Self-consistent interface properties of $d$ and $s$-wave superconductors.

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Abstract

We develop a method to solve the Bogoliubov de Gennes equation for superconductors self-consistently, using the recursion method. The method allows the pairing interaction to be either local or non-local corresponding to $s$ and $d$-wave superconductivity, respectively. Using this method we examine the properties of various $S-N$ and $S-S$ interfaces. In particular we calculate the spatially varying density of states and order parameter for the following geometries (i) $s$-wave superconductor to normal metal, (ii) $d$-wave superconductor to normal metal, (iii) $d$-wave superconductor to $s$-wave superconductor. We show that the density of states at the interface has a complex structure including the effects of normal surface Friedel oscillations, the spatially varying gap and Andeev states within the gap, and the subtle effects associated with the interplay of the gap and the normal van Hove peaks in the density of states. In the case of bulk $d$-wave superconductors the surface leads to mixing of different order parameter symmetries near the interface and substantial local filling in of the gap.

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I. INTRODUCTION.

Interfaces in superconductors, especially high temperature superconductors, are of considerable interest for both fundamental physics and for applications. Many experiments have used both single electron tunnelling and Josephson effects as probes of the energy gap and order parameter symmetry in the cuprates. For example Wollman et al. [1] and Sun et al. [2] constructed SQUID devices consisting of junctions between YBa$_2$Cu$_3$O$_7$ (YBCO) and Pb, while Tsuei et al. [3] constructed superconducting rings consisting of YBCO thin films with two or three grain boundary junctions. Theoretical analysis of experiments such as these relies to a large extent on macroscopic symmetry arguments and not on the microscopic details of the actual interfaces. However in some cases the microscopic physics at the interface can be an important factor in understanding the experimental results. For example, if mixing of different order parameter symmetries occurs at the interface (because the interface breaks the bulk tetragonal or orthorhombic symmetry) the extent of such mixing can only be determined from microscopic calculations. Similarly, suppression of the order parameter (either $d$-wave or $s$-wave) near an $S - N$ interface can lead to significant local density of states within the bulk energy gap, and this can complicate the analysis of single electron tunnelling spectra [4]. The microscopic physics of surfaces and interfaces of high $T_c$ superconductors are especially interesting because of the short coherence length, and the probable $d$-wave gap function.

In the past few years there have been a number of microscopic calculations of surfaces and interfaces in superconducting systems with a $d$-wave order parameter. Most of the theoretical results have been obtained using tunnelling theory, or Andreev’s approximation [5–11] in which the tunnelling barrier and the order parameter are not found self-consistently. For tunnel junctions these approximations may be adequate, but we show below that self-consistency has significant effects for interfaces with direct contact between the constituents. Self-consistent properties of interfaces have previously been computed using the Eilenberger equations [12–17], which are an approximation to the Bogoliubov de Gennes equation. These
self-consistent solutions to the Eilenberger equations have shown some interesting effects which have only arisen when the order parameter is calculated in a self-consistent manner.

In this paper we aim to show how to calculate self-consistent properties of superconducting interfaces by directly solving the Bogoliubov de Gennes equations. This approach has the advantage that self-consistency can be fully incorporated and also there are no need for the further approximations of the Eilenberger method. Our approach makes use of the recursion method [18] to solve the Bogoliubov de Gennes equation on an arbitrary tight binding lattice. Previously the recursion method has been used to examine the effects of disorder in s-wave [19,20] and d-wave [21] superconductors, and to determine the core structure of vortices and explain the origin of de Haas van Alphen oscillations in the superconducting state [22]. In particular Litak, Miller and Györffy [20] have given a detailed description of the application of the recursion method to local interactions, corresponding to s-wave superconductors. Here we extend this to the case of non-local interactions necessary to obtain d-wave superconductivity and apply the method to various interfaces of s and d-wave superconductors.

The method of performing our self-consistent calculations will be described in section II. Here we introduce the Bogoliubov de Gennes equation with a general interaction, $U_{ij}$, and demonstrate how this general Hamiltonian can be solved self-consistently using the recursion method [18,20]. A necessary and non-trivial step in the calculation, as described below, involves finding the density of states accurately by extrapolation of the recursion method continued fraction.

