The Bogoliubov–de Gennes and Andreev Equations: Andreev Reflection.

References: de Gennes ch. 5, Tinkham ch. 10 §1.

Consider the problem of a system described by a Hamiltonian of the generic form

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{1}$$

where $\hat{H}_0$ is a general single-particle Hamiltonian of the form

$$\hat{H}_0 = \sum_i \left[\frac{1}{2m}(\mathbf{p}_i - e\mathbf{A}(\mathbf{r}_i))^2 + U(\mathbf{r}_i, \sigma_i) - \mu \right] \tag{2}$$

and $\hat{V}$ is an interaction which may (inter alia) lead to pairing: we shall often use the specific 'contact' form

$$V = \frac{1}{2}\sum_{ij} V(\mathbf{r}_i - \mathbf{r}_j), \quad V(\mathbf{r}_i - \mathbf{r}_j) = -g\delta(\mathbf{r}_i - \mathbf{r}_j) \tag{3}$$

with some phenomenological energy cutoff, but the argument is actually more general.

Up to now we assumed that when Cooper pairs form, they form in eigenstates of $\hat{H}_0$ related by time reversal, i.e. that the many-body wave function is of the form

$$\Psi = \prod_n (u_n + v_n a_n^\dagger a_{\bar{n}}^\dagger)|\text{vac}\rangle \tag{4}$$

where n and $\bar{n}$ are eigenstates of $\hat{H}_0$ corresponding to the same eigenvalue $E_n = E_{\bar{n}}$.

In general, however, this scheme is either not possible or not optimal. If either $\mathbf{A} \neq 0$ or U is a (time reversal violating) functions of the spin σ, then in general eigenstates of $\hat{H}_0$ related by time reversal do not exist. Even for the case of no vector potential and a spin-independent $U(\mathbf{r})$, when time-reversed pairs do exist, the pairing scheme used in the last lecture may not be optimal, ever for the ground state; generally speaking, this tends to happen when the physical conditions vary over a length scale $\lesssim \xi_0$. Finally, even when the conditions are slowly varying over $\sim \xi_0$, we may wish to discuss states where the condensate is moving, which clearly breaks T-invariance. So a more general scheme is called for.

This more general scheme goes under the name of the Bogoliubov–de Gennes equation (or technique). For simplicity, I first just quote the principal results of the discussion *: The Hamiltonian can be cast in the form

$$\hat{H} = E_0 + \sum_{n\sigma} E_n \alpha_{n\sigma}^\dagger \alpha_{n\sigma} \tag{5}$$

*For simplicity I assume at this point (with de Gennes, section 5.1) that the potential term is spin-independent $U(\mathbf{r}, \sigma) \equiv U(\mathbf{r})$. The opposite case will be discussed in lecture 12.

where the α's are fermion quasiparticles operators satisfying the anti-commutation relations

$$[\alpha_{n\sigma}, \alpha^\dagger_{n'\sigma'}]_+ = \delta_{nn'}\delta_{\sigma\sigma'} \tag{6}$$

and the E_n are the positive solutions of the pair of equations (the BdG equations) for two functions $u_n(\mathbf{r})$, $v_n(\mathbf{r})$:

$$\hat{H}_0 u_n(\mathbf{r}) + \Delta(\mathbf{r})v_n(\mathbf{r}) = E_n u_n(\mathbf{r}) \tag{7}$$

$$-\hat{H}_0^* v_n(\mathbf{r}) + \Delta^*(\mathbf{r})u_n(\mathbf{r}) = E_n v_n(\mathbf{r}) \tag{8}$$

where the local energy gap must be self-consistently determined according to the prescription (given explicitly for the contact potential $-g\delta(\mathbf{r})$)

$$\boxed{\Delta(\mathbf{r}) = g\sum_n v_n^*(\mathbf{r})u_n(\mathbf{r})\tanh\beta E_n/2} \tag{9}$$

The ground state energy is given by the expression (relative to $N\mu$)

$$E_0 = -\sum_n E_n \int |v_n(\mathbf{r})|^2\, d\mathbf{r} + \frac{1}{2g}\int |\Delta(\mathbf{r})|^2\, d\mathbf{r} \tag{10}$$

Note that in the limit $\Delta(\mathbf{r}) \to 0$,the $v_n(\mathbf{r})$ are simply the single-particle eigenfunctions of the one-particle Schrödinger equation with negative energy (relative to μ), and since these are normalized (cf. below) the expression for E_0 reduces to $-\sum_{\epsilon_n<0}|\epsilon_n|$, as it should.

