Lecture 16 (Feb. 24)

BCS Theory of Superconductivity

- **Bound states**: Consider a ballistic particle in an attractive potential $V(\vec{x})$. The Schrödinger equation is

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(\vec{x}) + V(\vec{x})\,\psi(\vec{x}) = E\,\psi(\vec{x})$$

Fourier transform to obtain

$$\varepsilon(\mathbf{k})\,\hat{\psi}(\mathbf{k}) + \int\!\frac{d^dk'}{(2\pi)^d}\,\hat{V}(\mathbf{k}-\mathbf{k}')\,\hat{\psi}(\mathbf{k}') = E\,\hat{\psi}(\mathbf{k})$$

with $\varepsilon(\mathbf{k}) = \hbar^2\mathbf{k}^2/2m$. Since $\hat{V}_{\mathbf{k},\mathbf{k}'} \equiv \hat{V}(\mathbf{k}-\mathbf{k}')$ is a Hermitian matrix, we may express it as a sum over its eigenspace projectors, viz.

$$\hat{V}(\mathbf{k}-\mathbf{k}') = \sum_n \lambda_n\,\alpha_n(\mathbf{k})\,\alpha_n^*(\mathbf{k}')$$

Let's approximate the above sum by the contribution from the lowest eigenvalue, which we call λ. Thus, we take

$$\hat{V}(\mathbf{k},\mathbf{k}') \approx \lambda\,\alpha(\mathbf{k})\,\alpha^*(\mathbf{k}')$$

Such a potential is called **separable**. We then have

$$\varepsilon(\mathbf{k})\,\hat{\psi}(\mathbf{k}) + \lambda\,\alpha(\mathbf{k})\int\!\frac{d^dk'}{(2\pi)^d}\,\alpha^*(\mathbf{k}')\,\hat{\psi}(\mathbf{k}') = E\,\hat{\psi}(\mathbf{k}')$$

which entails

$$\hat{\psi}(\mathbf{k}) = \frac{\lambda\,\alpha(\mathbf{k})}{E-\varepsilon(\mathbf{k})}\int\!\frac{d^dk'}{(2\pi)^d}\,\alpha^*(\mathbf{k}')\,\hat{\psi}(\mathbf{k}')$$

Now multiply by $\alpha^*(\mathbf{k})$ and integrate to obtain

$$-\frac{1}{\lambda} = \int \frac{d^d k}{(2\pi)^d} \frac{|\alpha(\mathbf{k})|^2}{\varepsilon(\mathbf{k}) - E}$$

If $\hat{V}_{\mathbf{k},\mathbf{k}'}$ is isotropic, i.e. if $\hat{V}(\mathbf{k}-\mathbf{k}') = \hat{V}(R\mathbf{k}-R\mathbf{k}')$ where $R \in SO(d)$, then the lowest eigenvector $\alpha(\mathbf{k})$ is generally isotropic, i.e. we may write $\alpha(\mathbf{k}) = \alpha(\varepsilon(\mathbf{k}))$, which is a function only of the magnitude of $\mathbf{k}$. Then with $g(\varepsilon) = \int \frac{d^d k}{(2\pi)^d} \delta(\varepsilon - \varepsilon(\mathbf{k}))$ = DOS, we have

$$(\bullet) \qquad \frac{1}{|\lambda|} = \int_0^\infty d\varepsilon \, \frac{g(\varepsilon)}{|E| + \varepsilon} \, |\alpha(\varepsilon)|^2$$