In Sec. III we proceed to apply the method to several different problems. Firstly various test calculations are described, including: the local density of states for a uniform system with no interactions, the local density of states for a system with a local attractive interaction (local s-wave superconducting order parameter) and a system with a non-local attractive interaction. We show that for this non-local interaction there are two possible solutions, these solutions being a non-local s-wave superconducting order parameter (extended s-wave) and a non-local d-wave superconducting order parameter.
Having tested the method on uniform systems we present our self-consistent solutions for the interface between two different materials. We will consider three different interfaces. First we consider a normal metal to s-wave superconductor, $N - S^s$, interface where the pairing interaction is zero in the normal region ($N$) and purely local in the superconducting region ($S^s$). Then we will consider a $d$-wave to normal metal, $S^d - N$, interface where again the interaction in the normal region is zero and there is a non-local attractive interaction in the superconducting region ($S^d$). Finally a study of a $S^d - S^s$ interface will be described. These three calculations enable us to make a comparative study of how the local density of states and order parameter changes as a function of position across the different types of interface.

II. THEORY/MODEL.

A. The Bogoliubov de Gennes Equation.

The Bogoliubov de Gennes equation on a tight binding square lattice has the form

$$\sum_j H_{ij} \begin{pmatrix} u_{ij}^n \\ v_{ij}^n \end{pmatrix} = E_n \begin{pmatrix} u_i^n \\ v_i^n \end{pmatrix}$$

(1)

with

$$H_{ij} = \begin{pmatrix} H_{ij} & \Delta_{ij} \\ \Delta_{ij}^* & -H_{ij}^* \end{pmatrix}$$

(2)

where $u_i^n$ and $v_i^n$ are the particle and hole amplitudes, on site $i$, associated with an eigenenergy $E_n$ and where $\Delta_{ij}$ is the (possibly non-local) pairing potential or gap function.

In the fully self-consistent Bogoliubov de Gennes equation the normal state Hamiltonian $H_{ij}$ is given by

$$H_{ij} = (t_{ij} + \frac{1}{2}U_{ij} n_{ij})(1 - \delta_{ij}) + (\epsilon_i - \mu + \frac{1}{2}U_i n_i)\delta_{ij}$$

(3)

where $\mu$ is the chemical potential, $\epsilon_i$ is the normal on site energy of site $i$ and $t_{ij}$ is the hopping integral between site $i$ and site $j$, for the rest of this paper $t_{ij}$ is non zero for
nearest neighbours only. The on-site and off-site interaction terms $\frac{1}{2}U_{ii}n_{ii}$ and $\frac{1}{2}U_{ij}n_{ij}$ are the Hartree-Fock potentials corresponding to the on-site interaction $U_i$ and the non-local interaction $U_{ij}$. The charge density entering the Hartree-Fock terms $n_{ij}$ is given by

$$n_{ij} = \sum_\sigma \langle \Psi_{i\sigma}^\dagger \Psi_{j\sigma} \rangle = 2 \sum_n ((u_i^n)^* u_j^n f(E_n) + v_i^n (v_j^n)^* (1 - f(E_n))).$$  (4)

Similarly the pairing potentials are defined as

$$\Delta_{ij} = -U_{ij}F_{ij}$$  (5)

where the anomalous density is

$$F_{ij} = \langle \Psi_{i\uparrow} \Psi_{j\downarrow} \rangle = \sum_n (u_i^n (v_j^n)^* (1 - f(E_n)) - (v_i^n)^* (u_j^n) f(E_n)).$$  (6)

In equations (4) and (6) the sums only consider terms $E_n$ up to the condensate chemical potential ($\mu$).

A solution to the above system of equations will be fully self-consistent provided that both the normal ($U_{ij}n_{ij}$) and anomalous ($\Delta_{ij}$) potentials are determined consistently with the corresponding densities $n_{ij}$ and $F_{ij}$ via Eqs. (4) and (6). Note that the normal Hartree-Fock terms $U_{ij}n_{ij}$ play an important role and cannot be neglected. For on-site interactions these terms correspond to position dependent shifts in the on-site energy, while for non-local interactions these terms renormalise the hopping $t_{ij}$ leading to position dependent changes in the electronic bandwidth.

