SET 2 – due 16 September

Free spinless fermions in one dimension on a lattice of L lattice sites and lattice spacing a have a "hopping" or "tight-binding" Hamiltonian

$$H = -t_0 \sum_{m=0}^{L-1} c_{m+1}^\dagger c_m + c_{m-1}^\dagger c_m \tag{1}$$

where c_m annihilates an electron at site m and $c_{m+1}^\dagger$ creates an electron at site $m+1$. Assume that the sites form a ring of physical length aL where "a" is the lattice spacing.

(a) [4 points] Defining

$$c_k = \frac{1}{\sqrt{L}} \sum_m e^{ikam} c_m \tag{2}$$

where $k = 2\pi n_k/aL$, $n_k = -L/2, -L/2+1 \ldots L/2-1$, find an expression for H in momentum space. Sketch $E(k)$ vs. k. Note that for the case of periodic boundary conditions (particles on a ring) there is a useful identity

$$\frac{1}{L} \sum_k e^{ika(m-n)} = \delta_{m,n}. \tag{3}$$

(b)[5 points] Now define $|k_F|$ from $E(|k_F|) = 0$ and define particle and hole operators $c_{\pm(k_F+\kappa)} = b_{\pm\kappa}$ (annihilates a particle at κ) and $c_{\pm(k_F-\kappa)} = d_{\pm\kappa}^\dagger$ (creates a hole at κ). Measuring energies in terms of κ show

$$H = 2t_0 \sum_{\kappa=-k_F}^{\kappa=k_F} (b_\kappa^\dagger b_\kappa + d_\kappa^\dagger d_\kappa) \sin(|\kappa a|) + C \tag{4}$$

where C is a constant.

(c) [5 points] Show $[N, H] = 0$ where $N = \sum_m c_m^\dagger c_m$ (this is easiest in momentum space).

(d) [5 points] If we have a ground state consisting of a half-filled band, $c_k|0\rangle = 0$ for $|k| > k_F$ and $c_k^\dagger|0\rangle = 0$ ifor $|k| < k_F$, describe the first few excited states of the system with the same N as the ground state in terms of electrons and then in terms of particles and holes.

e) [6 points] If phonons are also present, an electron-phonon interaction might be $H_I = \sum_n c_n^\dagger c_n \phi_n$ with ϕ the phonon field. Writing

$$\phi_n = \sum_p a_p e^{-ipan} + a_p^\dagger e^{ipan}$$

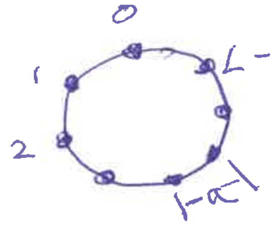
write out H_I in momentum space and describe the different kinds of interaction terms you get in terms of electrons and in terms of particle/hole creation and annihilation.

Comments:

- Many variations on this Hamiltonian are used in condensed matter physics
- Remember this problem set when we come to the Dirac equation

L1

$$H = -t_0 \sum_{m=0}^{N-1} c^\dagger_{m+1} c_m + c^\dagger_{m-1} c_m$$



Write $c_k = \frac{1}{\sqrt{L}} \sum_m e^{ikam} c_m$, $k = \frac{2\pi}{aL} n_k$.

A convenient set of n_k's is

$$n_k = -\frac{L}{2}, -\frac{L}{2}+1, -\frac{L}{2}+2 \dots \frac{L}{2}-1.$$

Pause to check Fourier conventions.

$$\sum_k c_k e^{-ikna} = \frac{1}{\sqrt{L}} \sum_m \sum_k c_m e^{ika(m-n)}$$

$$= \frac{1}{\sqrt{L}} \sum_m c_m \cdot L\,\delta_{m,n} = \sqrt{L}\, c_n$$

(since if $m=n$ there are L k's in the sum):

$$c_n = \frac{1}{\sqrt{L}} \sum_k c_k e^{-ikan} \qquad c_n^\dagger = \frac{1}{\sqrt{L}} \sum_k c_k^\dagger e^{+ikan}$$

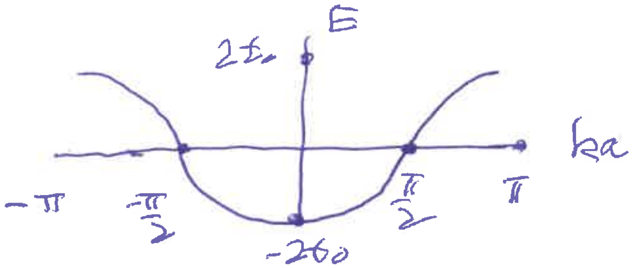
$$H = -\frac{t_0}{L} \sum_{m=0}^{L-1} \sum_k \sum_{k'} c_k^\dagger e^{ikam} \left[e^{ika} + e^{-ika} \right] c_{k'} e^{-ik'am}$$

$$= -t_0 \sum_{k,k'} \delta_{kk'} c_k^\dagger c_{k'} \cdot 2\cos ka$$

$$= -2t_0 \sum_k \cos ka \; c_k^\dagger c_k = \sum_k E(k)\, c_k^\dagger c_k$$

We have diagonalized H.

