HIGHLIGHT OF THE MONTH

THE BOGOLIUBOV - DE GENNES (BDG) EQUATIONS FOR SUPERCONDUCTORS : WHY AND HOW WE SOLVE THEM.

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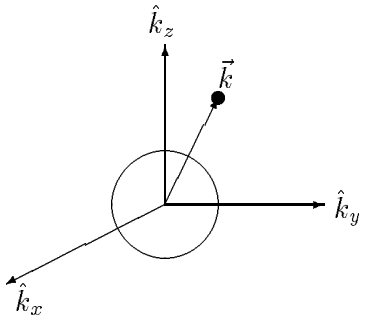
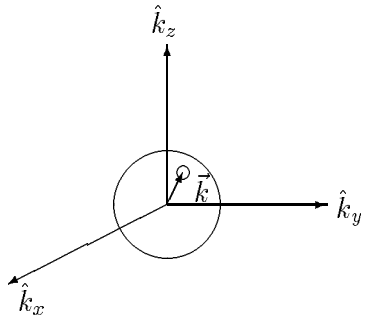
1 The Quasi-Particle Spectrum of Superconductors.

In the NORMAL STATE, the elementary excitations of a non interacting, degenerate Fermi system with a uniform background, are particles in the one particle plane wave states $|\vec{k}>$ for $|\vec{k}| > k_F$ and holes in the state $|\vec{k}>$ for $|\vec{k}| < k_F$ as shown below:





particle

$$\begin{aligned} \epsilon^p_{\vec{k}} &= E_0(N) + \varepsilon_{\vec{k}} - E_0(N+1) \\ &= \varepsilon_{\vec{k}} - \left(\frac{\partial E_0}{\partial N}\right)_N = \varepsilon_{\vec{k}} - \mu \end{aligned}$$

hole

$$\begin{aligned} \epsilon^h_{\vec{k}} &= E_0(N) - \varepsilon_{\vec{k}} - E_0(N-1) \\ &= -\varepsilon_{\vec{k}} + \left(\frac{\partial E_0}{\partial N}\right)_N = -\varepsilon_{\vec{k}} + \mu \end{aligned} \qquad (1)$$

where μ is the chemical potential.

Thus if we describe the particles by the wave function $u_{\vec{k}}(\vec{r})$ and the holes by $v_{\vec{k}}(\vec{r})$, we may say that the quasi-particle spectrum is given by the solutions of the following two component equations:

$$\begin{pmatrix} \epsilon + \mu - H_0 & 0 \\ 0 & \epsilon - \mu + H_0 \end{pmatrix} \begin{pmatrix} u_{\vec{k}}(\vec{r}) \\ v_{\vec{k}}(\vec{r}) \end{pmatrix} = 0 \qquad (2)$$

where $v_{\vec{k}}(\vec{r}) = 0$ for $|\vec{k}| > k_F$ and $u_{\vec{k}}(\vec{r}) = 0$ for $|\vec{k}| < k_F$, H_0 is the Hamiltonian for the non-interacting electrons and $\mu = \varepsilon_F$ is the Fermi energy.

In the SUPERCONDUCTING STATE an excitation will have both particle and hole amplitudes and the above equation generalizes to

$$\begin{pmatrix} \epsilon + \mu - H_0 & -\Delta(\vec{r}) \\ -\Delta^*(\vec{r}) & \epsilon - \mu + H_0 \end{pmatrix} \begin{pmatrix} u_{\vec{k}}(\vec{r}) \\ v_{\vec{k}}(\vec{r}) \end{pmatrix} = 0 \qquad (3)$$

where $\Delta(\vec{r})$ is the pairing potential. This is a fairly general form of the BdG equation [2] and as such it is the principle subject of this note.

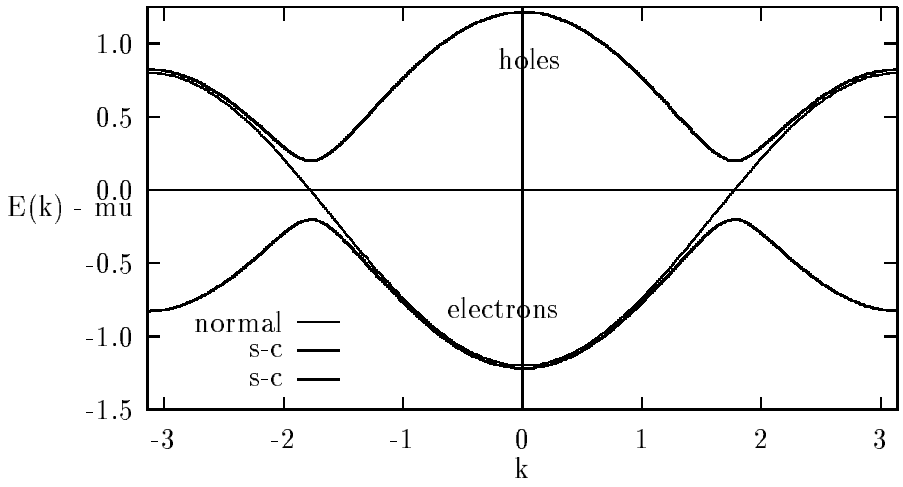


Figure 1: Normal, tight-binding band (continuous line) gapped by a pair potential, Δ (dashed lines).