Figure 1 illustrates the geometry corresponding to this system of equations. The tight-binding lattice has nearest neighbour hopping interactions ($t_{ij}$), as well as a coupling between particle and hole space, via a superconducting order parameter ($\Delta_{ij}$). If the interactions are purely on-site ($U_i$) attractions then the pairing potential will be purely local ($\Delta_{ii}$), corresponding to the dashed line in Fig. 1. On the other hand when the interaction is non-local ($U_{ij}, i \neq j$) the pairing potential $\Delta_{ij}$ will also be non-local, as illustrated by the solid lines in Fig. 1. For computational convenience we limit both the hopping and non-local interaction to nearest neighbours distances. We also need to specify over what energy range
the interaction has an effect, and as in BCS \cite{23}, we will assume that it only acts over a small energy range centred on the Fermi energy, $\mu \pm E_c$.

**B. The Recursion Method.**

The method we have adopted to solve the above system of equations is the recursion method \cite{18}. This method allows us to calculate the electronic Green’s functions

$$G_{\alpha \alpha'}(i, j, E) = \langle i\alpha | \frac{1}{E1 - H} | j\alpha' \rangle$$  \hspace{1cm} (7)

where the indices $i$ and $j$ denote sites, while $\alpha$ and $\alpha'$ represent the particle or hole degree of freedom on each site. We denote particle degrees of freedom by $\alpha = +$ and hole degrees of freedom by $\alpha = -$. For example $G_{++}(i, j, E)$ represents the Green’s function between the particle degree of freedom on site $i$ and the hole degree of freedom on site $j$.

To compute the Green’s functions (7) we can closely follow the method described by Litak, Miller and Györffy \cite{20} for the special case of a local interaction ($U_{ij} = U_{ii} \delta_{ij}$). Using their method we can transform the Hamiltonian to a block tridiagonal form

$$E1 - H = \begin{pmatrix} E1 - a_0 & -b_1 & 0 & 0 & 0 & 0 & 0 & \cdots \\ -b_1^\dagger & E1 - a_1 & -b_2 & 0 & 0 & 0 & 0 & \cdots \\ 0 & -b_2^\dagger & \ddots & \ddots & \ddots & \ddots & \ddots & \cdots \\ 0 & 0 & \ddots & \ddots & \ddots & \ddots & \ddots & \cdots \\ \vdots & \vdots & \vdots & 0 & \ddots & \ddots & \ddots & \cdots \\ 0 & 0 & 0 & -b_n^\dagger & E1 - a_n & -b_{n+1} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \cdots \end{pmatrix}$$  \hspace{1cm} (8)

where $a_n$ and $b_n$ are $2 \times 2$ matrices. Given this form for $\langle i\alpha | E1 - H | j\alpha' \rangle$ and expressing the Green’s function as

$$G_{\alpha \alpha'}(i, j, E) = \langle i\alpha | (E1 - H)^{-1} | j\alpha' \rangle,$$  \hspace{1cm} (9)

the Greens functions above can be evaluated as a matrix continued fraction so that
\[ G(i, j, E) = \left( E1 - a_0 - b_1^\dagger \left( E1 - a_1 - b_2^\dagger \left( E1 - a_2 - b_3^\dagger (E1 - a_3 - \ldots)^{-1} b_3 \right)^{-1} b_2 \right)^{-1} b_1 \right)^{-1} \]  

where

\[ G(i, j, E) = \begin{pmatrix} G_{\alpha \alpha}(i, i, E) & G_{\alpha \alpha'}(i, j, E) \\ G_{\alpha' \alpha}(j, i, E) & G_{\alpha' \alpha'}(j, j, E) \end{pmatrix}. \]  

Within equations (8) and (10) we have a formally exact representation of the Green’s functions. However in general both the tridiagonal representation of the Hamiltonian, and the matrix continued fraction (8) will be infinite. In practice one can only calculate a finite number of terms in the continued fraction exactly. In the terminology of the recursion method it is necessary to terminate the continued fraction \[18, 20, 24–28\].

