ICFP M1 - QUANTUM MATTER - TD n°1 - Solutions
Basics of Condensed Matter Theory

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Exercise 1: Avoided crossing at zone boundaries in 1d. Consider a fermionic non-interacting 1d system with inversion symmetry and the corresponding Hamiltonian for a set of bands which cross at the Brillouin zone boundary.

1. This will happen for example in the reduced band scheme for the Hamiltonian of (possibly spinless) free electrons in 1d. Why?

Let us first consider the free electron Hamiltonian is $H_{\text{free}} = \mathbf{p}^2/(2m)$. Its spectrum is $E_n(k) = (k + 2n\pi/a)^2/(2m)$ where k is quasimomentum (usually chosen to lie in the first Brillouin zone), n is an integer, and a is the lattice spacing. At $k = -\pi/a$, there exist a two-fold degeneracy of the spectrum $E_0(-\pi/a) = E_1(-\pi/a)$.

A more general (and elegant) argument (also in the continuum) goes as follows. In the continuum, the Hamiltonian is invariant under translations by an arbitrary distance d. Let us consider a translation by $d = a/2$. Using Bloch's form for the plane wave eigenstates $\psi = e^{ikx}u(x)$ with u being a-periodic, then $T_{a/2}P\psi = e^{ika}PT\psi$ where $T_{a/2}$ is a translation by $a/2$ and P is inversion (P for parity). Indeed,

$$\begin{aligned} T_{a/2}P\psi &= T_{a/2}Pe^{ikx}u(x) = T_{a/2}e^{-ikx}u(-x) = e^{-ik(x-a/2)}u(-(x-a/2)) && (1)\\ &= Pe^{ik(x+a/2)}u(x+a/2) = PT_{a/2}e^{ik(x+a)}u(x+a) = PT_{a/2}e^{ik(x+a)}u(x) = e^{ika}T_{a/2}P\psi. && (2)\end{aligned}$$

At the zone boundary where $k = \pm\pi/a$, this means $T_{a/2}P = -PT_{a/2}$, i.e. $\{T_{a/2}, P\} = 0$. Therefore, the two operations anticommute and there must be two degenerate states. Indeed, both P and $T_{a/2}$ are symmetries of the system, *i.e.* they commute with H. In particular, they stabilise the eigenspaces of H. If the eigenvalue was not degenerate, the eigenspace would be of dimension one and all operators stabilising this space would commute in it. Since P and $T_{a/2}$ anticommute, the eigenspace cannot be of dimension 1.

2. Write down an "effective" Hamiltonian which describes two of the bands at and near their crossing (i.e. a 2×2 matrix).

Generically, in the eigenbasis where we've shifted the labeling of the momentum,

$$H_{2\times 2}(\pi/a + \delta k) = \begin{pmatrix} \epsilon_1(\frac{\pi}{a} + \delta k) & 0 \\ 0 & \epsilon_2(\frac{\pi}{a} + \delta k) \end{pmatrix}, \tag{3}$$

and unless linear-in-k terms are forbidden by symmetry, then $\epsilon_i(\frac{\pi}{a} + \delta k) \approx \epsilon_0(\frac{\pi}{a}) + v_i\delta k$, $i = 1, 2$.

3. Now add to the free electron Hamiltonian a periodic potential $\hat{V}$, $\hat{V}(x + a) = \hat{V}(x)$, where a is the lattice spacing. Write this potential in second quantification.

In second quantized form, $\hat{V}(x)$ is $\hat{V}(x) = c_x^\dagger V(x) c_x$, where $c_x, c_x^\dagger$ are the fermion annihilation and creation operators at site x. Because of the translation symmetry with period a, V can be written as a Fourier series (up to proper normalization):

$$V(x) = \sum_m e^{i2\pi mx/a} V_m. \tag{4}$$

4. Write this potential in Fourier space and deduce that it introduces a coupling between states at k-points separated by $2\pi/a$. How does this translate into our effective 2-band matrix?

We now have, up to proper normalization...

$$H_V = \sum_{\mathbf{x}} c_x^\dagger V(x) c_x = \sum_{\mathbf{x}} \sum_{k,k',k''} c_k^\dagger V(k'') c_{k'} e^{i(-k+k''+k')x} = \sum_{k,k'} c_k^\dagger V(k-k') c_{k'} = \sum_k \sum_m c_k^\dagger V_m c_{k+2\pi m/a}. \tag{5}$$

This introduces in particular a coupling between momenta at k and $k + 2\pi/a$, for all k, and so one between the degenerate states at $\pm\pi/a$. In our effective 2-band matrix, which focuses on just one pair of states, this introduces off-diagonal terms.