In the Bardeen Cooper Schrieffer (BCS) theory the pairing potential is proportional to the pairing amplitude, $\langle \Psi_\uparrow(\vec{r})\Psi_\downarrow(\vec{r})\rangle$, an anomalous average which is zero in the normal state. It works out to be

$$\begin{aligned} \Delta(\vec{r}) &= -\lambda \langle \Psi_\uparrow(\vec{r})\Psi_\downarrow(\vec{r})\rangle \\ &= \sum_n u_n(\vec{r})v_n(\vec{r})\left[1-2f(E_n)\right] \end{aligned} \tag{4}$$

where λ is the strength of the model electron-electron potential : $V^p(\vec{r}-\vec{r'})$, which is attractive for $\lambda > 0$, $\begin{pmatrix} u_n(\vec{r}) \\ v_n(\vec{r}) \end{pmatrix}$ is an eigensolution of the BdG equation in Eq. 3 corresponding to the quasi-particle energy eigenvalue E_n and $f(E)$ is the usual Fermi function. It should be stressed that Eq. 3 is to be solved self-consistently using Eq. 4 in each iteration.

If we assume that Δ is a constant, Eq. 3 leads to the well known BCS-formula

$$E_{\vec{k}} = \sqrt{\left(\varepsilon_{\vec{k}} - \mu\right)^2 + \Delta^2} \tag{5}$$

where $\varepsilon_{\vec{k}}$ is the dispersion relation, corresponding to H_0, in the normal state. This is displayed in Fig. 1.

What lends particular significance to the BdG equation in Eq. 3 is that it holds much more generally than the above simple BCS model implies. Indeed the recently formulated Density Functional Theory for superconductors [3] yields an Euler-Lagrange (Kohn-Sham) equation which is precisely of this form. Moreover, as is usual in density functional theories, it supplies exact recipes for calculating the effective one electron potential in H_0 and the pairing potential, $V^p(\vec{r},\vec{r'})$. When these are approximated, in an LDA-like fashion for instance [4], the way is open to calculations of the ground state energy or ground potential as well as the quasi-particle spectrum in the superconducting states on a first principles basis.

Whilst from the point of view of our present concern the above generalization is decisive, it is relevant to note that the BdG equations are also studied in Nuclear Physics [1] and Astrophysics [5].

In summary, the BdG equations are of general significance in describing degenerate Fermi systems with anomalous pairing amplitudes like $\chi(\vec{r},\vec{r'})$. Since their structure is rather similar to those usually studied in calculation of the electronic structure of the normal state it is natural to deploy the powerful methods of 'band theory' for solving them. In what follows we shall describe some interesting examples of doing that. As it turns out these examples are the principle activities of Working Group Va in the Ψ_k-Network.

2 Density Functional Theory for Superconductors

For conventional superconductors the coherence length, $\xi_0 = \frac{\hbar v_F}{\pi\Delta}$, is large ($\approx 1000$Å) and therefore, $\Delta(\vec{r}) = \Delta$ a constant, is a good approximation. Consequently Eq. 5 describes well the quasi-particle spectra and it is sufficient to calculate $\varepsilon_{\vec{k},\nu}$, the normal state electronic structures. Indeed, when energies are rescaled by Δ and distances by ξ_0, the superconducting properties of most superconductors appear to be very similar. By contrast the new so-called 'high T_c' superconductors have short coherence length, $\xi_0 \approx 10 - 30\mathring{A}$, and their superconducting properties appear to be as varied among materials as the magnetic properties of itinerant magnets. Thus, in this case we may expect that first principles calculation may play an important role. In particular, since now $\Delta(\vec{r})$ will depend on $\vec{r}$, the quasi-particle spectra which has the general form

$$E_{\vec{k},\nu} = \sqrt{\left(\varepsilon_{\vec{k},\nu} - \mu\right)^2 + \left|\Delta_{\vec{k},\nu}\right|^2} \tag{6}$$

contains the 'gap' function, $\Delta_{\vec{k},\nu}$, as a new $\vec{k}$-dependent superconducting property. (Note that it is not the Fourier transform of $\Delta(\vec{r})$). The point is that, at least in principle, this most interesting quantity can be measured in angle-resolved photoemission [6], quantum oscillation [7] and neutron scattering experiments [8] and hence its study could provide the much needed differentiation between contending models.

Another novel feature of superconductors with small coherence length, like the superconducting cuprates, is that Δ may be different on inequivalent sites. This would show up in NMR experiments [9] and would be a natural consequence of a first-principles calculations.

