omega - i\sqrt{1 + \Omega^2} r_3 + \tau_1}}{\sqrt{1 + \Omega^2}}$$

(186)
Combining Eqs. 165, 182, 185, and 186, we find

\[ G(i\omega, r\hat{x}) = \frac{-2N_0}{\pi} \times \]

\[ \left[ \frac{\pi}{2} \left( \frac{\sqrt{1 + \Omega^2} - 1}{1 + \Omega^2} \right)^{1/4} \right] \left( \frac{8\pi}{k_{FR}} \right)^{1/2} \text{exp}\left( -\frac{u}{2} \sqrt{1 + \Omega^2} \right) \times \]

\[ [(i \text{ sgn } \Omega - i\tau_1) \exp\left( -\frac{iu}{2} \sqrt{1 + \Omega^2} + 1 \right) \]

\[ + (i \text{ sgn } \Omega + i\tau_1) \exp\left( \frac{iu}{2} \sqrt{1 + \Omega^2} + 1 \right)] \]

\[ + \frac{(1 - i)\pi}{2} \sqrt{\frac{\pi}{k_{FR}}} e^{ik_{FR}e^{-\sqrt{1+\Omega^2\Delta_{or}/v_F}i\Omega + i\sqrt{1+\Omega^2\tau_3 + \tau_1}} \frac{\sqrt{1 + \Omega^2}}{\sqrt{1 + \Omega^2}}} \]

\[ + \frac{(1 - i)\pi}{2} \sqrt{\frac{\pi}{k_{FR}}} e^{-ik_{FR}e^{-\sqrt{1+\Omega^2\Delta_{or}/v_F}i\Omega - i\sqrt{1+\Omega^2\tau_3 + \tau_1}} \frac{\sqrt{1 + \Omega^2}}{\sqrt{1 + \Omega^2}}} \]

\[ (187) \]

From this Eq. 141 follows immediately.

The Green’s function for the direction along the node is more easily computed. We have, from Eq. 142, that

\[ G(i\omega, r\hat{x} + \hat{y}\sqrt{2}) = \frac{-2N_0}{\pi} \int d\epsilon \int_{-1}^{1} dv \frac{i\omega + \epsilon\tau_3 + \Delta_0 \tau_1 v\sqrt{1 - v^2}}{\sqrt{1 - v^2} \omega^2 + \epsilon^2 + 2\Delta_0^2 v^2(1 - v^2)} e^{iuv}, \]

\[ (188) \]

where the part proportional to \( \tau_1 \) vanishes by symmetry. and with the usual breakup:

\[ G(i\omega, r\hat{x} + \hat{y}\sqrt{2}) = \frac{-2N_0}{\pi} \int ds(I_1 + I_2 + I_3). \]

\[ (189) \]

Now

\[ I_1 = \oint dz \frac{i\Omega + s\tau_3}{\sqrt{1 - z^2} \Omega^2 + s^2 + 2z^2(1 - z^2)} e^{iuz} \]

\[ = -\frac{1}{4} \oint \frac{i\Omega + s\tau_3 + \tau_1 z\sqrt{1 - z^2}}{(z - z_1)(z - z_2)(z - z_3)(z - z_4)} e^{iuz}, \]

\[ (190) \]

where the roots are

\[ z_1 = \frac{i}{\sqrt{2}}(\sqrt{1 + t^2} - 1)^{1/2} \]

\[ z_2 = -z_1 \]

\[ z_3 = -\frac{1}{\sqrt{2}}(\sqrt{1 + t^2} + 1)^{1/2} \]

\[ z_4 = -z_3. \]

\[ (191) \]
We shall also need:

\[ \sqrt{1 - z_1^2} = z_4 \]  

(192)

Only \( z_1 \) lies in the contour. Evaluating the integral:

\[
I_1 = -\frac{2\pi i}{4} (1 - z_1^2)^{-1/2} \frac{i\Omega + s\tau_3}{(z_1 - z_2)(z_1 - z_3)(z_1 - z_4)} e^{iuz_1} 
\]

\[ = -\pi i \frac{i\Omega + s\tau_3}{2z_4(2z_1)(z_1^2 - z_4^2)} e^{iuz_1} 
\]

\[ = \pi(i\Omega + s\tau_3) \left| t \right| \sqrt{\Omega} \exp\left[\frac{-u}{\sqrt{2}} (\sqrt{1 + t^2} - 1)^{1/2} \right] \]  

(193)