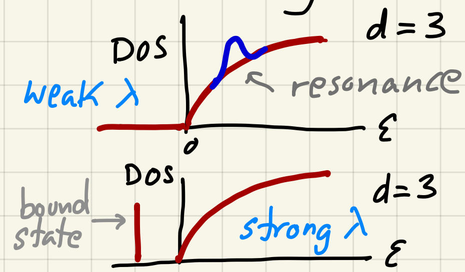
where we assume $\lambda < 0$ and $E < 0$. If $\alpha(\varepsilon)$ and $g(\varepsilon)$ are finite as $\varepsilon \to 0$, then we have, as $E \to 0^-$,

$$\frac{1}{|\lambda|} = g(0)\, |\alpha(0)|^2 \ln\left(\frac{B}{|E|}\right) + \text{finite}$$

where B is the bandwidth (i.e. $g(\varepsilon) = 0$ for $\varepsilon > B$). This equation has a solution for arbitrily small values of $|\lambda|$, since the RHS diverges logarithmically as $E \to 0^-$. Thus, as $\lambda \to 0^-$ we have

$$E(\lambda) = -c\,B \exp\left(-\frac{1}{g(0)\,|\alpha(0)|^2 |\lambda|}\right)$$

where $c > 0$ is a constant. If $g(\varepsilon) \propto \varepsilon^p$ with $p > 0$, then the RHS of $(\bullet)$ is finite as $E \to 0^-$. In this case, a bound state solution with $E<0$ exists only for $|\lambda| > \lambda_c$, where

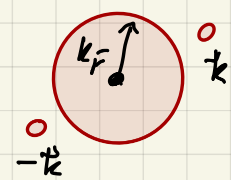


$$\lambda_c = 1 \Big/ \int_0^\infty d\varepsilon \, \frac{g(\varepsilon)}{\varepsilon} \, |\alpha(\varepsilon)|^2$$

For a ballistic dispersion, $g(\varepsilon) \propto \varepsilon^{(d-2)/2}$, so $g(0)$ vanishes for $d>2$ and is finite for $d=2$. For $d<2$, $g(\varepsilon \to 0^+)$ diverges as $g(\varepsilon) \propto \varepsilon^{-p}$ with $p = 1 - \frac{1}{2}d$, i.e. $p = \frac{1}{2}$ in $d=1$. The RHS of $(\bullet)$ then diverges as $|E|^{-p}$ as $E \to 0^-$ and so $E(\lambda) = -c\,|\lambda|^{1/p}$ as $\lambda \to 0^-$.

- **Cooper's problem (1956)**: Cooper considered the problem of two electrons with a weak attraction in the presence of a quiescent Fermi sea, described by a variational wavefunction

$$|\Psi\rangle = \frac{1}{\sqrt{2}} \sum_{|\mathbf{k}|>k_F} A_{\mathbf{k}} \left(c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} - c^\dagger_{\mathbf{k}\downarrow} c^\dagger_{-\mathbf{k}\uparrow} \right) |F\rangle$$



where $|F\rangle$ is the filled Fermi sphere. Note that $|\Psi\rangle$ has total momentum $\vec{K}=0$ and total spin $S=0$ (i.e. a singlet). The electrons in the Fermi sea only enter the problem through Pauli blocking. In real space, the wavefunction for Cooper's pair is

$$\Psi(\vec{x}_1, \vec{x}_2) = \frac{1}{\sqrt{2}} \sum_{|k|>k_F} A_k e^{ik\cdot(\vec{x}_1 - \vec{x}_2)} \left(|\uparrow_1 \downarrow_2\rangle - |\downarrow_1 \uparrow_2\rangle \right)$$

where $A_k = A_{-k}$. The Hamiltonian is

$$\hat{H} = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \frac{1}{2} \sum_{k_1,\sigma_1} \cdots \sum_{k_4,\sigma_4} \langle k_1\sigma_1, k_2\sigma_2 | v | k_3\sigma_3, k_4\sigma_4 \rangle$$
$$\times\, c^\dagger_{k_1\sigma_1} c^\dagger_{k_2\sigma_2} c_{k_4\sigma_4} c_{k_3\sigma_3}$$

We treat $|\Psi\rangle$ as a variational state, so we set

$$\delta \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\delta\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} - \underbrace{\frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle}}_{E} \cdot \frac{\delta\langle\Psi|\Psi\rangle}{\langle\Psi|\Psi\rangle} = 0$$