The structure of the above density functional theory is very similar to that of Spin Density Functional Theory with the pairing amplitude $\chi(\vec{r})$ playing the role of the magnetization $m(\vec{r})$. Indeed, the Kohn-Sham equations of this theory for the two component wave-function $\begin{pmatrix} \Psi_\uparrow(\vec{r}) \\ \Psi_\downarrow(\vec{r}) \end{pmatrix}$ are very similar to the BdG equations given by Eq. 3 both in mathematical form and self-consistency logic. Thus the computational techniques necessary for solving the former can be expected to be a generalized version of 'spin-polarized band theory'.

Evidently, to get started we need a recipe, analogous to LSDA for an effective potential functional $V_{eff}\,(\vec{r},[n,\chi])$, to be used in H_0 of Eq. 3 and a pairing functional $V_p\left(\vec{r},\vec{r'};[n,\chi]\right)$. For the former we use the usual LDA and for the latter we take the following BCS-like form [4] :

$$V_p\left(\vec{r},\vec{r'};[n,\chi]\right) \equiv \frac{\delta E_{xc}[n,\chi]}{\delta\chi(\vec{r},\vec{r'})} = \lambda_i\delta(\vec{r}-\vec{r'}) \tag{7}$$

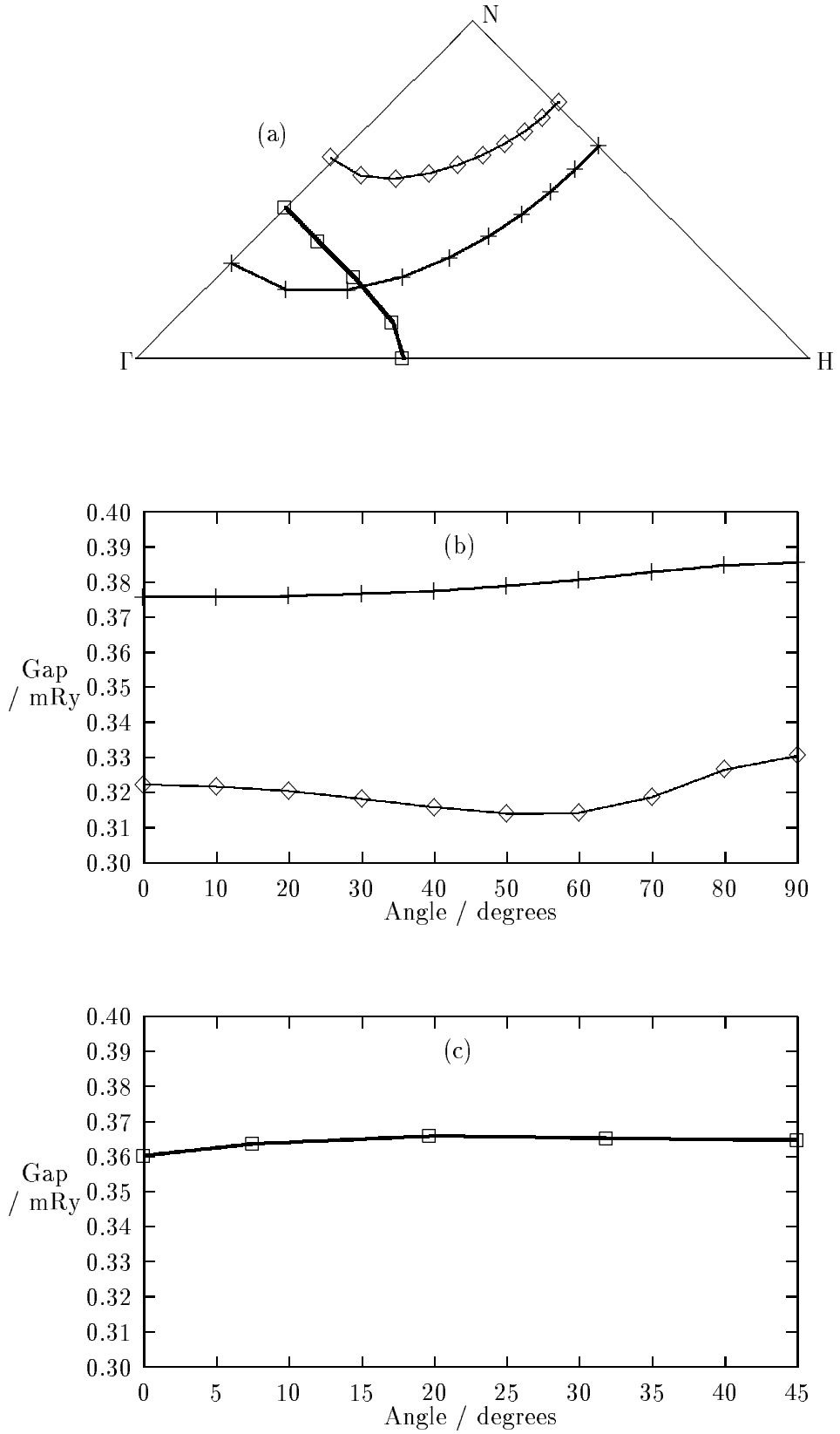


Figure 2: (a) Positions of sheets of Fermi surface in Nb, and (b), (c) the respective gaps for the directions indicated in (a). For (b) 0^o indicates the Γ-N line, while 90^o is on the N-H line. For (c) 0^o indicates the Γ-N line, while 45^o is on the Γ-H line.