Integrating over energy:

\[
\int ds I_1 = \pi \int_{-\infty}^{\infty} ds \frac{i\Omega + s\tau_3}{\sqrt{\Omega^2 + s^2\sqrt{1 + \Omega^2 + s^2}}} \exp\left[\frac{-u}{\sqrt{2}} (\sqrt{1 + \Omega^2 + s^2} - 1)^{1/2} \right] 
\]

\[ = \pi \frac{i\Omega}{|\Omega|\sqrt{1 + \Omega^2}} \exp\left[\frac{-u}{\sqrt{2}} (\sqrt{1 + \Omega^2} - 1)^{1/2} \right] \times 
\]

\[ \int_{-\infty}^{\infty} ds \exp\left[\frac{-us^2}{4\sqrt{2}} (\sqrt{1 + \Omega^2} - 1)^{1/2}\sqrt{1 + \Omega^2} \right] 
\]

\[ = \left( \frac{4\pi^3 \sqrt{2}}{k_F} \right)^{1/2} \frac{i \text{sgn} \Omega}{(1 + \Omega^2)^{1/4}} (\sqrt{1 + \Omega^2} - 1)^{1/4} e^{-k_F r (\sqrt{1 + \Omega^2} - 1)^{1/2}/\sqrt{2}}. \]  

(194)

The other integrals are simpler, as usual.

\[
I_2 = -i \int_0^{\infty} dy \frac{i\Omega + s\tau_3}{\sqrt{1 - (1 + iy)^2}} \Omega^2 + s^2 + 2(1 + iy)^2(1 - (1 + iy)^2) e^{i\Omega(1 + iy)}, 
\]

\[ \approx -i e^{iu} \int_0^{\infty} dy \frac{e^{-uy} i\Omega + s\tau_3}{s^2 + \Omega^2} \]

\[ = \frac{1 - i}{2} e^{ik_F r} \frac{i\Omega + s\tau_3}{s^2 + \Omega^2} e^{ik_F s \Delta_0 F/r \sqrt{\frac{v}{F}}}, \]  

(195)

and

\[
I_3 = i \int_0^{\infty} dy \frac{i\Omega + s\tau_3}{\sqrt{1 - (-1 + iy)^2}} \Omega^2 + s^2 + 2(-1 + iy)^2(1 - (-1 + iy)^2) e^{i\Omega(-1 + iy)}, 
\]

\[ \approx i e^{-iu} \int_0^{\infty} dy \frac{e^{-uy} i\Omega + s\tau_3}{s^2 + \Omega^2} \]

\[ = \frac{1 + i}{2} e^{-ik_F r} \frac{e^{ik_F s \Delta_0 F/r \sqrt{\frac{v}{F}}}}{s^2 + \Omega^2} e^{-i k_F s \Delta_0 F/r \sqrt{\frac{v}{F}}}. \]  

(196)

The energy integrals are easily done:
\[
\int ds I_2 = \frac{(1 - i)\pi}{2} \frac{e^{ik_FR} (i \ sgn \ \Omega + i\tau_3) e^{-|\omega|/v_F}}{\sqrt{k_{FR}}} , \quad (197)
\]
and
\[
\int ds I_3 = \frac{(1 + i)\pi}{2} \frac{e^{-ik_FR} (i \ sgn \ \omega - i\tau_3) e^{-|\omega|/v_F}}{\sqrt{k_{FR}}} . \quad (198)
\]

From Eqs. 189, 194, 197, and 198, the Green’s function is

\[
G(i\omega, r \hat{x} + \hat{y}) = -\frac{2N_0}{\pi} \times 
\left[ \frac{4\pi^3 \sqrt{2}}{k_{FR}} \right]^{1/2} \frac{i \ sgn \ \Omega}{(1 + \Omega^2)^{1/4}} (\sqrt{1 + \Omega^2} - 1)^{1/4} e^{-k_{FR}(\sqrt{1+\Omega^2}-1)^{1/2}/\sqrt{2}}
\]

\[
+ \frac{(1 - i)\pi}{2} \frac{e^{ik_FR}}{\sqrt{k_{FR}}} (i \ sgn \ \Omega + i\tau_3) e^{-|\omega|/v_F}
\]

\[
+ \frac{(1 + i)\pi}{2} \frac{e^{-ik_FR}}{\sqrt{k_{FR}}} (i \ sgn \ \omega - i\tau_3) e^{-|\omega|/v_F} \right]. \quad (199)
\]

From this, Eq. 143 follows immediately.