We take the variation wrt A^*_k. We have

$$\langle\Psi|\Psi\rangle = \sum_k A^*_k A_k$$
$$\langle\Psi|\hat{H}|\Psi\rangle = E_0 + \sum_k 2\varepsilon_k |A_k|^2 + \frac{1}{2}\sum_{k,k'} V_{k,k'} A^*_k A_{k'}$$

where $E_0 = \langle F|\hat{H}|F\rangle$ and

$$V_{k,k'} = \langle k\uparrow, -k\downarrow | v | k'\uparrow, -k'\downarrow\rangle = \frac{1}{V}\int d^3x\, v(\vec{x})\, e^{i(k-k')\cdot\vec{x}}$$

Thus, we obtain the eigenvalue equation

prime means $|k'|>k_F$

$$(E_0 + 2\varepsilon_k) A_k + \sum_{k'}{}' V_{k,k'} A_{k'} = E A_k$$

Now define $\varepsilon_k \equiv \varepsilon_F + \xi_k$ and $E \equiv E_0 + 2\varepsilon_F + W$, so that

$$2\xi_k A_k + \sum_{k'}{}' V_{k,k'} A_{k'} = W A_k$$

Assuming $v(\vec{x}) = v(|\vec{x}|)$, we may write

$$V_{\mathbf{k},\mathbf{k}'} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} V_l(k,k')\, Y_{l,m}(\hat{k})\, Y^*_{l,m}(\hat{k}')$$

We further assume separability, i.e.

$$V_l(k,k') = \frac{1}{V} \lambda_l\, \alpha_l(k)\, \alpha^*_l(k')$$

and we seek a solution $A_{\mathbf{k}} = A_k Y_{l,m}(\hat{k})$ in the angular momentum l channel. This results in

$$2\xi_k A_k + \lambda_l\, \alpha_l(k) \cdot \frac{1}{V} \sum_{\mathbf{k}'}{}' \alpha^*_l(k')\, A_{k'} = W_l A_k$$