Although the eigenvalues E_n of the BdG equations are independent of normalization, the value $\Delta(\mathbf{r})$ depends on it: we have implicitly chosen the normalization

$$\int \left[|u_n(\mathbf{r})|^2 + |v_n(\mathbf{r})|^2\right]\, d\mathbf{r} = 1 \tag{11}$$

This is a special case of a more general orthonormality relation, see below.

In the literature the BdG equations are almost invariably derived by writing down the Hamiltonian in second-quantized form, making a generalized mean-field approximation so that

$$g\psi^\dagger_\uparrow(\mathbf{r})\psi^\dagger_\downarrow(\mathbf{r})\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}) = \Delta(\mathbf{r})\psi^\dagger_\uparrow(\mathbf{r})\psi^\dagger_\downarrow(\mathbf{r}) + \text{h.c.}, \quad \text{where } \Delta(\mathbf{r}) \equiv g\langle\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r})\rangle \tag{12}$$

and diagonalizing the resulting 'mean-field' Hamiltonian (which contains of course both the above terms and the usual ones $\propto \psi^\dagger(\mathbf{r})\psi(\mathbf{r})$) by the generalized Bogoliubov transformations

$$\psi_\sigma(\mathbf{r}) = \sum_n \left[\alpha_{n\sigma}u_n(\mathbf{r}) - \sigma\alpha^\dagger_{n\sigma}v_n^*(\mathbf{r})\right] \tag{13}$$

etc.

This procedure is very standard and is well explained e.g. in de Gennes §5.1; however, it does not by itself give much into the nature of the groundstate, so I shall take an alternative route.

Let's first consider an even number of fermions at $T = 0$ and thus consider a single state of the system (which need however not necessarily be the ground state). As in lecture 5 we *assume* the general form of the wave function corresponds to the formation of Cooper pairs; explicitly

$$\Psi_N = \mathcal{N}\mathcal{A}\left[\phi(\mathbf{r}_1\sigma_1;\mathbf{r}_2\sigma_2)\phi(\mathbf{r}_3\sigma_3;\mathbf{r}_4\sigma_4)\ldots\phi(\mathbf{r}_{N-1}\sigma_{N-1};\mathbf{r}_N\sigma_N)\right] \tag{14}$$

where all the ϕ's are exactly the same. In second-quantized notation this reads:

$$\Psi_N = \mathcal{N}\left\{\sum_{\sigma\sigma'}\iint d\mathbf{r}d\mathbf{r}'\,K_{\sigma\sigma'}(\mathbf{r},\mathbf{r}')\psi^\dagger_\sigma(\mathbf{r})\psi^\dagger_{\sigma'}(\mathbf{r}')\right\}^{N/2}|\text{vac}\rangle \tag{15}$$

where $K_{\sigma\sigma'}(\mathbf{r},\mathbf{r}')$ may be taken antisymmetric under the exchange $\mathbf{r}\sigma \rightleftharpoons \mathbf{r}'\sigma'$. If we introduce an arbitrary orthonormal one-particle basis $\chi_i(\mathbf{r},\sigma)$ then

$$\Psi_N = \mathcal{N}\Big\{\sum_{ij}K_{ij}a^\dagger_i a^\dagger_j\Big\}^{N/2}|\text{vac}\rangle \tag{16}$$

where $K_{ij} = -K_{ji}$. Now, there is a general theorem that any antisymmetric even-rank square matrix can be 'skew-diagonalized', that is written in the form

$$\begin{bmatrix} 0 & K_1 & 0 & 0 & \\ -K_1 & 0 & 0 & 0 & \\ 0 & 0 & 0 & K_2 & \\ 0 & 0 & -K_2 & 0 & \\ & & & & \ddots \end{bmatrix} \tag{17}$$