If we were to calculate up to and including \( a_n \) and \( b_n \) and then simply set subsequent coefficients to zero then the Green’s function would have \( 2n \) poles along the real axis. The density of states would then correspond to a set of \( 2n \) delta functions. Integrated quantities such as the the densities \( n_{ij} \) and \( F_{ij} \) could depend strongly on \( n \), especially since only a few of the \( 2n \) delta functions would be within the relevant energy range within the BCS cut off, \( E_c \). In order to obtain accurate results it would be necessary to calculate a large number of exact levels, which would be expensive in terms of both computer time and memory.

As a more efficient alternative we choose to terminate the continued fraction using the extrapolation method, as used previously by Litak, Miller and Gyorffy \[20\]. We calculate the values for \( a_n \) and \( b_n \) exactly up to the first \( m \) coefficients using the recursion method. Then, noting the fact that the elements of the matrices \( a_n \) and \( b_n \) vary in a predictable manner \[20\], we extrapolate the elements of the matrices for a further \( k \) iterations, where \( k \) is usually very much greater than \( m \). This enables us to compute the various densities of states, and the charge densities \( n_{ij} \) and \( F_{ij} \) accurately with relatively little computer time and memory.

In terms of the Green’s functions \( G_{\alpha \alpha'}(i, j, E) \) the pairing and normal Hartree-Fock potentials \( \Delta_{ij} \) and \( \frac{1}{2}U_{ij}n_{ij} \) are given by
\[ \Delta_{ij} = \frac{1}{2\pi} U_{ij} \int_{-E_c}^{E_c} \left( G_{-}(i, j, E + \eta) - G_{+}(i, j, E - \eta) \right) (1 - f(E)) dE \]  

(12)

and

\[ \frac{1}{2} U_{ij} n_{ij} = \frac{1}{2\pi} U_{ij} \int_{-E_c}^{E_c} \left( G_{++}(i, j, E + \eta) - G_{++}(i, j, E - \eta) \right) f(E) dE. \]  

(13)

where \( \eta \) is a small positive number.

To obtain the above equations we have used the fact that

\[
\begin{pmatrix}
  u^n_i \\
  v^n_i
\end{pmatrix}
\quad \text{and} \quad
\begin{pmatrix}
  -(v^n_i)^* \\
  (u^n_i)^*
\end{pmatrix}
\]

are the eigenvectors of equation (11) with eigenvalues \( E_n \) and \( -E_n \) has been used. Also note that the integrals in equations (12) and (13) are bounded by the cut-off \( E_c \), corresponding to the energy dependent interaction

\[ U_{ij}(E) = \begin{cases} 
-|U| & \text{for } |E - \mu| \leq E_c \\
0 & \text{for } |E - \mu| > E_c
\end{cases}, \]  

(15)

as in BCS theory. Our cut-off \( E_c \) can correspond to the BCS cut-off \( \hbar \omega_D \) arising from retardation of the electron-phonon interaction, or any other energy scale cut-off for the interaction which may be applicable for high temperature superconductors

C. Achieving Self-consistency.

Using the above methods to calculate \( \Delta_{ij} \) and \( U_{ij} n_{ij} \) we need to achieve a fully self-consistent solution. Firstly we make use of any symmetries in the system in order to minimise the number of calculations which are necessary. For example on an infinite square lattice with no variation in any of the potentials only one independent site needs to be calculated since this site can be mapped onto all of the other sites. Secondly, once we have decided which sites need to be calculated self-consistently \( \Delta_{ij} \) and \( n_{ij} \) can be calculated for those sites, remembering that on a square lattice each site will have four nearest neighbours. This implies that in general we will have to calculate equation nine different Green’s functions in
order to calculate $\Delta_{ij}$ and $n_{ij}$. This can be seen by considering site $i$ in figure 1 and noting that we need to calculate the Greens functions shown in table I, depending on whether the interaction is purely local, purely non-local, or both local and non-local. Having calculated the appropriate Green’s functions new values for $\Delta_{ij}$ and $n_{ij}$ can be calculated, which we will denote as $\Delta_{ij}^{(1)}$ and $n_{ij}^{(1)}$. Inserting these into the Hamiltonian and repeating the calculation of then Green’s functions leads to a new set $\Delta_{ij}^{(2)}$ and $n_{ij}^{(2)}$ and so on. We repeat this iteration for all $i$ and $j$ until

$$\left| \frac{|\Delta^{(n-1)}| - |\Delta^{(n)}|}{|\Delta^{(n)}|} \right| \leq 0.001$$

and

$$\left| \frac{|n^{(n-1)}| - |n^{(n)}|}{|n^{(n)}|} \right| \leq 0.001.$$  

Since $\Delta_{ij}$ and $n_{ij}$ can be complex we need to also check for convergence in their associated phases. We do this and find that convergence in the phase gradient of the complex parameters is much more rapid than the convergence in the magnitude.