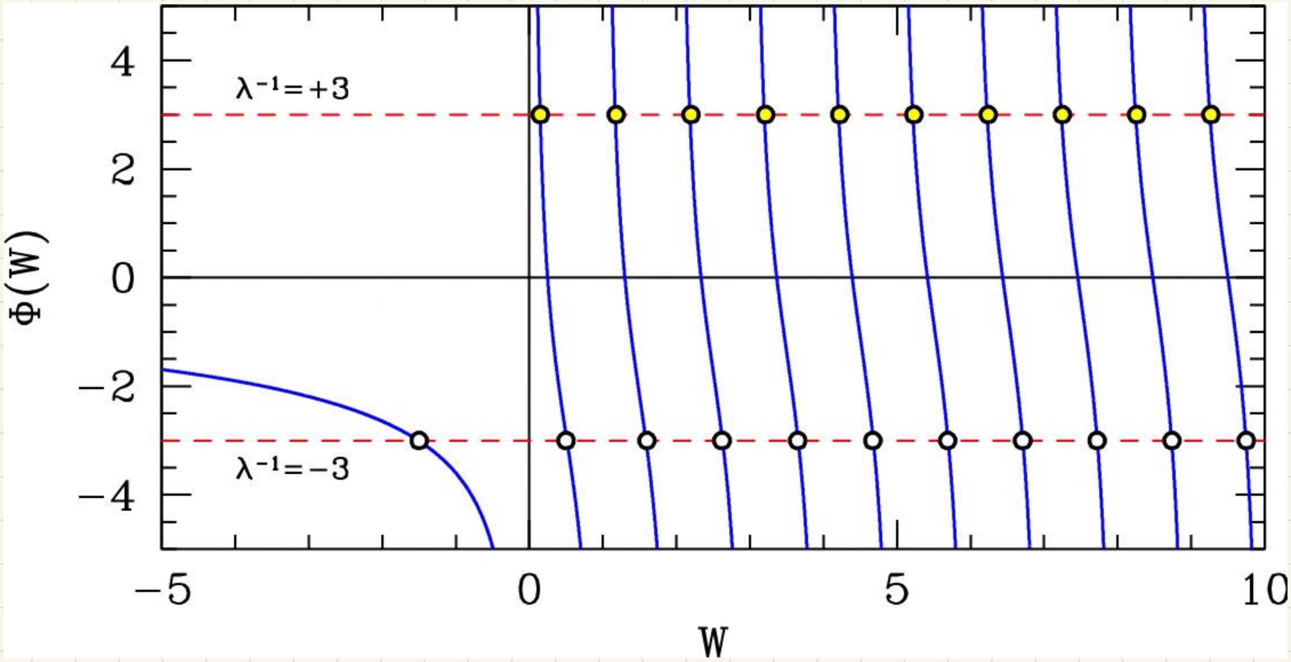
This may be recast as

$$A_k = \frac{\lambda_l\, \alpha_l(k)}{W_l - 2\xi_k} \cdot \frac{1}{V} \sum_{\mathbf{k}'}{}' \alpha^*_l(k')\, A_{k'}$$

Now multiply by $\alpha^*_l(k)$ and sum over $|\mathbf{k}| > k_F$ to obtain

$$\frac{1}{\lambda_l} = \frac{1}{V} \sum_{\mathbf{k}}{}' \frac{|\alpha_l(k)|^2}{W_l - 2\xi_k} \equiv \Phi(W_l)$$

We can solve this graphically. Since $|\mathbf{k}| > k_F$, $\xi_k > 0$. The denominator passes through zero as W_l passes through each value of ξ_k. As we see from the plot below, when $\lambda_l < 0$ there is a bound state solution with $W_l < 0$. This is true for arbitrarily weak attractive λ_l.



We saw previously how in $d=3$ dimensions bound states require a critical attraction strength. The difference here is that we are not interested in states near $\mathbf{k}=0$, where the DOS vanishes as $\sqrt{\varepsilon}$, but rather in states near $|\mathbf{k}|=k_F$, where $g(\varepsilon_F)=m^* k_F/\pi^2\hbar^2$ is constant, as it is for a $d=2$ system near $\varepsilon=0$.

To solve further, assume $\alpha_\ell(k)=\Theta(B_\ell-\xi_k)$ so

because $g(\varepsilon)$ includes spin

$$1=\frac{1}{2}|\lambda_\ell|\int_0^{B_\ell} d\xi\,\frac{g(\varepsilon_F+\xi)}{|W_\ell|+\xi}$$

Now assume $g(\varepsilon_F+\xi)\approx g(\varepsilon_F)$, integrate, and find

$$|W_\ell|=\frac{2B_\ell}{\exp\left(4/|\lambda_\ell|g(\varepsilon_F)\right)-1}$$

weak coupling

In the weak coupling limit, where $|\lambda_\ell|g(\varepsilon_F)\ll 1$,

$$W_\ell \simeq -2B_\ell\, e^{-4/|\lambda_\ell|\, g(\varepsilon_F)}$$

As we shall see when we study BCS theory, the factor of 4 in the exponent is twice too large. For strong coupling, $|\lambda_\ell|\, g(\varepsilon_F) \gg 1$, and

$$W_\ell \simeq -\tfrac{1}{2}\,|\lambda_\ell|\, B_\ell\, g(\varepsilon_F)$$

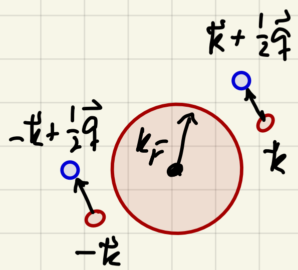
strong coupling

The energy scale B_ℓ will be shown to be the Debye energy of the phonons for conventional phonon-mediated superconductivity. The effective attractive interaction exists only over a very thin energy shell about the Fermi surface. Two additional features of the Cooper problem:

- One can construct a finite momentum Cooper pair, viz.