where $\vec{r}$ and $\vec{r'}$ are within the muffin-tin well surrounding the i-th inequivalent site. Presently, we take the parameters λ_1, λ_2, *etc.*, one for each inequivalent site, as phenomenological parameters to be determined by requiring that some calculated properties like T_c, *etc.* agree with experiments. As was argued in the paper by Suvasini et al. [4] this semi-phenomenological, yet first principles, approach can be useful if there is a rich structure in $\Delta_{\vec{k},\nu}$ and only a few coupling constants, λ_1, λ_2, *etc.*, are needed.

The above strategy was fully implemented by Suvasini et al. [4] for Nb using the LMTO method. As an illustration of the results we show $\Delta_{\vec{k},\nu}$ on three sheets of the Fermi surface in Fig. 2. Since the coherence length of Nb is large ($\xi_0 \approx 1000\mathring{A}$) and hence Eq. 7 is not likely to be a good approximation, this example is only of computational interest. The code is now in the process of being scaled up to the HTC cuprates (YBCO *etc.*). The motivation behind such calculations is the hope that $\lambda_{Cu} \neq 0$, $\lambda_O = 0$ and $\lambda_{Cu} = 0$, $\lambda_O \neq 0$ in the CuO_2 planes will give sufficiently different quasi-particle spectra to enable us to identify which of the two configurations are favoured by experiments. Moreover, recently we began to experiment with finite range pairing potentials which are attracting for electrons on different sites. These have interestingly dramatic effects on the quasi-particle spectra [14]. Clearly, the novelty of this work is the fact that a very simple phenomenological pairing interaction, of unknown origin, is treated in the context of a realistic complex band structure. Viewed in this light this approach is very similar in spirit to the X_α method of Slater before the invention of proper density functional theory. Hopefully, some later time, we shall have a parameter-free local density approximation for the exchange-correlation energy functional $E_{xc}[n, \chi]$ in the superconducting phase. Thanks to our current work the numerical technique to exploit such circumstance will be available.

3 The Quasi-Particle Spectrum of the Abrikosov Flux Lattice

Type-II superconductors in magnetic fields $H > H_{c1}$ - the lower critical field - do not expel all external flux completely, but allow it to pass through in units of the flux quanta, $\Phi_0 = \frac{h}{2e}$. This is illustrated in Fig. 3. Where the flux is admitted the order parameter, $\Delta(\vec{r})$, drops to zero and the magnetic field reaches its external value. Such a configuration is called a vortex and, as was discovered theoretically by Abrikosov, these vortices form a two dimensional, usually triangular, lattice frequently referred to as the Abrikosov flux lattice [10]. His and almost all subsequent work on the subject was based on the phenomenological Ginzburg-Landau theory which describes the spatial variation of the order parameter $\Delta(\vec{r})$, or, to put it another way, the condensate of the Cooper pairs, but not the quasi-particle excitations of the superconducting ground state. The latter are described only by the fully microscopic BdG equations in a magnetic field. In this section we shall be concerned with the solutions of these.

Whilst such a fully microscopic theory of the flux state is clearly desirable in its own right, the recent discovery of de Haas-van Alphen oscillations [8] in the superconducting state makes this problem one of the burning issues of solid-state physics. Briefly, on the one hand even the precise mechanism of these oscillations is highly controversial, on the other, one would expect that seeing de Haas-van Alphen oscillations in the high $T_c$superconductors would prove that their normal state