The general direction is given by the equation:

\[
G(i\omega, r \cos(\frac{\pi}{4} - \psi)\hat{x} + r \sin(\frac{\pi}{4} - \psi)\hat{y}) = -\frac{N_0}{\pi} \times 
\int ds \int_{-1}^{1} \frac{dv}{\sqrt{1 - v^2}} \int_{v}^{1} \frac{d\omega}{\omega^2 + \epsilon^2 + 2\Delta_0^2 v^2 (1 - v^2)} \times 
\]

\[
e^{iu(\cos \psi + \sqrt{1 - v^2} \sin \psi)}
\]

\[
+ (\sin \psi \to -\sin \psi, \ \tau_1 \to -\tau_1). \]

\[
= \int ds (I_1 + I_2 + I_3) \quad (200)
\]

The two integrals come from the regions \(\phi = (0, \pi)\) and \(\phi = (\pi, 2\pi)\). Then we find

\[
I_1 = \frac{\pi i \Omega + s\tau_3 + i|\tau_1|}{2 |\tau_1|} \exp[iu(z_1 \cos \psi + z_4 \sin \psi)]
\]

\[
+ \frac{\pi i \Omega + s\tau_3 - i|\tau_1|}{2 |\tau_1|} \exp[iu(z_1 \cos \psi - z_4 \sin \psi)] , \quad (201)
\]

where the result is obtained by the same method as that in Eq. 193. The energy integral is:

\[
\int ds I_1 = \left(\frac{4\pi^3 \sqrt{2}}{k_{FR} |\cos \psi|}\right)^{1/2} \frac{i \ sgn \ \Omega + i\tau_1}{(1 + \Omega^2)^{1/4}} (\sqrt{1 + \Omega^2} - 1)^{1/4} \times 
\]

\[
\exp[iu(z_1 \cos \psi + z_4 \sin \psi)]
\]

\[
+ \frac{\pi i \Omega + s\tau_3 - i|\tau_1|}{2 |\tau_1|} \exp[iu(z_1 \cos \psi - z_4 \sin \psi)] , \quad (201)
\]

where the result is obtained by the same method as that in Eq. 193. The energy integral is:
\begin{align*}
e^{-k_F r |\cos \psi(\sqrt{1+\Omega^2}-1)^{1/2}/\sqrt{2}} & \exp [ik_F r \sin \psi(\sqrt{1+\Omega^2}-1)^{1/2}/\sqrt{2}] \\
+ \left( \frac{4\pi^3 \sqrt{2}}{k_F r |\cos \psi|} \right)^{1/2} & \frac{i \operatorname{sgn} \Omega - i\tau_1}{(1 + \Omega^2)^{1/4}} (\sqrt{1 + \Omega^2} - 1)^{1/4} \times \\
e^{-k_F r |\cos \psi(\sqrt{1+\Omega^2}-1)^{1/2}/\sqrt{2}} & \exp [-ik_F r \sin \psi(\sqrt{1+\Omega^2}-1)^{1/2}/\sqrt{2}]. \quad (202)
\end{align*}

Similarly, from Eqs. 197 and 198, we have
\begin{equation}
\int ds I_2 = \frac{(1-i)\pi}{2} \frac{e^{ik_F r \cos \psi}}{\sqrt{k_F r |\cos \psi|}} (i \operatorname{sgn} \Omega + i\tau_3) e^{-|\omega \cos \psi| r/v_F}, \quad (203)
\end{equation}
and
\begin{equation}
\int ds I_3 = \frac{(1+i)\pi}{2} \frac{e^{-ik_F r \cos \psi}}{\sqrt{k_F r |\cos \psi|}} (i \operatorname{sgn} \omega - i\tau_3) e^{-|\omega \cos \psi| r/v_F}. \quad (204)
\end{equation}

Finally, let us define
\begin{equation}
G_-(i\omega, \psi) = G(i\omega, r \cos(\frac{\pi}{4} - \psi)\hat{x} + \sin(\frac{\pi}{4} - \psi)\hat{y}). \quad (205)
\end{equation}