$$|\Psi_{\vec{q}}\rangle = \frac{1}{\sqrt{2}} \sum_{\vec{k}} A_{\vec{k}} \left(c^\dagger_{\vec{k}+\frac{1}{2}\vec{q}\uparrow}\, c^\dagger_{-\vec{k}+\frac{1}{2}\vec{q}\downarrow} - c^\dagger_{\vec{k}+\frac{1}{2}\vec{q}\downarrow}\, c^\dagger_{-\vec{k}+\frac{1}{2}\vec{q}\uparrow} \right) |F\rangle$$

The total momentum is $\vec{P} = \hbar\vec{q}$. This results in the eigenvalue equation



$$\left(\xi_{\vec{k}+\frac{1}{2}\vec{q}} + \xi_{\vec{k}-\frac{1}{2}\vec{q}}\right) A_{\vec{k}} + \sum_{\vec{k}'}{}' V_{\vec{k},\vec{k}'}\, A_{\vec{k}'} = W A_{\vec{k}}$$

Now

$$\left(\xi_{\vec{k}+\frac{1}{2}\vec{q}} + \xi_{\vec{k}-\frac{1}{2}\vec{q}}\right) = 2\xi_{\vec{k}} + \frac{1}{4}\, \frac{\partial^2 \xi_{\vec{k}}}{\partial k_\alpha\, \partial k_\beta}\, q_\alpha q_\beta + \ldots$$

and thus the binding energy is reduced by $\mathcal{O}(q^2)$. The $\vec{q}=0$ Cooper pair has the greatest binding energy.

- The mean square radius of the Cooper pair is

$$\langle \vec{r}^{\,2} \rangle = \frac{\int d^3r \, |\Psi(\vec{r})|^2 \, \vec{r}^{\,2}}{\int d^3r \, |\Psi(\vec{r})|^2} = \frac{\int d^3k \, |\vec{\nabla}_{\vec{k}} A_{\vec{k}}|^2}{\int d^3k \, |A_{\vec{k}}|^2}$$

$$\simeq \frac{g(\varepsilon_F)\, \xi'(k_F)^2 \int_0^\infty d\xi \, |\partial A/\partial \xi|^2}{g(\varepsilon_F) \int_0^\infty d\xi \, |A(\xi)|^2}$$

We have $A(\xi) = -C\lambda_2 \alpha(\xi)/(|W| + 2\xi)$, and $\xi'(k_F) = \hbar v_F$. For weak binding, $W \to 0^-$, and we have

$$\langle \vec{r}^{\,2} \rangle \simeq \frac{4}{3} (\hbar v_F)^2 |W|^{-2}$$

Thus, for weak attractive interactions, $W \to 0^-$ and the radius of the Cooper pair diverges. This is why BCS turns out to be such a successful mean field theory. The **Ginzburg criterion** (§11.4.5) says that mean field theory is qualitatively accurate down to a reduced temperature

$$t_G = \frac{|T - T_c|}{T_c} = \left(\frac{a}{R_*}\right)^{2d/(4-d)}$$

where a is a microscopic length (e.g., the lattice constant) and R_* the mean Cooper pair size. Typically we have $R_*/a \approx 10^2 - 10^3$, so in $d=3$, $t_G \approx 10^{-6} - 10^{-9}$.

- **Phonon-mediated attraction**

Please read §12.3 for details. The electron-phonon Hamiltonian for small momentum transfer and longitudinal phonons is

$$\hat{H}_{el\text{-}ph} = \frac{1}{\sqrt{V}} \sum_{\vec{k},\vec{q}} \sum_{\sigma} g_{\vec{q}} \left(a^\dagger_{\vec{q}} + a_{-\vec{q}}\right) c^\dagger_{\vec{k}\sigma} c_{\vec{k}+\vec{q}\sigma}$$

with $g_{\vec{q}} = \lambda_{el\text{-}ph} \hbar c_L q / g(\varepsilon_F)$. We compute an effective indirect electron-electron interaction by working to second order in $\hat{H}_{el\text{-}ph}$. Starting with a pair of electrons in states $|\vec{k}\sigma, -\vec{k}-\sigma\rangle$, we transition to either of the two intermediate states