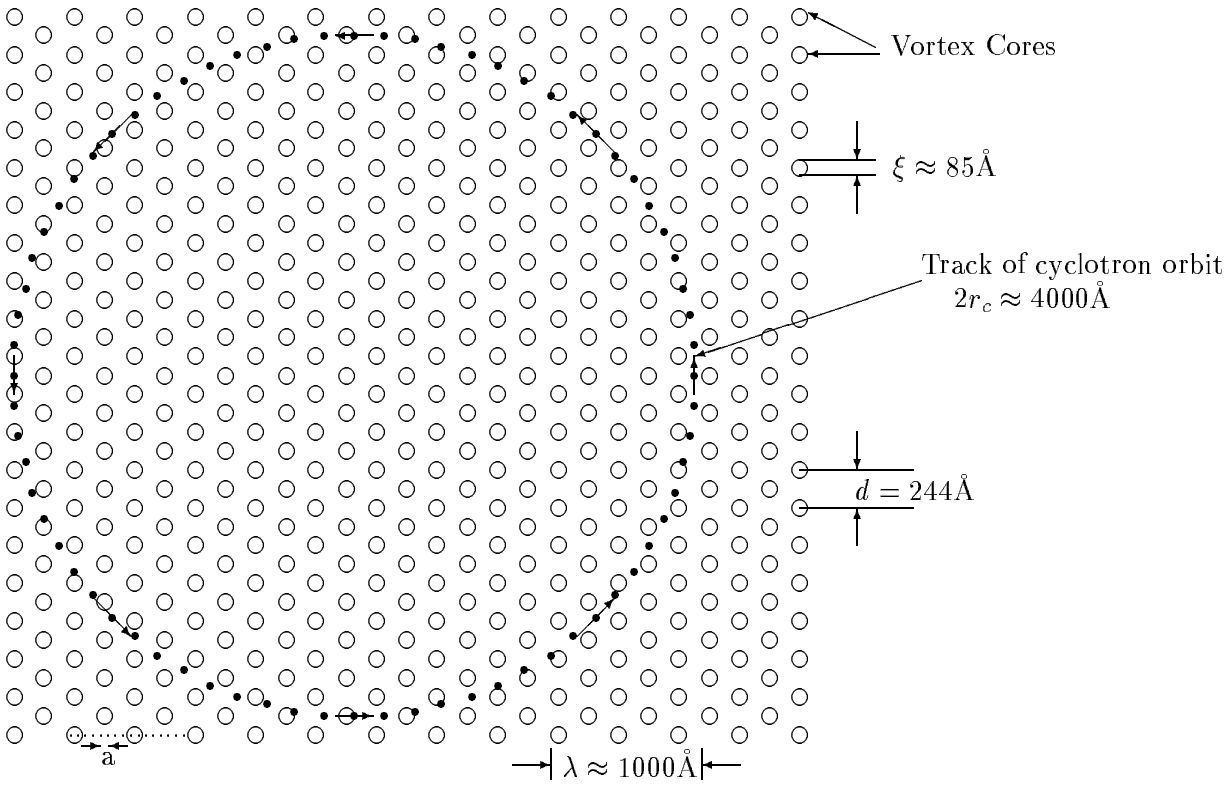


Figure 3: The various length scales for a field of 8 Tesla in $NbSe_2$

is a Fermi Liquid (since H_{c2} is several 100 Tesla and $T_c \approx 100K$, the only hope of seeing the de Haas-van Alphen effect in these materials is in the superconducting state) and their observation in the Heavy Fermion Superconductors like UPt_3 could be the 'smoking gun' experiment for exotic (p- or d-wave) pairing. To appreciate the difficulty of the problem at hand we illustrate the four different length scale on which we must do justice to the complexity of the electronic motion in Fig. 3.

They are the lattice parameter, a, the lattice parameter of the flux lattice, d, the size of the vortex cores, ξ_0 and the radius, r_c of the Landau orbits which, at least in the normal state, govern the dHvA oscillations. Note also that there are two separate flux quantizations in this problem: one is to do with the motion of the Cooper pairs and gives rise to the flux quanta, each Φ_0, piercing the superconductors at the vortices. The other is associated with the motion of individual electrons or quasi-particles, in Landau orbits which encircle integer multiples of the flux unit, $\frac{h}{e}(= 2\Phi_0)$.

Given the above complicated but interesting circumstances, an effective strategy is to take a simple model which contains all the principle ingredients of the physics and solve it exactly. In the present case such a model is a single band, tight-binding Bogoliubov-de Gennes equation with a magnetic field.

This may be written as follows :

$$\sum_j \begin{pmatrix} \left(\epsilon_0 + \frac{Un_i}{2} - \mu\right)\delta_{ij} + t_{ij} & \Delta_i\delta_{ij} \\ \Delta_i^*\delta_{ij} & -\left(\epsilon_0 + \frac{Un_i}{2} - \mu\right)\delta_{ij} - t_{ij}^* \end{pmatrix} \begin{pmatrix} u_j \\ v_j \end{pmatrix} = E \begin{pmatrix} u_i \\ v_i \end{pmatrix} \tag{8}$$

where the hopping amplitude, t_{ij}, is given in terms of the vector potential, $\vec{A}(\vec{r})$, by

$$t_{ij} = -t \exp\left\{-i\frac{e}{\hbar}\int_{\vec{R}_i}^{\vec{R}_j} \vec{A}(\vec{r})\cdot d\vec{r}\right\} \qquad \text{for } i \text{ and } j \text{ nearest neighbours,} \tag{9}$$