Hence we can rewrite Ψ_N in the form

$$\Psi_N = \mathcal{N}\Big\{\sum_n c_n a^\dagger_n a^\dagger_{\bar{n}}\Big\}^{N/2}|\text{vac}\rangle \tag{18}$$

where the sets n and $\bar{n}$ have zero intersection and together form an orthonormal basis. The simple BCS form of Ψ_N is clearly a special form of (18) with $n = (\mathbf{k}\uparrow)$, $\bar{n} = (-\mathbf{k}\downarrow)$. Just as in that case, we can relax particle number conservation and replace (18) by the form

$$\Psi = \prod_n(\mathrm{U}_n + \mathrm{V}_n a^\dagger_n a^\dagger_{\bar{n}})|\text{vac}\rangle, \quad |\mathrm{U}_n|^2 + |\mathrm{V}_n|^2 = 1, \quad \frac{\mathrm{V}_n}{\mathrm{U}_n} = c_n \tag{19}$$

We use capital letters for the U_n and V_n to emphasize that these will not necessarily have all the properties associated with u_n and v_n which we met e.g. in lecture 9.

We can follow the original argument a little further. We define the 'pair wave function' $F(\mathbf{r}\mathbf{r}',\sigma\sigma') \equiv \langle\psi_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r})\rangle$, and find that it is given by the expression

$$F(\mathbf{r}\mathbf{r}',\sigma\sigma') = \sum_n \mathrm{U}_n\mathrm{V}_n\,\chi_n(\mathbf{r}\sigma)\chi_{\bar{n}}(\mathbf{r}'\sigma') \tag{20}$$

We now write down the expectation value of the Hamiltonian as a function of the trial functions $\chi_n(\mathbf{r})$, $\chi_{\bar{n}}(\mathbf{r})$ and the constants (which, we must remember, are in general complex, though the U_n can always be chosen real by convention). The pairing term is a simple generalization of the form in lecture 10:

$$\langle V\rangle_{\rm pair} = -g\int |F(\mathbf{r},\mathbf{r})|^2\, d\mathbf{r} = -g\int d\mathbf{r}\,\Big|\sum_n \mathrm{U}_n\mathrm{V}_n\chi_n(\mathbf{r})\chi_{\bar{n}}(\mathbf{r})\Big|^2 \tag{21}$$

The single-particle energy has the form

$$\langle\hat{H}_0\rangle = \sum_{n\sigma}|\mathrm{V}_n|^2\big[(\chi_n,\hat{H}_0,\chi_n)+(\chi_{\bar{n}},\hat{H}_0,\chi_{\bar{n}})\big] \tag{22}$$

This can be cast in a more useful form by adding and subtracting a term

$$K_0 = \frac{1}{2}\sum_{n\sigma}\Big[|\mathrm{U}_n|^2(\chi_n,\hat{H}_0,\chi_n)+|\mathrm{V}_n|^2(\chi_{\bar{n}},\hat{H}_0,\chi_{\bar{n}})\Big] \tag{23}$$

The quantity in brackets turns out (see below) to be just the trace of $\hat{H}_0$ which is simply a constant (infinite, if no cutoff is imposed): compare the addition and subtraction of the term $\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}$ in the translation-invariant case. Thus we can ignore this term in the expectation value of $\langle\hat{H}_0\rangle$ which then takes the form

$$\langle\hat{H}_0\rangle = \sum_n\Big[-|\mathrm{U}_n|^2(\chi_n,\hat{H}_0,\chi_n)+|\mathrm{V}_n|^2(\chi_{\bar{n}},\hat{H}_0,\chi_{\bar{n}})\Big] \tag{24}$$

where the factor of $1/2$ has been cancelled against the sum over spins.

Thus, the expectation value of the total Hamiltonian in the ground state* has the form

$$\langle\hat{H}\rangle = \sum_n\Big[-|\mathrm{U}_n|^2\int\chi_n^*\hat{H}_0\chi_n\,d\mathbf{r}+|\mathrm{V}_n|^2\int\chi_{\bar{n}}^*\hat{H}_0\chi_{\bar{n}}\,d\mathbf{r}\Big]-g\int d\mathbf{r}\,\Big|\sum_n\mathrm{U}_n\mathrm{V}_n^*\chi_n(\mathbf{r})\chi_{\bar{n}}(\mathbf{r})\Big|^2 \tag{25}$$

It is now tempting to try to minimize expression (25) with respect to *a)* the form of the functions $\chi_n(\mathbf{r}\sigma)$, $\chi_{\bar{n}}(\mathbf{r}\sigma)$ and *b)* the coefficients V_n and U_n. Indeed we shall see below that the result of doing so without additional constraints is precisely the BdG equations. Unfortunately, however, we now come to a major difference with the simple BCS case (or generalizations of it such as that of lecture 9): *In general, the BdG equations do not guarantee that the χ_n and $\chi_{\bar{n}}$ individually form a complete orthonormal set.* Thus, if we want to preserve this state of affairs (as we must), it is necessary to introduce the constraint of orthogonality explicitly, e.g. by means of appropriate Lagrange multipliers, and the resulting equations are so messy as to make explicit solution usually impossible. Thus, although we can always write the ground state in the form (19), there is in general *no simple relation between the quantities occurring in that equation and the solution of BdG equations.* (Cf. PS 3, problem 1)

*or more generally in the 'completely paired' state we are considering.