### III. NUMERICAL RESULTS.

#### A. Uniform Systems.

As a first test of the above methods let us examine a bulk superconductor, corresponding to an infinite 2-d square lattice with either local or non-local attraction. These examples will show how well such quantities as the local particle density of states can be calculated and how the extrapolation of the elements of the matrices $a_n$ and $b_n$ is performed.

The quantity of interest is the local particle density of states, which can be calculated from the following expression

$$N_i(E) = \frac{1}{2\pi} (G_{++}(i, i, E + i\eta) - G_{++}(i, i, E - i\eta)).$$

Consider first a non-interacting system where $U_{ij} = 0$, $\mu = 0$, $\epsilon_i = 0$, and $t_{ij} = 1$ for nearest neighbours and zero everywhere else. Figure 2 shows the local particle density of
states for a calculation where the number of exact continued fraction levels was $m = 50$ and the elements of $a_n$ and $b_n$ were extrapolated for 2000 more values. For this calculation the convergence parameter $\eta$ was chosen as $\eta = 0.02$. Fig. 2 shows that using the extrapolation method the central logarithmic van Hove singularity and the sharp band edges can be resolved very well. Figure 3 shows the first 100 continued fraction coefficients $\Re b_{11}^n$, where the first 50 are calculated directly using the recursion method and the rest are the extrapolated values. It is clear from the figure that the oscillations in $\Re b_{11}^n$ still persist after the first 50 continued fraction levels. In fact these oscillations die off slowly as $1/n$ and it is critical to include them correctly. From figure 3 it is clear that the first 50 levels provide enough information about the decaying oscillation that the $\Re b_{11}^n$ can be extrapolated quite easily.

Having considered a system where the interaction is zero the next step is to consider systems where the interaction is uniform and finite. For such systems the local particle density of states can be calculated, for different types of interaction. In figure 4 we have plotted two different local particle densities of states for a local interaction $U_{ij} = -2.5\delta_{ij}$ (dashed line) and $U_{ij} = -2.5(1 - \delta_{ij})$ for nearest neighbours (solid line). In each case $E_c = 4$ and $t_{ij} = 1$ (for nearest neighbours) and all other parameters were set to zero throughout the lattice.

The dashed line in figure 4 clearly shows the energy gap at the Fermi energy, characteristic of $s$-wave superconductivity. The van Hove peak in the density of states is also very clearly resolved. The solid line in Fig. 4 shows the local particle density of states going to zero at the Fermi energy, in a manner which is typical of the local particle density of states for a $d$-wave superconductor. In this case of the non-local interaction the order parameter changes sign we as rotate by $\pi/2$ around a site, ie. in reference to figure 1 $\Delta_{ij1} = -\Delta_{ij2}$, $\Delta_{ij2} = -\Delta_{ij3}$ and $\Delta_{ij4} = -\Delta_{ij3}$. The way we have performed the calculation is to keep the Fermi energies the same in the two calculations but change, in the case of the local interaction (dashed line), the density and, in the case of the non-local interaction (solid line), the width of the band self-consistently. This has the effect of moving the system away from half filling in the case of the local interaction, and, broadening the band in the case of the non-local interaction,
because of the local and non-local Hartree-Fock terms in the Hamiltonian $U_{ii}n_{ii}$ and $U_{ij}n_{ij}$ respectively.

At this point one should note that in the case of a non-local interaction one can as well as having a $d$-wave self-consistent solution to the Bogoliubov de Gennes equation, it is also possible to obtain an extended $s$-wave solution, i.e. $\Delta_{ij_1} = \Delta_{ij_2}$, $\Delta_{ij_3} = \Delta_{ij_4}$ and $\Delta_{ij_4} = \Delta_{ij_3}$. However we find that such solutions are less stable than the $d$-wave solutions, this is only true at or near half filling of the band.