$$= 0 \qquad \text{otherwise} \tag{10}$$

ϵ_0 is the site energy, n_i is the charge density and Δ_i the pairing potential at the site i, and U is the electron-electron coupling constant in the negative-U Hubbard model, from which the above equation has been derived. As usual in electronic structure problems, Eq. 8 has to be solved self-consistently. Namely, for a set of $\{n_i, t_{ij}, \Delta_i\}$ one solves for $\{u_i, v_i\}$ and recalculates n_i , t_{ij} and Δ_i, using standard formulae (not given here) repeating this procedure until convergence. The most novel feature of such a calculation is the need to re-compute the hopping integral, t_{ij}, at each iteration. This involves finding the current, I_{ij}, on all the links $(i-j)$ and solving Ampères law for flux through each plaquette and the vector potential. In other words we are solving not only the usual electrostatic, but also the magnetostatic Maxwell equations self-consistently with the Many-Body Schrödinger's equation.

If the external magnetic field is such that the flux per plaquette is not a rational number times Φ_0, there is no lattice periodicity left in the above problem. This suggests that in solving it we throw out $\vec{k}$-space [11] altogether and solve the problem entirely in real space, by adopting the Recursion Method of Haydock and others [12] to deal with it. This turns out to be a very efficient procedure.

In the normal state $\Delta_i = 0$ and the energy eigenvalues of Eq. 8 are that of the celebrated Azbel'-Hofstadter spectra displayed in Fig. 4. Our real-space, Recursion-Method, solution for the local density of states $N_0(\varepsilon)$ at the centre of our coordinate system is shown in Fig. 5. Evidently the presence of the magnetic field has broken up the zero-field, square lattice band into sharp states. These are the tight-binding analogues of the Landau levels in the free electron (no periodic potential) limit. This is particularly clear near the band edges where the peak separations are quite uniform and are close to $\hbar\omega_c$ $\left(\omega_c = \frac{eB}{m^*}\right)$. Note that in the zero field case, our real space calculation reproduces satisfactorily the sharp features of the density of states due to van Hove singularities of the $\vec{k}$-space band structure. To achieve such accuracy we had to go to 10^3-10^4 approximate levels in the continued fraction representation of local density of states.

To solve the fully self-consistent superconducting version of the above problem is a very much greater computational task. However, it follows the logic of a real space, order N, self-consistent Density-Functional Calculation and it is particularly susceptible to treatment by parallel algorithms. In fact solutions were found for flux lattice unit cells containing up to 900 real lattice sites, by using up to 136 nodes of the Oak Ridge National Laboratory Paragon machine. For particular, unphysically large but computationally very convenient fields the solutions were for smaller flux lattice cells, and the density of states shown in figure 6 is for a vortex cell consisting of 16 unit cells of real lattice. The attractive interaction energy, $-U$, was also chosen to be unreasonably large,