It may however be instructive to consider to consider the special case defined by the requirement that the solutions $u_n(\mathbf{r})$, $v_n(\mathbf{r})$ of the BdG equations have the properties (which, we repeat, is *not* guaranteed by the equations themselves)

$$\big(u_n(\mathbf{r}\sigma), u_{n'}(\mathbf{r}\sigma)\big) = \big(v_n(\mathbf{r}\sigma), v_{n'}(\mathbf{r}\sigma)\big) = \delta_{nn'}, \quad \big(u_n(\mathbf{r}\sigma), v_{n'}(\mathbf{r}\sigma)\big) = 0 \tag{26}$$

(The second equation is automatically satisfied if, for example, all the u_n correspond to spin up and all the v_m to spin down; but the first need not be satisfied even under that condition). If these conditions are satisfied, then it turns out (and can be checked a posteriori) that the orthogonality of the χ_n's and $\chi_{\bar{n}}$'s individually is automatically satisfied and does not have to be enforced by Lagrange multipliers (the normalization condition still needs one, however: cf. below). It is then convenient to introduce the notation

$$u_n(\mathbf{r}) \equiv \mathrm{U}_n \chi_n(\mathbf{r}), \quad v_n(\mathbf{r}) \equiv \mathrm{V}_n^* \chi_{\bar{n}}^*(\mathbf{r}) \tag{27}$$

Notice that association of $u_n(\mathbf{r})$ and $v_n(\mathbf{r})$ with $\chi_n(\mathbf{r})$ and $\chi_{\bar{n}}(\mathbf{r})$ respectively (rather than the other way around) is purely conventional, and that even though we can always choose the U_n real by convention, $u_n(\mathbf{r})$ may be nontrivially complex because we are not guaranteed that $\chi_n(\mathbf{r})$ is real. In terms of the functions $u_n(\mathbf{r})$, $v_n(\mathbf{r})$ the expectation value of the energy takes the form

$$\langle \hat{H} \rangle = \sum_n \Big\{ -\int d\mathbf{r}\, u_n^*(\mathbf{r}) \hat{H}_0 u_n(\mathbf{r}) + \int d\mathbf{r}\, v_n(\mathbf{r}) \hat{H}_0 v_n^*(\mathbf{r}) \Big\} - g \int d\mathbf{r} \Big| \sum_n u_n(\mathbf{r}) v_n^*(\mathbf{r}) \Big|^2 \tag{28}$$

and the normalization conditions on the χ's and U_n, V_n above are equivalent to the single condition

$$K_n \equiv \int d\mathbf{r} \left\{ |u_n(\mathbf{r})|^2 + |v_n(\mathbf{r})|^2 \right\} = 1 \tag{29}$$

As usual, we handle the constraint by introducing a Lagrange multiplier λ_n for each n and minimizing the quantity $\langle \hat{H} \rangle - \sum_n \lambda_n K_n$. Anticipating the result, it is convenient to relabel the λ_n as E_n. Then explicit minimization of $\langle \hat{H} \rangle - \sum_n \lambda_n K_n$ with respect to $u_n^*(\mathbf{r})$ and $v_n(\mathbf{r})$ separately gives two equations for each n:

$$\begin{aligned} \hat{H}_0 u_n(\mathbf{r}) + \Delta(\mathbf{r}) v_n(\mathbf{r}) &= E_n u_n(\mathbf{r}) \\ \Delta(\mathbf{r}) u_n(\mathbf{r}) - \hat{H}_0 v_n^*(\mathbf{r}) &= E_n v_n^*(\mathbf{r}) \end{aligned} \tag{30}$$

where $\Delta(\mathbf{r})$ is a shorthand for the quantity

$$\Delta(\mathbf{r}) \equiv g \sum_n u_n(\mathbf{r}) v_n^*(\mathbf{r}) \quad \big(\equiv g F^*(\mathbf{r}, \mathbf{r}) \big) \tag{31}$$

The first of eqns. (30) is the first BdG equation, and the second is turned into the second BdG equation by complex conjugation (note that e.g. in the presence of a vector potential, the Hamiltonian is Hermitian but not real, so in the general case it is necessary to complex-conjugate it.) Thus for the special case considered we recover in this way complete argument with the usual textbook treatment, and there is a simple correspondence

between the GSWF and the solution of the BdG equations. Again we emphasize this is not the generic case.

