Phys 726 — Lecture 21

Electron bound states

* Attractive interactions are fundamentally different from repulsive ones

→ competition between kinetic (+ve) and potential (−ve) energy

→ possibility of bound states

* Consider two quantum particles described by coordinates $\vec{r}_1$ and $\vec{r}_2$ interacting via a potential $V(\vec{r}_2 - \vec{r}_1)$

→ the pair has a wave function $\Psi(\vec{r}_1, \vec{r}_2)$ obeying

$$-\frac{\hbar^2}{2m_1}\nabla_1^2\Psi(\vec{r}_1,\vec{r}_2) - \frac{\hbar^2}{2m_2}\nabla_2^2\Psi(\vec{r}_1,\vec{r}_2) + V(\vec{r}_1-\vec{r}_2)\Psi = E\Psi$$

→ Switch to relative ($\vec{r} = \vec{r}_1 - \vec{r}_2$) and center-of-mass ($\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2)$) coordinates

$$-\frac{\hbar^2}{2M}\nabla_R^2 \psi(\vec{r},\vec{R}) - \frac{\hbar^2}{2\mu}\nabla_r^2 \psi(\vec{r},\vec{R}) + V(\vec{r})\psi(\vec{r},\vec{R}) = E\psi$$

$M = m_1 + m_2$ $\qquad$ $\mu = \left(\frac{1}{m_1} + \frac{1}{m_2}\right)^{-1}$

→ Since V depends on $\vec{r}$ only, the equation is separable, and we can factor out the wave function of the center-of-mass

$$\psi(\vec{r},\vec{R}) = e^{i\vec{K}\cdot\vec{R}}\psi(\vec{r})$$

where $\hbar\vec{K}$ is the momentum of the particle pair

→ Substitution gives

$$-\frac{\hbar^2}{2\mu}\nabla_r^2\psi + V(r)\psi = \underbrace{\left(E - \frac{\hbar^2 K^2}{2M}\right)}_{\text{energy in the center-of-mass frame}}\psi = \tilde{E}\psi$$

→ Fourier transform

$$\psi(\vec{r}) = \int \frac{d^3r}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}} \psi(\vec{k})$$

to get a k-space Schrödinger eq.

$$\tilde{E}\psi(k) = \frac{\hbar^2 k^2}{2\mu}\psi(\vec{k}) + \int \frac{d^3k'}{(2\pi)^3} V(\vec{k}-\vec{k}')\psi(\vec{k}')$$

Let's suppose $m_1 = m_2 = m$
so that $\mu = m/2$.
Then $\frac{\hbar^2 k^2}{2\mu} = 2\frac{\hbar^2 k^2}{2m} \equiv 2\varepsilon_k$

→ Define a "gap function"

$$\Delta(\vec{k}) = (\tilde{E} - 2\varepsilon_k)\psi(\vec{k})$$

so that

$$(\tilde{E} - 2\varepsilon_k)\psi(k) = \Delta(k) = \int \frac{d^3k'}{(2\pi)^3} V(\vec{k}-k')\psi(k')$$

$$= \int \frac{d^3k'}{(2\pi)^3} \frac{V(k-k')\Delta(k')}{\tilde{E} - 2\varepsilon_{k'}}$$

* The Schrödinger equation turns into a self-consistent equation for the gap function

$$\Delta(\vec{k}) = \int \frac{d^3k'}{(2\pi)^3} \frac{V(\vec{k}-\vec{k}')\,\Delta(\vec{k}')}{\tilde{E} - 2\varepsilon_{k'}}$$

$$= -\int \frac{d^3k'}{(2\pi)^3} \frac{V(\vec{k}-\vec{k}')\,\Delta(\vec{k}')}{2\varepsilon_{k'} - \tilde{E}}$$

→ Consider a special case: Sp. that $v(r)$ is a contact potential. Then

$$v(r) = U\delta(r) \Rightarrow V(k) = \text{const} = U$$

(no k-dependence!)