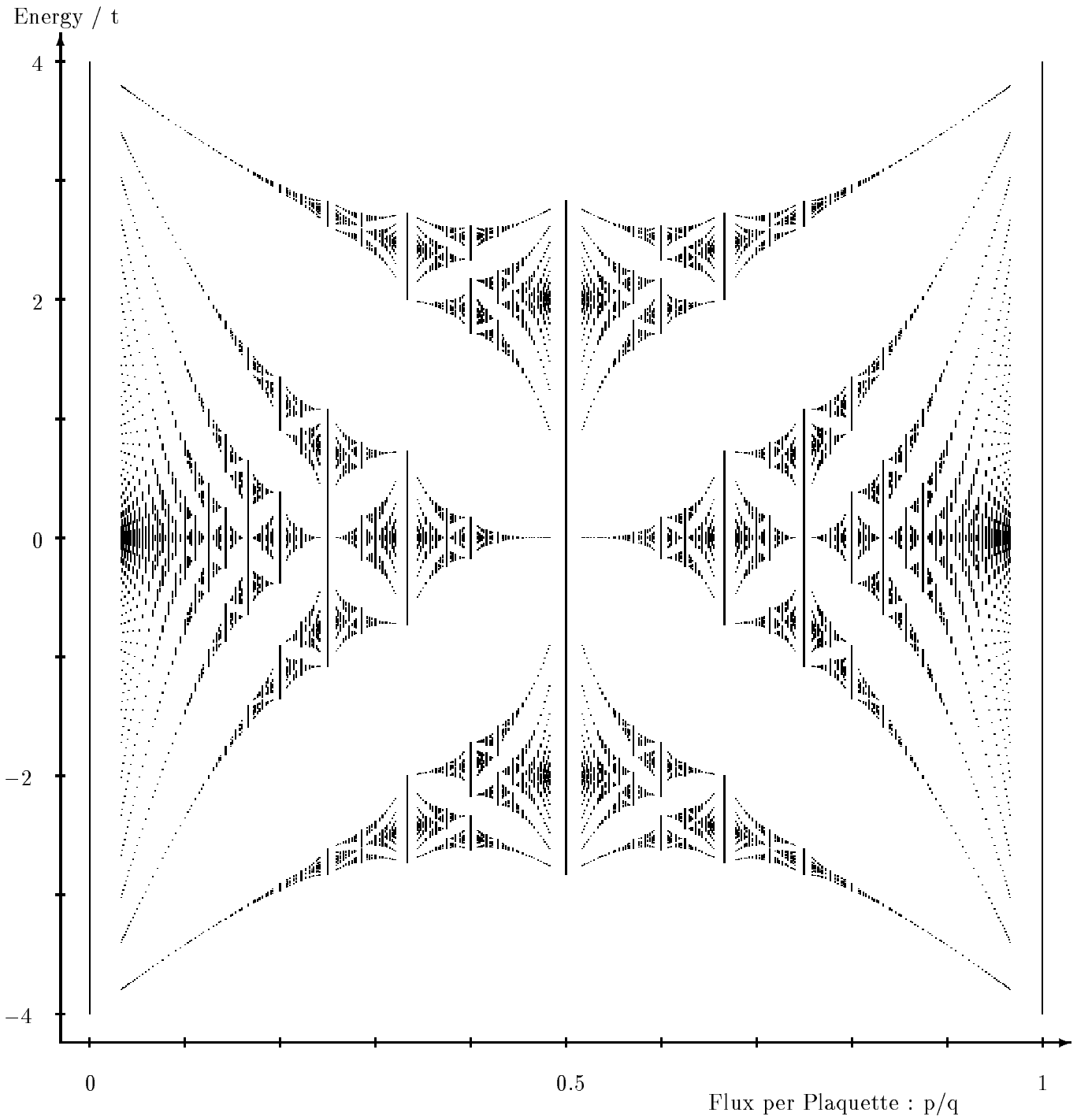


Figure 4: The Hofstatder Spectrum

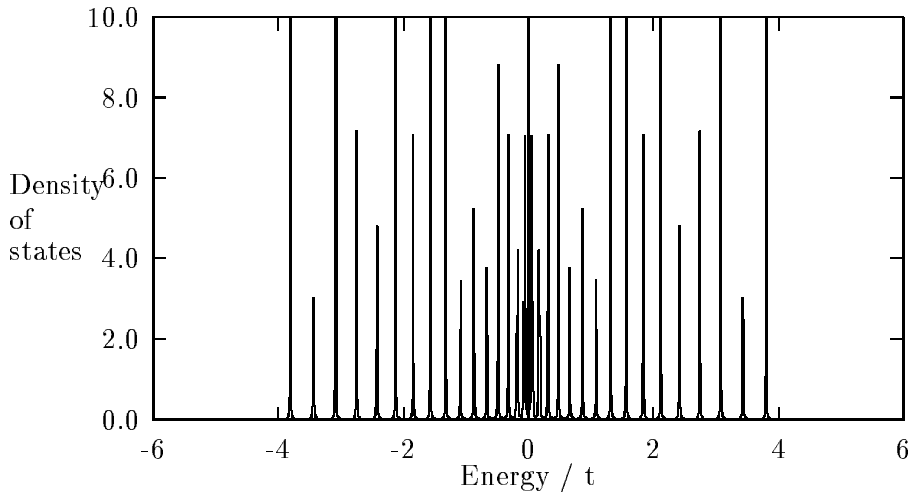


Figure 5: Normal state with a magnetic field, such that the flux per lattice plaquette, $Ba^2 = 1/32(h/e)$.

leading to a very large self-consistent order parameter, $\Delta(\vec{r})$, so that the coherence length, ξ_0, would be of the order a. The phase of the order parameter, $|\Delta_i|\, e^{i\theta_i}$ and the current vary cylindrically about the vortex core where the amplitude $|\Delta_i| = 0$. Away from the core, $|\Delta_i|$ recovers to more or less its value without the magnetic field in one step. In Fig.6 we show the quasi-particle density of states at such a healed lattice site (2,0) halfway between two vortex cores.

The quasi-particle local density of states, $N_{2,0}(\varepsilon)$ shown in Fig. 6 illustrates the central results of these calculations. Namely, as in the normal state the effect of a magnetic field in the superconducting state is that it breaks up the appropriate density of states into 'Landau level like' peaks. Of course these peaks are now pushed out from the gap region and squeezed together. The main point is that if a Landau level was below the Fermi energy, ε_F in the normal state it will be pushed down and will be found below the gap in the superconducting state. On the other hand if it was above ε_F, it will get pushed to energies above the gap as the system goes superconducting. Thus with increasing field there will be a steady migration of 'Landau levels' across the Fermi energy, ε_F, and the total energy will oscillate with changing $\frac{1}{B}$ as in the normal state. Naturally, the presence of the gap will change the phase and the amplitude of these oscillations, hopefully as observed in experiments, but the frequency remains the same.