longitudinal phonon

$$|I_1\rangle = |\vec{k}'\sigma, -\vec{k}-\sigma\rangle \otimes |-\vec{q}\rangle$$
$$|I_2\rangle = |\vec{k}\sigma, -\vec{k}'-\sigma\rangle \otimes |+\vec{q}\rangle$$

where $\vec{q} = \vec{k}' - \vec{k}$. Another application of $\hat{H}_{el\text{-}ph}$ takes us to $|\vec{k}'\sigma, -\vec{k}'-\sigma\rangle$. The intermediate state energies are given by

$$E_1 = \xi_{-\vec{k}} + \xi_{\vec{k}'} + \hbar\omega_{-\vec{q}}$$

$$E_2 = \xi_{\vec{k}} + \xi_{-\vec{k}'} + \hbar\omega_{\vec{q}}$$

The second order matrix element is then

$$\langle \vec{k}'\sigma, -\vec{k}'-\sigma | \hat{H}_{indirect} | \vec{k}\sigma, -\vec{k}-\sigma \rangle = \sum_n \langle \vec{k}'\sigma, -\vec{k}'-\sigma | \hat{H}_{el-ph} | n \rangle$$

$$\times \langle n | \hat{H}_{el-ph} | \vec{k}\sigma, -\vec{k}-\sigma \rangle \times \left(\frac{1}{E_f - E_n} + \frac{1}{E_i - E_n} \right)$$

$$= |g_{\vec{q}}|^2 \left(\frac{1}{\xi_{\vec{k}'} - \xi_{\vec{k}} - \hbar\omega_{\vec{q}}} + \frac{1}{\xi_{\vec{k}} - \xi_{\vec{k}'} - \hbar\omega_{\vec{q}}} \right)$$

Adding in the direct Coulomb interaction $\hat{v}(\vec{q}) = \frac{4\pi e^2}{\vec{q}^2}$, we obtain the effective interaction

$$\langle \vec{k}'\sigma, -\vec{k}'-\sigma | \hat{H}_{eff} | \vec{k}\sigma, -\vec{k}\sigma \rangle = \hat{v}(\vec{q}) + |g_{\vec{q}}|^2 \times \frac{2\hbar\omega_{\vec{q}}}{(\xi_{\vec{k}} - \xi_{\vec{k}'})^2 - (\hbar\omega_{\vec{q}})^2}$$

Thus for $|\xi_{\vec{k}} - \xi_{\vec{k}'}| < \hbar\omega_{\vec{q}}$ the second term is negative and can dominate the first, yielding an effective attraction.

- **Reduced BCS Hamiltonian:** The operator that creates a Cooper pair with total momentum $\hbar\vec{q}$ is $b^\dagger_{\vec{k},\vec{q}} + b^\dagger_{-\vec{k},\vec{q}}$

$$b_{\vec{k},\vec{q}} = c^\dagger_{\vec{k}+\frac{1}{2}\vec{q}\uparrow} c^\dagger_{-\vec{k}+\frac{1}{2}\vec{q}\downarrow}$$

Since $\vec{q}=0$ pairs have the greatest binding energy, we consider the **reduced BCS Hamiltonian**,

$$\hat{H}_{red} = \sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + \sum_{\vec{k},\vec{k}'} V_{\vec{k},\vec{k}'} b^\dagger_{\vec{k},0} b_{\vec{k}',0}$$

We may assume $V_{\vec{k},\vec{k}'} = V_{\vec{k},-\vec{k}'} = V_{-\vec{k},\vec{k}'}$, which is required by spin rotational invariance. Since

$$2\underbrace{c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}}_{b^\dagger_{k,0}} \underbrace{c_{-k\downarrow} c_{k\uparrow}}_{b_{k,0}} |\psi\rangle = (c^\dagger_{k\uparrow} c_{k\uparrow} + c^\dagger_{-k\downarrow} c_{-k\downarrow}) |\psi\rangle$$

provided all the pair states $(k\uparrow, -k\downarrow)$ in $|\psi\rangle$ are either empty or doubly occupied. Thus, we consider

$$\hat{H}^0_{red} = \sum_k 2\varepsilon_k b^\dagger_{k,0} b_{k,0} + \sum_{k,k'} V_{k,k'} b^\dagger_{k,0} b_{k',0}$$