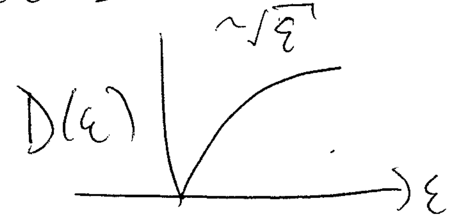
$\Rightarrow \Delta(k) = \Delta_0$ also is independent of the wave vector

So $$\cancel{\Delta_0} = -\int \frac{d^3k'}{(2\pi)^3} \frac{U\cancel{\Delta_0}}{2\varepsilon_{k'} - \tilde{E}}$$

or $$1 = -U \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\varepsilon_k - \tilde{E}}$$

$$= -U \int \frac{d^3k}{(2\pi)^3} \int d\varepsilon\, \delta(\varepsilon - \varepsilon_k) \frac{1}{2\varepsilon - \tilde{E}}$$

$$= -U \int_0^\infty d\varepsilon \frac{D(\varepsilon)}{2\varepsilon - \tilde{E}}$$



EXERCISE: ① Convince yourself that a bound state in this context means $\hat{E} < 0$ and that the equality is only possible if $U < 0$

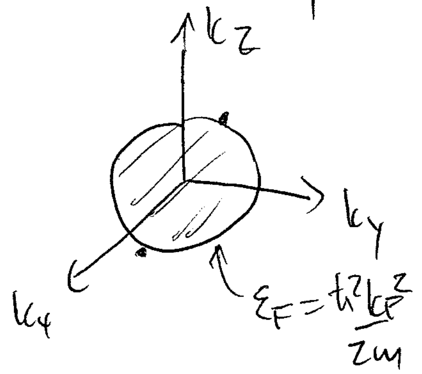
② In dimensions $D = 1, 2, 3$, use the relation

$$1 = |U_c| \int d\varepsilon \frac{D(\varepsilon)}{2\varepsilon}$$

to determine if there is a critical attractive threshold for forming a bound state

* The nature of the pairing problem changes if we add back the many-particle Fermi Sea and the underlying lattice

→ The lowest energy state for two additional particles is $2\varepsilon_F$, where ε_F is the Fermi energy



→ So the binding energy is now $\varepsilon_b = 2\varepsilon_F - \tilde{E}$

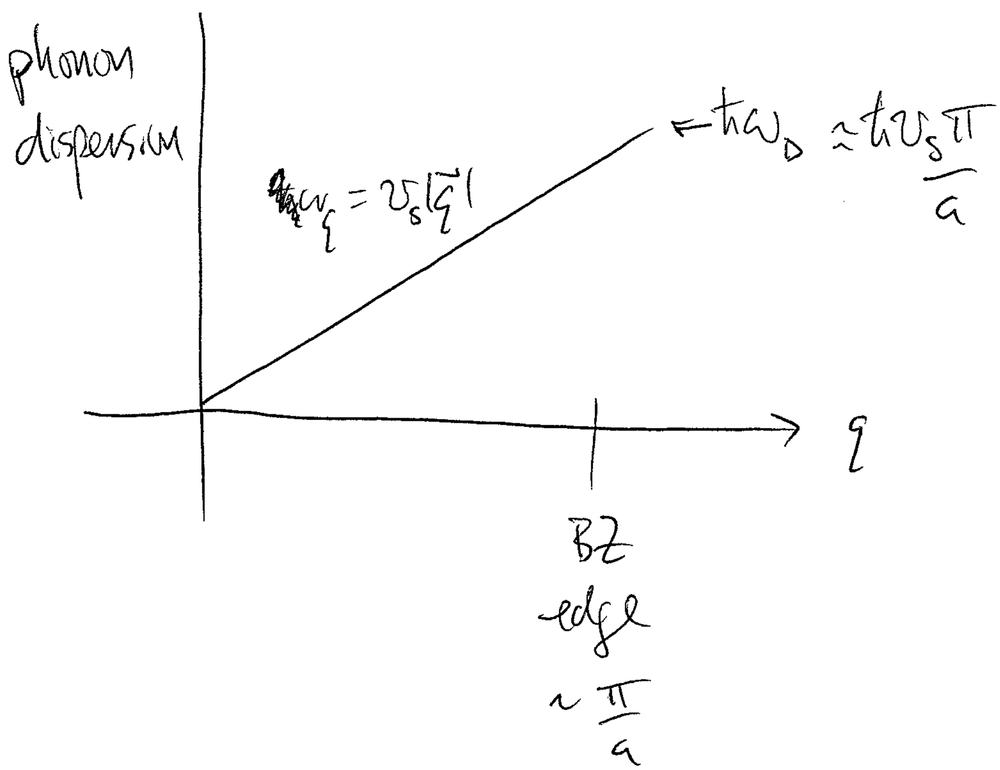
→ The filled fermi sea excludes most intermediate states from the k summations