At this point it is useful to note some general properties of the solutions to the BdG equations. We can regard the $u_n(\mathbf{r})$ and $v_n(\mathbf{r})$ as respectively the upper and lower components of a 'spinor' $\psi_n(\mathbf{r})$ and the effective Hamiltonian acting on this spinor is then of the form of a matrix:

$$\begin{bmatrix} \hat{H}_0 & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -\hat{H}_0^* \end{bmatrix} \tag{32}$$

This matrix operator is Hermitian, and therefore by the usual theorems the solutions can be chosen to form a complete orthonormal set, in the sense that

$$\big(\psi_n(\mathbf{r}), \psi_{n'}(\mathbf{r})\big) \equiv \big(u_n(\mathbf{r}), u_{n'}(\mathbf{r})\big) + \big(v_n(\mathbf{r}), v_{n'}(\mathbf{r})\big) = \delta_{nn'} \tag{33}$$

Because of the completeness, the trace of any single-particle operator $\hat{Q}$ can be written in the form

$$\mathrm{Tr}\,\hat{Q} = \sum_n \big\{(u_n, \hat{Q}\, u_n) + (v_n, \hat{Q}\, v_n)\big\} \tag{34}$$

which is what justified us earlier in asserting that the expression (23) above was just the trace of $\hat{H}_0$. A further conclusion follows from the observation that if (u_n, v_n) is a spinor satisfying the BdG equations with eigenvalue E_n, then the spinor $(v_n^*, -u_n^*)$ is equally a solution with eigenvalue $-E_n$. Since spinors with eigenvalues E_n and $-E_{n'}$ must be orthogonal, this gives a second orthogonality condition, namely

$$(u_n, v_{n'}^*) - (v_n, u_{n'}^*) = 0 \quad (\text{all } n, n') \tag{35}$$

Note that eqns. (33) and (35), while generally true, *do not* in general imply eqns. (26).

It is often asserted in the literature that the negative-energy solutions of the BdG equations correspond to the states occupying the 'filled Fermi sea'. Personally I find this point of view more confusing than helpful, and find it more informative simply to regard the 'creation operators' associated with them as annihilating the groundstate.

The Andreev equations

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The Andreev equations are the 'semiclassical limit' of the more general BdG equations. Consider a situation where the 'diagonal' potential $U(\mathbf{r})$ can be taken as a constant (and thus absorbed in the zero of energy) and the gap $\Delta(\mathbf{r})$ is slowly varying over scales of the order of ${k_\mathrm{F}}^{-1}$ (though it may very appreciably over scales $\sim \xi_0$). Such a situation may obtain, for example, in the intermediate state of a type-I superconductor near an N-S interface (Andreev's original problem), in the case of a vortex in a type-II superconductor or (a case of great current interest) in an 'exotic' superconductor near a so-called pair-breaking surface.

Under these conditions the single-particle Hamiltonian reduces simply to the kinetic energy operator $-(\hbar^2/2m)\boldsymbol{\nabla}^2 - \mu$. It is convenient to take out a 'fast oscillating' piece

of the BdG functions $u_n(\mathbf{r})$, $v_n(\mathbf{r})$. Let us in fact concentrate on a particular pair n and make the ansatz

$$\begin{aligned} u(\mathbf{r}) &\equiv f(\mathbf{r}) \exp ik_{\mathrm{F}} \hat{\mathbf{n}} \cdot \mathbf{r} \\ v(\mathbf{r}) &\equiv g(\mathbf{r}) \exp ik_{\mathrm{F}} \hat{\mathbf{n}} \cdot \mathbf{r} \end{aligned} \tag{36}$$