To obtain the results shown in figure 4 we have again calculated 50 levels of the recursion method exactly and then extrapolated for further 2000 levels. This can easily be done because the elements of $a_n$ and $b_n$ vary in a predictable manner, as has already been seen for the case without interactions.

**B. Interfaces.**

Having considered systems where the interactions remain uniform throughout the structure the next step is to consider systems which contain interaction strengths which vary in real space. The most simple case one can conceive for this scenario is an interface. We will simply model the interface by allowing the interaction to change in a step like manner.

We will consider three separate situations, $N - S^s$, $S^d - N$ and $S^d - S^s$. In the normal region we shall set $U_{ij} = 0$, hence the order parameter in this region will be zero, (but one should note that this does not imply that $F_{ij}$ is zero). Before we look at the numerical results it is worthwhile considering what one may expect to find. In the case of a local interaction the results are well documented, i.e. the magnitude of the superconducting order parameter reaches a maximum at the bulk value a few coherence lengths in the superconducting region away from the normal interface. In the case of the non-local interaction we would also expect the amplitude of the superconducting order parameter to reach a maximum several coherence lengths away from the interface, but the problem of how to define the magnitude of the superconducting order parameter now arises. Going back to figure 1 we can see that
for each site $i$ there are five $\Delta_{ij}$’s, so hence for each site we can define five order parameters per site. We can also combine these different order parameters on each site in the following manner

\[ |\Delta_i^{(s_{local})}| = |\Delta_i| \quad (19) \]

\[ |\Delta_i^{(d)}| = \frac{1}{4}|\Delta_{ij_1} - \Delta_{ij_2} + \Delta_{ij_3} - \Delta_{ij_4}| \quad (20) \]

\[ |\Delta_i^{(s_{non-local})}| = \frac{1}{4}|\Delta_{ij_1} + \Delta_{ij_2} + \Delta_{ij_3} + \Delta_{ij_4}| \quad (21) \]

so that each equation defines a different type of symmetry for that site. Since the systems we are interested in change in the $x$-direction only it is possible, when one is considering the properties of that interface, to look along one line of sites in the $x$-direction and note that for any other $y$ coordinate the properties of the system are the same, so $\Delta_i \rightarrow \Delta(x)$.

Having defined all the quantities of interest the next step is to specify some of the systems of interest. The three systems we are going to consider are as already pointed out $N - S^s$, $S^d - N$ and $S^d - S^s$, to set up these systems we used the parameters shown in table II.

Figures 5(a-c) plot the three main symmetry components of the order parameter $|\Delta^{(s_{local})}(x)|$ (dashed line), $|\Delta^{(d)}(x)|$ (circles) and $|\Delta^{(s_{non-local})}(x)|$ (solid line) for the three different geometries $N - S^s$ (figure 5(a)), $S^d - N$ (figure 5(b)) and $S^d - S^s$ (figure 5(c)). The interface corresponds to $x = 100$ on the figures. Figure 5(a) shows, as expected, that the $s$-wave order parameter, $|\Delta^{(s_{local})}(x)|$, simply rises over a coherence length to a maximum at the bulk superconducting order parameter. Because the interaction is purely on-site in Fig. 5(a) $|\Delta^{(d)}(x)| = |\Delta^{(s_{non-local})}(x)| = 0$.

In figure 5(b) we see that for the $d$-wave to normal metal interface $|\Delta^{(d)}(x)|$ also drops to zero at the interface. However, unlike the $s$-wave case, it does not simply drop to zero smoothly but has a sharp peak structure right at the interface. The origin of this peak is explained by looking at the extended $s$-wave component, $|\Delta^{(s_{non-local})}(x)|$ (solid line in Fig. 5(b)). We see that the extended $s$-wave gap function is finite near the interface. This is due to
The fact that the order parameter varies near the interface and hence $\Delta_{j_1}(x) \neq \Delta_{j_3}(x)$, making the values of $|\Delta^{(s(\text{non-local}))}(x)|$. This is emphasised in figure 5(d) where $\Delta_{j_3}(x) - \Delta_{j_1}(x)$ is plotted, from this graph one can see that the peak in $|\Delta^{(d)}(x)|$, in figure 5(b), near the interface is due to the component in the the $x$ direction.