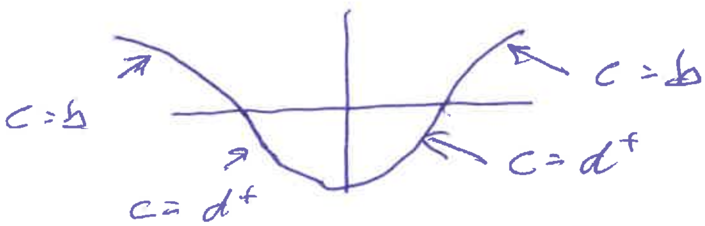
$E(k) = -2t_0 \cos ka.$



Other choices for n_k, for example $n_k = 0$ to $L-1$, just shift the picture in k.

b) From the picture, $E(|k_F|) = 0$ at $k_F a = \frac{\pi}{2}$.
As we continue, 1-d is messy:

$$c_\pm(k_F + K) \equiv b_{\pm K}, \quad c_\mp(k_F - K) = d^\dagger_{\pm k}.$$



We can rewrite H as

$$H = -2t_0 \sum_{|k|<k_F} (\cos ka)\, c_k^\dagger c_k - 2t_0 \sum_{|k|>k_F} (\cos ka) \times c_k^\dagger c_k$$

In the first term, $c_k^\dagger c_k = d_k d_k^\dagger = 1 - d_k^\dagger d_k$, anticommuting the d and $d^\dagger$. Then, $k = k_F - K$,

$$-2t_0 \cos(k_F - K)a = -2t_0 \cos\left(\frac{\pi}{2a} - K\right)a$$

$= -2t_0 \sin|Ka|$. The absolute value is needed to handle the left side of the Brillouin zone correctly. The second term is

$$-2t_0 \cos(k_F + K)\, b_K^\dagger b_K = -2t_0 \cos\left(\frac{\pi}{2a} + K\right)a\, b_K^\dagger b_K$$

$= 2t_0 \sin|Ka|$ so

$$H = 2t_0 \sum_{k=-k_F}^{k_F} \left(b_k^+ b_k + d_k^+ d_k \right) \sin|ka| + E_0$$

and $E_0 = -2t_0 \sum_{|k|<k_F} \cos ka.$

We have rewritten H to count the number of <u>particles</u> (states with electrons with $|k| > k_F$) and <u>holes</u> (states with missing electrons with $|k| < k_F$) — both terms contribute positive quantities to H.

c) $[N, H] = ?$ $N = \sum_n c_n^+ c_n = \sum_k c_k^+ c_k$

(basically the same calculation as in (a)!)

Then $N = \sum_k c_k^+ c_k$ and $H = \sum_k E(k)\, c_k^+ c_k$ obviously commute — work it out if it isn't obvious! Note $N = \sum_k \left(b_k^+ b_k - d_k^+ d_k \right) + \frac{N}{2}$

or $N = \#$ of particles $- \#$ of holes $+ \frac{N}{2}$.

$\frac{N}{2}$ counts the number of states with $|k| < k_F$

d) For the half-filled band, the electronic ground state $|\Phi\rangle$ (better to call it $|0\rangle$!) is $c_k^+|0\rangle = 0$ for $|k| < k_F$, $c_k|0\rangle = 0$ if $k > k_F$

and this is $b_k|0\rangle = 0$, $d_k|0\rangle = 0$ for all k - a state with zero particles, zero holes.

Excited states with the same N as $|0\rangle$ are

$$c_p^+ c_q |0\rangle \quad \text{or} \quad b^+_{p-k_F} d^+_{k_F-q} |0\rangle.$$

You can think of these as states with the same number of electrons, or as one-particle, one hole states. Examples of higher energy states are

$$c^+_{p_1} c^+_{p_2} c_{q_1} c_{q_2} |0\rangle \quad \text{or} \quad b^+_{k_1} b^+_{k_2} d^+_{k_3} d^+_{k_4} |0\rangle,$$