This has the alluring appearance of a noninteracting bosonic Hamiltonian, which would render it exactly solvable. However, $b_{k,0}$ is a composite operator that is not a true boson in that it doesn't satisfy bosonic commutation relations. If $\beta^\dagger_k$ is a bosonic creation operator, then $[\beta_k, \beta_{k'}] = [\beta^\dagger_k, \beta^\dagger_{k'}] = 0$, $[\beta_k, \beta^\dagger_{k'}] = \delta_{kk'}$. But while $[b_{k,0}, b_{k',0}] = [b^\dagger_{k,0}, b^\dagger_{k',0}] = 0$,

$$[b_{k,0}, b^\dagger_{k',0}] = (1 - c^\dagger_{k\uparrow} c_{k\uparrow} - c^\dagger_{-k\downarrow} c_{-k\downarrow})\, \delta_{kk'}$$

Furthermore, $(b^\dagger_{k,0})^2 = (b_{k,0})^2 = 0$. So we need another approach, as $\hat{H}^0_{red}$ can't be diagonalized by any known methods.

Mean field theory: While $b_{k,0}$ doesn't satisfy bosonic commutation relations, it is still a

composite boson and can take on an expectation value. So let's do the mean field thing and write

$$b_{\vec{k},0} = \langle b_{\vec{k},0} \rangle + \underbrace{\left(b_{\vec{k},0} - \langle b_{\vec{k},0} \rangle \right)}_{\delta b_{\vec{k},0}}$$

We now have

$$\hat{H}_{red} = \sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + \sum_{\vec{k},\vec{k}'} V_{\vec{k},\vec{k}'} \Big(- \overbrace{\langle b^\dagger_{\vec{k},0} \rangle \langle b_{\vec{k},0} \rangle}^{c\text{-number}}$$
$$+ \langle b^\dagger_{\vec{k},0} \rangle b_{\vec{k}',0} + b^\dagger_{\vec{k},0} \langle b_{\vec{k}',0} \rangle + \underbrace{\delta b^\dagger_{\vec{k},0}\, \delta b_{\vec{k}',0}}_{(\text{flucts})^2 \text{ drop!}} \Big)$$

Thus our mean field Hamiltonian is

$$\hat{H}^{MF}_{red} = \sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + \sum_{\vec{k}} \left(\Delta_{\vec{k}} c^\dagger_{\vec{k}\uparrow} c^\dagger_{-\vec{k}\downarrow} + \Delta^*_{\vec{k}} c_{-\vec{k}\downarrow} c_{\vec{k}\uparrow} \right)$$
$$- \sum_{\vec{k},\vec{k}'} V_{\vec{k},\vec{k}'} \langle c^\dagger_{\vec{k}\uparrow} c^\dagger_{-\vec{k}\downarrow} \rangle \langle c_{-\vec{k}'\downarrow} c_{\vec{k}'\uparrow} \rangle$$

where

$$\Delta_{\vec{k}} = \sum_{\vec{k}'} V_{\vec{k},\vec{k}'} \langle c_{-\vec{k}'\downarrow} c_{\vec{k}'\uparrow} \rangle \quad , \quad \Delta^*_{\vec{k}} = \sum_{\vec{k}'} V^*_{\vec{k},\vec{k}'} \langle c^\dagger_{\vec{k}\uparrow} c_{-\vec{k}'\downarrow} \rangle$$

One highly noteworthy aspect of $\hat{H}_{red}$: it does not conserve particle number! Therefore we need to work in the grand canonical ensemble, with

$$\hat{K}_{BCS} = \hat{H}^{MF}_{red} - \mu \hat{N} \quad , \quad \hat{N} = \sum_{\vec{k},\sigma} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma}$$