Figure 5(c) shows the $d$-wave to $s$-wave superconductor interface. Again we can see that the extended $s$-wave component $|\Delta^{(s(\text{non-local}))}(x)|$ is non-zero at the interface, even though it is zero in the bulk on both sides, and that this leads to sharp features in both the local $s$-wave and $d$-wave order parameters near the interface.

Having seen how the profiles of the superconducting order parameters are affected by the proximity of different materials, we now look at how the local particle density of states changes as we move across the various interfaces. Figures 6, 7 and 8 are contour plots of the local particle densities of states for the three interfaces of interest. Figure 6 shows a contour plot for the $N - S^s$ interface. Looking at this plot one can see that as we move across the interface, at $x = 100$, the superconducting gap opens up within a couple of atomic sites. On the normal metal side, for $x < 100$, the van Hove singularity in the centre of the band can be clearly seen, but as we move into the superconducting region the band edges are shifted (due to the Hartree-Fock potential term) and the superconducting gap opens up at $E = 0$. In the superconducting region the van-Hove singularity is shifted away from $E = 0$ as can also be seen in figure 3 (dashed line). Due to the mismatch in the band edges we see oscillations in the local particle density of states near the band edges; these are simply Friedel oscillations.

Figure 7 shows a similar contour plot of the local particle density of states for an $S^d - N$ interface. Again we can clearly see the gap in the superconducting region and the van Hove singularity in the normal region. In this system the Hartree-Fock potential term leads to an increase in overall band width on the d-wave side. Again since the band edges do not match up we see Friedel oscillations in the local particle density of states near the band edges.

Finally in figure 8 we have plotted the local particle density of states as we move across the $S^d - S^s$ interface. This plot has many interesting features, the first to note is that again
due to the mismatch in the band edges oscillations appear in the local particle density of states. Secondly for $x < 100$ ($S_d$ region) the density of states gradually goes to zero at $E = 0$ (typical of d-wave superconductivity (see figure 4 (solid line))). Whereas for the $S^s$ region the local particle density of states drops to zero very sharply. The main points of interest is what happens at the interface itself. In plane of the interface there are states in the gap, as both the d-wave and s-wave order parameters are suppressed. At $x = 100$ there are two peaks in the density of states just above and below $E = 0$, which as we move further into the $S^s$ region are shifted to become the BCS density of states singularities just above and below the superconducting gap. Note that the parameters for the calculation in Fig. 8 were chosen so that $|\Delta^{(d)}| >> |\Delta^{s(\text{local})}|$ as would be the case for a YBCO-Pb junction such as those used by Wollman et al. [1].

IV. CONCLUSIONS.

In this paper we have shown how it is possible to perform self-consistent calculations of the Bogoliubov de Gennes equation, using the recursion method. This method has the advantage of being an order $N$ method and hence allows us to tackle problems with a relatively small amount of computational effort. A key to obtaining accurate densities of states with relatively little computational effort is the extrapolation procedure we have used to terminate the matrix continued fraction. Our method is fully self-consistent, including both self-consistency in the order parameter and in the normal Hartree-Fock potentials. As we have shown these normal potentials make significant contributions by shifting or widening the density of states in a spatially dependent manner. Our method can deal with both local attractive interactions, corresponding to local s-wave superconductivity, or non-local interactions corresponding to d-wave or extended s-wave pairing. In our system we found that the d-wave is more stable.

As a first application of the method we examined three simple interfaces, corresponding to an s-wave $S-N$ junction, a d-wave $S-N$ junction and an s-wave to d-wave $S-S$
juncture. The numerical results show a number of interesting features, including a non-monotonic variation of the order parameters near the interface, a surface layer of extended s-wave pairing (even though it is not stable in the bulk), and subtle effects of the self-consistent Hatree-Fock terms in the Bogoliubov de Gennes Hamiltonian leading to Friedel oscillations and spatially dependent shifts in the van Hove singularities near the interfaces, as highlighted by the contour plot in figure 8.

In future we hope to apply our method to more complex interfacial phenomena in superconductors, such as junctions carrying supercurrent (e.g. to look for \( \pi \)-junctions), superconducting twin boundaries and grain boundary junctions. Our methods can also be applied to many other problems in superconductivity such as the structure of vortex cores in s or d-wave superconductors, the effects of impurities and so on.