Clearly, there is no hope of repeating the above calculation for such first principles Bogoliubov-de Gennes equation as we have discussed in Sec. 2. Yet if we are to interpret the very interested experimental data that is now beginning to be available we must make contact between them and quantitative calculations based on realistic models. To do this we retraced the history of the de Haas-van Alphen effect in the normal state during the late 50's and developed a semi-classical theory of the superconducting quasi-particle motion in a magnetic field.

In short, we took the solution of the Bogoliubov-de Gennes equation to be in the semi-classical

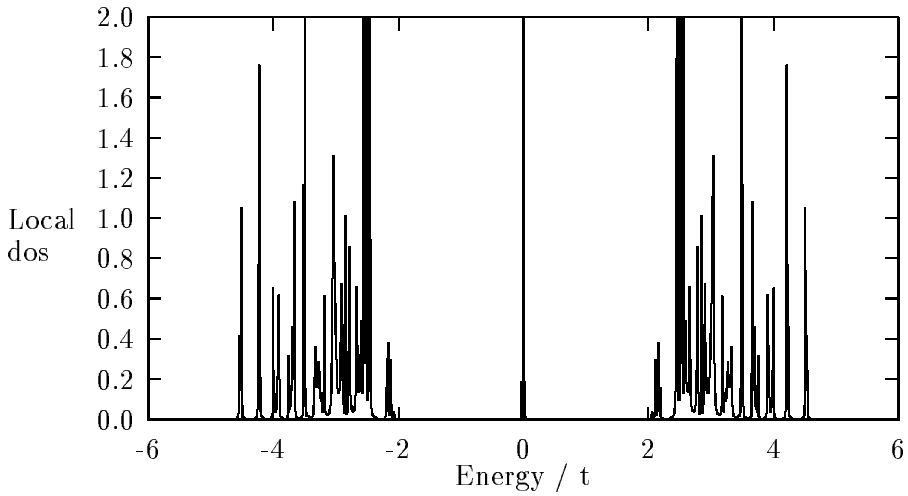


Figure 6: The local density of states on site (2,0) of a fully self-consistent solution with 16 lattice sites per vortex cell.

form

$$\begin{pmatrix} u(\vec{r}) \\ v(\vec{r}) \end{pmatrix} = \begin{pmatrix} u^0(\vec{r}) \\ v^0(\vec{r}) \end{pmatrix} \mathrm{e}^{\frac{i}{\hbar}\left[S(\vec{r})\underline{\underline{1}} + \Sigma(\vec{r})\underline{\underline{\tau}}_z\right]} \tag{11}$$

where u^0 and v^0 are slowly varying functions of $\vec{r}$, $\underline{\underline{1}}$ and $\underline{\underline{\tau}}_z$ are the unit matrix and z-component Pauli matrix respectively, and the phase functions, $S(\vec{r})$ and $\Sigma(\vec{r})$, are determined by the Bogoliubov-de Gennes equation to lowest order in $\hbar$. (To treat Eq. 8 we generalized the semi-classical theory of Wilkinson [5] for a tight binding model). An interesting novel feature of the theory is the presence of the two phase functions $S(\vec{r})$ and $\Sigma(\vec{r})$. They represent the sum and the difference phases of the two amplitudes, u and v, and give rise to the two, Landau and Abrikosov, flux quantizations.

As in the case of semi-classical theory for normal electrons, the Bohr-Sommerfeld quantization rules which follow from the requirement that $S(\vec{r})$ and $\Sigma(\vec{r})$ describe a single valued quasi-particle amplitude, $\underline{\Psi}(\vec{r}) = \begin{pmatrix} u(\vec{r}) \\ v(\vec{r} \end{pmatrix}$, determine the quasi-particle energies in terms of the band structure without the magnetic field. In the present, superconducting, case this is described by the normal state spectra $\varepsilon_{\vec{k},\nu}$ and the gap function $\Delta_{\vec{k},\nu}$, both of which we can aspire to calculate for a variety of pairing mechanisms.

The most remarkable upshot of this theory is that it relates the de Haas-van Alphen signal to extremal orbits on the Fermi Surface (in the normal state) and the average of the gap $\Delta_{\vec{k},\nu}$ over such orbits. This means that these experiments measure the gap average over selected portions of the Fermi Surface, namely the extremal orbits transverse to the external magnetic field. Given the track record of the de Haas-van Alphen measurements in providing detailed quantitative information about the shape and size of the normal state Fermi Surface, the above effect in the superconducting state can be expected to become a uniquely powerful probe of the superconducting gap's variation over the Fermi Surface. In particular, it is likely to be the 'smoking gun experiment' for detecting lines on the Fermi Surface along which $\Delta_{\vec{k},\nu} = 0$ and hence anisotropic superconductivity such

as expected in the high-T_c materials (d-wave pairing) and heavy fermion superconductors (UPt_3, UBe_{13} *etc.*).

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