where $\hat{\mathbf{n}}$ is a unit vector on the Fermi surface. On substituting these forms into the BdG equations and noting that $\hbar^2 {k_{\mathrm{F}}}^2/2m = \mu$ we obtain a term proportional to $k_{\mathrm{F}}|\boldsymbol{\nabla} f|$ (etc.) and one proportional to $\nabla^2 f$. Assuming that f and g themselves vary on the scale of the variation of $\Delta(\mathbf{r})$, i.e. slowly on the scale of ${k_{\mathrm{F}}}^2$, we can drop the second term in comparison to the first. Then, introducing the notation $v_{\mathrm{F}} \equiv \hbar k_{\mathrm{F}}/m$ as usual, we obtain the *Andreev equations*[§]

$$\begin{aligned} -i\hbar v_{\mathrm{F}}\, \hat{\mathbf{n}} \cdot \boldsymbol{\nabla} f(\mathbf{r}) + \Delta(\mathbf{r}) g(\mathbf{r}) &= E f(\mathbf{r}) \\ -i\hbar v_{\mathrm{F}}\, \hat{\mathbf{n}} \cdot \boldsymbol{\nabla} g(\mathbf{r}) + \Delta^*(\mathbf{r}) f(\mathbf{r}) &= E g(\mathbf{r}) \end{aligned} \tag{37}$$

Being linear rather than quadratic in the gradients, these equations are usually easier to solve than the full BdG equations. A crucial point is that since the combined equations are second order, we expect in general 2 solutions for each energy eigenvalue E.

Andreev reflection

Consider a situation in which the gap $\Delta(\mathbf{r})$ is either constant (in magnitude and phase) or very slowly varying, let us say for definiteness in the z-direction. Under these conditions the Andreev equations can be combined to give a single Schrodinger-like equation for $f(\mathbf{r})$, namely

$$-(\hbar v_{\mathrm{F}})^2 \big(\hat{\mathbf{n}} \cdot \boldsymbol{\nabla}\big)^2 f + |\Delta(\mathbf{r})|^2 f = E^2 f \tag{38}$$

and an identical equation for g. The general solution involves a dependence on x and y of the form $\exp i(q_x x + q_y y)$, where q_x, q_y are constants, but it is clear that this can be removed by an appropriate choice of $\hat{\mathbf{n}}$, so we can take f to be a function only of z and to satisfy the equation

$$-(\hbar v_{\mathrm{F}} n_z)^2 \frac{\partial^2 f}{\partial z^2} + |\Delta(z)|^2 f = E^2 f(z) \tag{39}$$

This second-order equation has two independent solutions, which in the limit of slowly varying $\Delta(z)$ have the semiclassical form $\exp \pm i \int k(z)\, dz$, where

$$\boxed{k(z) \equiv \frac{1}{\hbar v_{\mathrm{F}} n_z} \sqrt{E^2 - |\Delta(z)|^2}} \tag{40}$$

The two solutions represent 'particle-like' and 'hole-like' states: if n_z is positive, the $+$ sign corresponds to the particle. This can be seen most easily by taking the limit $\Delta(z) \to 0$, when $E \to |\epsilon_{\mathbf{k}}|$.

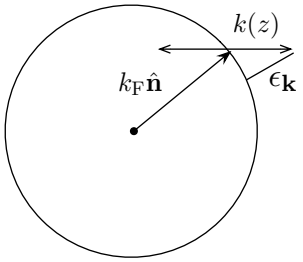
Consider the momentum and velocity of these two states. The momentum is $\hbar[k_{\mathrm{F}} \hat{\mathbf{n}} \pm k(z)\hat{\mathbf{z}}]$, and thus is little different for the two. However, the *velocity* is given by the

[§]In the literature one sometimes finds slightly different (but equivalent) forms, which result e.g. from a different choice of phase for $\Delta(\mathbf{r})$.

standard expression $1/\hbar\,\partial E(\mathbf{k})/\partial\mathbf{k}$, where $\mathbf{k} = k_{\rm F}\hat{\mathbf{n}} \pm k(z)\hat{\mathbf{z}}$. Here we have to be a little careful, since a dependence on $\mathbf{k}$ arises through $\hat{\mathbf{n}}$. The easiest technique is to define the normal-state KE $\epsilon_{\mathbf{k}}$ by $\epsilon_{\mathbf{k}} \equiv \pm\hbar v_{\rm F} n_z k(z)$; since $\partial\epsilon_{\mathbf{k}}/\partial\mathbf{k} = \hbar^2\mathbf{k}/m \approx \hbar v_{\rm F}\hat{\mathbf{n}}$, we have

$$\mathbf{v} \approx \frac{\partial E_{\mathbf{k}}}{\partial\epsilon_{\mathbf{k}}}\, v_{\rm F}\hat{\mathbf{n}} = \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\, v_{\rm F}\hat{\mathbf{n}} = \pm\frac{\hbar v_{\rm F} k(z)}{E_{\mathbf{k}}} v_{\rm F}\hat{\mathbf{n}} \tag{41}$$

Thus the velocity is (nearly) *opposite* on the two branches.