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FIGURES

FIG. 1. This is a schematic diagram of a tight binding lattice, with particle and hole degrees of freedom, $\Delta_{ij}$ couples particles on site $i$ to holes on site $j$. The difference between local and non-local pairing is highlighted by the dashed (local pairing) and solid (non-local pairing) lines.

FIG. 2. The local particle density of states for a 2-D tight binding lattice with no interactions ($U_{ij} = 0$). For this system $t_{ij} = 1$ for nearest neighbours only, $\mu = 0$ and $\epsilon_i = 0$.

FIG. 3. A plot of the real part of $b(n)^{11}$ for the same system which was used to calculate the local particle density of states in figure 2.

FIG. 4. Two plots of the local particle density of states for, a local interaction ($U_{ij}\delta_{ij} = -2.5, U_{ij}(1 - \delta_{ij}) = 0$ (dashed line)) and a non-local interaction ($U_{ij}\delta_{ij} = 0, U_{ij}(1 - \delta_{ij}) = -2.5$ (solid line)), all the other parameters are equal to those used to obtain figure 2.

FIG. 5. Figures 5(a-c) plot the profiles of different symmetries of the superconducting order parameter ($|\Delta^{(s(non-local))}(x)|$ (solid line), $|\Delta^{(s(local))}(x)|$ (dashed line) and $|\Delta^{(d)}(x)|$ (circles)) for different interfaces. Figures 5(a), (b) and (c) are for $N - S^s$, $S^d - N$ and $S^d - S^s$ interfaces respectively. Figure 5(d) plots $\Delta_{j1}(x) - \Delta_{j3}(x)$ for the $N - S^d$ interface. The parameters used to obtain the figures are given in table II.

FIG. 6. This is a contour plot of the local particle density of states as a function of position, as one move across the $N - S^s$ interface. The steps in the contour plot are in units of 0.4, ie. white represents $N(E) < 0.4$ and black represents $N(E) > 0.32$. The parameters used to obtain this graph are given in table II.

FIG. 7. This is a contour plot of the local particle density of states as a function of position, as one move across the $S^d - N$ interface. The steps in the contour plot are in units of 0.4, ie. white represents $N(E) < 0.4$ and black represents $N(E) > 0.32$. The parameters used to obtain this graph are given in table II.
FIG. 8. This is a contour plot of the local particle density of states as a function of position, as one move across the $S^d - S^s$ interface. The steps in the contour plot are in units of 0.4, i.e. white represents $N(E) < 0.4$ and black represents $N(E) > 0.32$. The parameters used to obtain this graph are given in table II.
TABLES

| Interaction Type | $G_{+-}(i, i, E)$ | $G_{++}(i, j_1, E)$ | $G_{+-}(i, j_2, E)$ | $G_{++}(i, j_3, E)$ | $G_{++}(i, j_4, E)$ |
|------------------|-------------------|---------------------|---------------------|---------------------|---------------------|
| $U_{ii}$         | Y                 | N                   | N                   | N                   | N                   |
| $U_{ij}(1 - \delta_{ij})$ | N                 | Y                   | Y                   | Y                   | Y                   |
| $U_{ii} + U_{ij}(1 - \delta_{ij})$ | Y                 | Y                   | Y                   | Y                   | Y                   |

TABLE I. This table shows which Greens functions need to be calculated for systems with interactions which are local, $U_{ii}$, non-local, $U_{ij}(1 - \delta - ij)$, or both. The site labels correspond to the notation of Fig. 1.

| System          | $x < 100$ | $x \geq 100$ | $E_c$ | $x < 100$ | $x \geq 100$ | $E_c$ |
|-----------------|-----------|--------------|-------|-----------|--------------|-------|
| $N - S^s$       | 0         | 0            | 0     | -2.5      | 0            | 4.0   |
| $S^d - N$       | 0         | -3.5         | 4.0   | 0         | 0            | 0     |
| $S^d - S^s$     | 0         | -3.5         | 4.0   | -2.5      | 0            | 4.0   |

TABLE II. This table defines how the interactions vary in real space for the three different interfaces. All energies are given in units where the nearest neighbour hopping $t_{ij} = 1$. Also $\mu = 0$ everywhere and $T = 0.01$. 