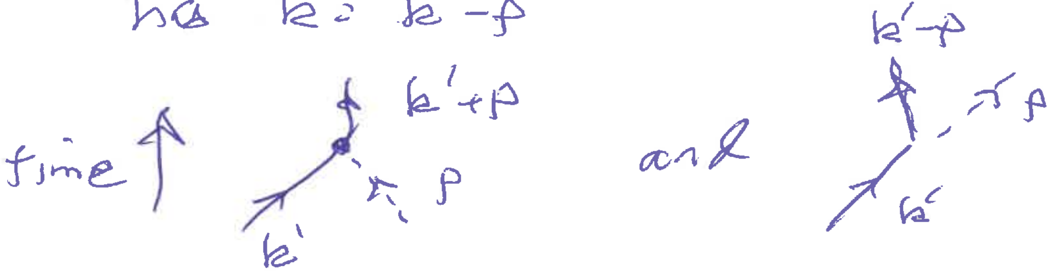
2 particle - 2 hole states. Remember - the energy associated with both particles and holes is <u>positive</u>.

e) $H_I = \sum_n c_n^+ c_n \phi_n$, $\phi_n = \sum_p a_p e^{-ipan} + a_p^+ e^{ipan}$

$$H_I = \frac{1}{L} \sum_n \sum_{kk'p} c_k^+ c_{k'} e^{-i(k'-k)an} \left[a_p e^{-ipan} + a_p^+ e^{ipan} \right]$$

$$= \sum_{kk'p} \left\{ \delta(k'-k+p)\, c_k^+ c_{k'} a_p + \delta(k'-k-p)\, c_k^+ c_{k'} a_p^+ \right\}$$

the interpretation: In the first term, an electron with k' absorbs a phonon with p to create an electron at $k = k'+p$.
In the second term, the electron at k' emits a photon at p and the final electron has $k = k'-p$



The particle-hole vertices are messy to write but easy to ~~enumerate~~ enumerate–
c can be b or $d^\dagger$, $c^\dagger$ can be $b^\dagger$ or d.
Let's look at the phonon absorption terms– $\delta(k'+p-k)\, c^\dagger_k c_{k'} a_p$:

a) $k = k_F + K$, $k' = k_F + K'$

$$\rightarrow \delta(k_F + K' + p - k_F - K)\, b^\dagger_K b_{K'} a_p$$

$$= \delta(K' + p - K)\, b^\dagger_K b_{K'} a_p$$

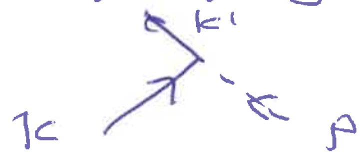
A particle absorbs a phonon and scatters.

b) $k = k_F - K$, $k' = k_F - K'$

$$\delta(k_F - K' + p - k_F + K)\, d_K\, d^+_{K'}\, a_p$$

$$= \delta(K + p - K')\, d_K\, d^+_{K'}\, a_p$$

A hole absorbs a phonon, scatter

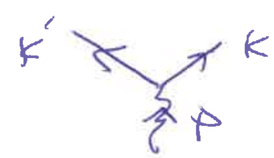


c) $k = k_F + K$, $k' = k_F - K'$

$$\delta(k_F - K' + p - k_F - K)\, b^+_K\, d^+_{K'}\, a_p$$

$$= \delta(p - K - K')\, b^+_K\, d^+_{K'}\, a_p$$

The phonon converts to an electron-hole pair.



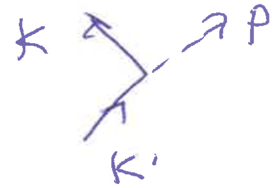
d) $k = k_F - K$ $k' = k_F + K'$

$$\delta(k_F + K' + p - k_F + K)\, d_K\, b_{K'}\, a_p$$

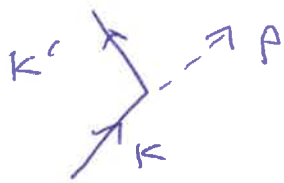
$$= \delta(K' + p + K)\, d_K\, b_{K'}\, a_p$$

All 3 annihilate at a point. This peculiar process cant occur if all 3 momenta are positive, but we have the two ~~sides of the~~ "sides" of the dispersion relation, the two separate k_F's $= \pm \pi/2a$. In solid state physics this is called "umklapp scattering." Note you need $p > 2k_F$ to drive it

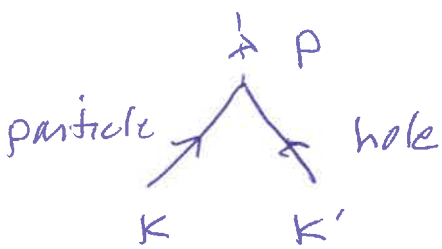
Emission is similar



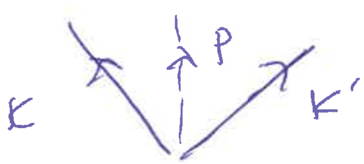
particle emits phonon



hole emits phonon



particle-hole annihilation



umklapp

Remember this problem when we study the Dirac equation.