Lets consider a situation where $\Delta(z) \to 0$ as $z \to -\infty$ and $\to$ some finite value Δ_0 as $z \to +\infty$ (such a situation might arise, for example, near an N-S interface in a type-I superconductor). It is clear that for $E < \Delta_0$, there exist solutions of (39) for $z \to -\infty$ but not for $z \to +\infty$, so that the packet properties towards positive z: in the region $\Delta(z) = 0$, which is simply a normal metal, these are simply 'electron-like' wave packets. Now, it is clear that for $E < \Delta_0$ the packet cannot propagate to $z = +\infty$. On the other hand, it apparently cannot be reflected in any ordinary sense either: a 'single-shot' reflection in which $\mathbf{k} \to -\mathbf{k}$ corresponds (at best) to a matrix element of the form $\int\Delta(z)\exp 2ik_{\rm F}z\,dz$, which since Δ is assumed slowly varying over a range $\sim {k_{\rm F}}^{-1}$ is exponentially small, while a process of gradual reflection in which $\mathbf{k}$ changed step by step to $-\mathbf{k}$ is blocked by the Fermi sea (Pauli principle). So the only possibility is that the 'electron-like' wave packet is reflected as a 'hole-like' packet! ('Andreev reflection') Formally, this is possible because the true eigenstates are of the form of definite linear combinations of the electronlike and holelike solutions, i.e.

$$f(z) = A\exp +i\int k(z)\,dz \;+\; B\exp i\int k(z)\,dz \tag{42}$$

where the magnitudes of A and B are equal but the relative phase is determined by the condition that $f(z) \to 0$ for $z \to +\infty$ (where of course the simple form (42) is not valid).

A rather easier way of understanding Andreev reflection is to treat the wave packet semiclassically. Write

$$E(k,z) = \left(\epsilon_k^2 + |\Delta(z)|^2\right)^{1/2}, \quad (\epsilon_k = \hbar n_z k) \tag{43}$$

(so that conservation of E leads to the boxed equation). For simplicity let's take $\Delta(z)$ real and $n_z = +1$ (particle propagating normal to interface). Then we can write for the position $z(t)$ and k-vector (relative to $k_{\rm F}$) $k(t)$ the semiclassical equations

$$\begin{aligned} \frac{dz(t)}{dt} &= \frac{1}{\hbar}\frac{\partial E}{\partial k} = v_{\rm F}\frac{\hbar v_{\rm F}}{E}\,k(t) \\ \frac{dk(t)}{dt} &= -\frac{1}{\hbar}\frac{\partial E}{\partial z} = -\frac{1}{\hbar}\frac{\Delta(z)}{E}\frac{\partial\Delta(z)}{\partial z} \end{aligned} \tag{44}$$

It is clear that $k(t)$ decreases uniformly in time, and eventually goes through zero at the point where $\Delta(z) = E$ ('classical turning point'). At this point the velocity of the packet reverses, and it emerges as a hole-like packet propagating back towards $z = -\infty$. It is important to note that in the more general case not only the z-component *but also the transverse components* of the velocity are reversed, in contrast to the familiar case of specular reflection. Note also that although the packet undergoes some change of momentum on Andreev reflection, this is small compared to that ($\sim 2\hbar k_{\rm F}$) on ordinary reflection.

The semiclassical description is of course not a complete account: even for $E < \Delta$ it must fail very close to the classical turning point, and moreover it would predict that for $E > \Delta$ we get 100% transmission. whereas a proper quantum-mechanical solution of the Andreev equations show that even for $E > \Delta$ we can get a finite reflection amplitude(the exact value depends on the shape of the function $\Delta(z)$; generally speaking, the sharper the spatial variation of Δ the greater the reflection amplitude).