Collecting results, we have
\begin{align*}
G_-(i\omega, \psi) &= -\frac{2N_0}{\pi} \times \\
& \left\{ \left( \frac{4\pi^3 \sqrt{2}}{k_F r |\cos \psi|} \right)^{1/2} \frac{i \operatorname{sgn} \Omega + i\tau_1}{(1 + \Omega^2)^{1/4}} (\sqrt{1 + \Omega^2} - 1)^{1/4} \times \\
&e^{-k_F r |\cos \psi(\sqrt{1+\Omega^2}-1)^{1/2}/\sqrt{2}} \exp [ik_F r \sin \psi(\sqrt{1+\Omega^2}-1)^{1/2}/\sqrt{2}] \\
+ \left( \frac{4\pi^3 \sqrt{2}}{k_F r |\cos \psi|} \right)^{1/2} \frac{i \operatorname{sgn} \Omega - i\tau_1}{(1 + \Omega^2)^{1/4}} (\sqrt{1 + \Omega^2} - 1)^{1/4} \times \\
e^{-k_F r |\cos \psi(\sqrt{1+\Omega^2}-1)^{1/2}/\sqrt{2}} \exp [-ik_F r \sin \psi(\sqrt{1+\Omega^2}-1)^{1/2}/\sqrt{2}] \\
+ \frac{(1-i)\pi}{2} \frac{e^{ik_F r \cos \psi}}{\sqrt{k_F r |\cos \psi|}} (i \operatorname{sgn} \Omega + i\tau_3) e^{-|\omega \cos \psi| r/v_F} \\
+ \frac{(1+i)\pi}{2} \frac{e^{-ik_F r \cos \psi}}{\sqrt{k_F r |\cos \psi|}} (i \operatorname{sgn} \omega - i\tau_3) e^{-|\omega \cos \psi| r/v_F} \right\}. \quad (206)
\end{align*}

This is Eq. 143.
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FIGURES

FIG. 1. Density of states for a model semiconductor with a band structure which is symmetric about the gap midpoint. This system contains a single impurity which is a unitary scatterer. This results in a midgap state.

FIG. 2. Density of states for a model semiconductor with a band structure which is not symmetric about the gap midpoint. This system contains a single impurity which is a unitary scatterer. This results in a bound state which is not at midgap. This is the generic case.

FIG. 3. Density of states for an artificial semiconductor with nearest-neighbor tight-binding dispersion and a gap. This density of states has an asymmetry factor of 0.25 t / unit cell. The asymmetry factor is defined in the text.

FIG. 4. Density of states for a semiconductor with many impurities using the usual impurity averaging procedure. The impurity density is above the critical value, so the gap has filled in. The even density of states is for a semiconductor with a band structure which is symmetric about the gap midpoint. The parameters, referring to Figure 1, are $\epsilon_1/\Delta = 5$ and $n_{imp} V^2 N_0 / \Delta = 0.8$. The asymmetric density of states is for an asymmetric density of states. The parameters, referring to Fig. 2, are $\epsilon_\ell / \Delta = 5$, $\epsilon_u / \Delta = 8$, and $n_{imp} V^2 N_0 / \Delta = 0.8$.

FIG. 5. The density of states for a model semiconductor with many impurities. The calculation combines the results of the T-matrix and the impurity averaging. The concentration is subcritical, so the gap is not completely closed. The bound states are shown in black. Note that the total number of bound states is proportional to the number of impurities, whereas the number of states in a fixed energy range around the chemical potential is proportional to the total number of orbitals.
FIG. 6. The density of states for a model semiconductor with many impurities. The calculation combines the results of the T-matrix and the impurity averaging. The concentration is supercritical, so the gap is closed. The bound states, shown in black, become resonances. Note that the total number of states in the resonance peak is proportional to the number of impurities, whereas the number of states in a fixed energy range around the chemical potential is proportional to the total number of orbitals.

FIG. 7. Contour for the angular integrals involved in calculating the impurity wavefunction in real space.

FIG. 8. Diagram (a), which contains no crossed impurity lines, is counted in the usual calculations of transport properties in unconventional superconductors. Diagram (b), with crossed lines, is usually neglected.

FIG. 9. The diagrams of the previous figure in momentum space in the normal state. The justification for the neglect of (b) is that one of the momenta is off the Fermi surface unless an additional constraint is applied.

FIG. 10. The same diagrams in momentum space, but now in the superconducting state at low temperatures. All momenta must be near the nodes, which are situated on the diagonals. The justification for the neglect of (b) no longer applies.

FIG. 11. The density of states for a d-wave superconductor with many impurities. The calculation combines the results of the T-matrix and the impurity averaging. The broadening of the resonance is shown. Note that the total number of states in the resonance peak is proportional to the number of impurities, whereas the number of states in a fixed energy range around the chemical potential is proportional to the total number of orbitals.