$$\Delta(\vec{k}) = -\int \frac{d^3k'}{(2\pi)^3} \frac{V(\vec{k}-\vec{k}')\Delta(\vec{k}')}{2\varepsilon_{k'} - \tilde{E}}$$

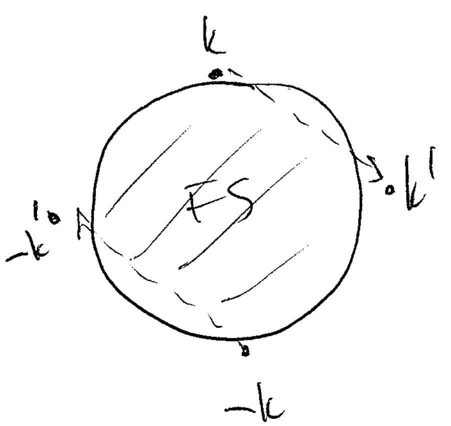
$$\rightarrow -\sum_{k'} \frac{V(\vec{k}-\vec{k}')\Delta(\vec{k}')}{2(\varepsilon_{k'} - \varepsilon_F) + \varepsilon_b}$$

restricted sum over unoccupied states in the BZ

→ Acoustic phonons set the Debye energy scale, which serves as an upper limit on the strength of phonon-mediated electron-electron attraction



→ Model of Cooper pair scattering



$$V(\vec{k}-\vec{k}') = \begin{cases} -V_0 & \text{if } \varepsilon_F < |\vec{k}| < \varepsilon_F + \hbar\omega_D \\ & \text{and } \varepsilon_F < |\vec{k}'| < \varepsilon_F + \hbar\omega_D \\ 0 & \text{otherwise} \end{cases}$$

$$\Delta(\vec{k}) = -\sum_{k'} \frac{V(\vec{k}-\vec{k}')\,\Delta(\vec{k}')}{2(\varepsilon_{k'}-\varepsilon_F)+\varepsilon_b}$$

becomes

$$1 = V_0 \int_{\varepsilon_F}^{\varepsilon_F+\hbar\omega_D} d\varepsilon \, \frac{D(\varepsilon)}{2(\varepsilon-\varepsilon_F)+\varepsilon_b}$$

$$= \frac{V_0}{2}\int_0^{\hbar\omega_D} d\varepsilon \, \frac{D(\varepsilon_F+\varepsilon)}{\varepsilon+\varepsilon_b/2}$$

negligible over small energy window $[0,\hbar\omega_D]$

$$= \frac{V_0}{2}\int_0^{\hbar\omega_D} d\varepsilon \, \frac{D(\varepsilon_F)+D'(\varepsilon_F)\varepsilon+\cdots}{\varepsilon+\varepsilon_b/2}$$

$$\simeq \frac{V_0}{2} D(\varepsilon_F) \log\left(\frac{\hbar\omega_D+\varepsilon_b/2}{\varepsilon_b/2}\right)$$

$$\Rightarrow \exp\left(\frac{2}{V_0 D(\varepsilon_F)}\right) = \frac{2\hbar\omega_D+\varepsilon_b}{\varepsilon_b} \simeq \frac{2\hbar\omega_D}{\varepsilon_b}$$

$$\Rightarrow \varepsilon_b \simeq 2\hbar\omega_D \, e^{-2/V_0 D(\varepsilon_F)}$$

exponentially small gap for arbitrarily small $V_0 D(\varepsilon_F)$

* Energy of the electron pair

$$E_{pair} = 2\varepsilon_F - 2\hbar\omega_D e^{-2/(V_0 D(\varepsilon_F))}$$

falls below the Fermi level

→ Cooper pair formation destabilizes the Fermi Sea