5. What are the consequences on the band "crossing"?

This should be straightforward from class! We are left with a "generic" 2×2 Hermitian matrix, which in general does not have degenerate eigenvalues.

Exercise 2: Collapse of the bosonic matter. First let us recall the situation of a single atom,

$$H = \sum_{i=1}^{Z} \left(\frac{p_i^2}{2m_r} - \frac{Ze^2}{|\mathbf{x}_i|} \right) + \sum_{i<j=1}^{Z} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|}, \tag{6}$$

where we separated and eliminated the center of mass coordinate, and $m_r \approx m_e$ is the reduced mass (in the Born-Oppenheimer approximation, $m_r = m_e$, which is seen to be very accurate).

The next step is the many-electron atom. This raises a new fundamental question: how does the size of matter change as you increase the number of charges? We are familiar with conventional matter, which is *extensive*: the volume of material is proportional to the number of electrons and protons in it, i.e. to its mass. How does this end up being the case? If one proton attracts one electron, more protons will attract more electrons more strongly, so why would matter not *decrease* in size as we add more electrons and protons? What prevents such a many-particle *collapse* of matter?

In the context of a multi-electron atom, the question becomes: how does the atomic radius depend upon the atomic number Z? In fact, it is easy to show that avoiding many-particle collapse relies not only on uncertainty but also on Fermi-Dirac statistics and the Pauli exclusion principle. If electrons were bosons, then actually collapse would indeed occur! Let us see this by constructing a bosonic variational wavefunction for Eq. (6) which puts every electron in the same, spherically symmetric, state: $\Psi = \prod_i \psi(r_i)$, where $r_i = |\mathbf{x}_i|$.

1. Recall the definition of a variational energy, and evaluate it in the "Ansatz" state $|\Psi\rangle$.

Using $\hbar = 1$ for simplicity,

$$\begin{aligned}
\langle\Psi|H|\Psi\rangle =& \frac{4\pi Z}{2m_r} \int_0^\infty dr r^2 \left(\frac{d\psi}{dr}\right)^2 - 4\pi Z^2 e^2 \int_0^\infty dr r |\psi(r)|^2 \\
&+ 8\pi^2 e^2 \frac{Z(Z-1)}{2} \int_0^\infty dr_1 dr_2 r_1^2 r_2^2 |\psi(r_1)|^2 |\psi(r_2)|^2 \int_{-1}^1 \frac{d\cos\theta}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta}} \\
=& \frac{4\pi Z}{2m_r} \int_0^\infty dr r^2 \left(\frac{d\psi}{dr}\right)^2 - 4\pi Z^2 e^2 \int_0^\infty dr r |\psi(r)|^2 \\
&+ 16\pi^2 e^2 \frac{Z(Z-1)}{2} \int_0^\infty dr_1 dr_2 \frac{r_1^2 r_2^2}{\max(r_1, r_2)} |\psi(r_1)|^2 |\psi(r_2)|^2.
\end{aligned} \tag{7}$$

Now we choose a specific form, which is just that of the ground state of the hydrogen atom:

$$\psi(r) = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{r}{a}}, \tag{8}$$

where a will determine the "size" of the atom and is a variational parameter.

2. Check that this is a normalized wavefunction.

Just integrate.

3. What is the form of the variational energy for this specific wavefunction? Identify the physical origin of each term.

We obtain then

$$\langle\Psi|H|\Psi\rangle = \frac{Z}{2m_r a^2} - \frac{Z^2 e^2}{a} + \frac{5Z(Z-1)e^2}{16a}. \tag{9}$$

Here the first term is the kinetic energy, the second term is the attraction of the electrons to the nuclei, and the third is the electron-electron repulsion.

4. What does this predict when $Z \gg 1$ (and in fact for any $Z \geq 1$)?

The crucial fact is that for large $Z \gg 1$, the Coulomb terms become dominant and scale as Z^2, and moreover the coefficient of the Z^2 term from the attraction, -1, is larger in magnitude than the coefficient of the Z^2 term from the repulsion, $5/16 < 1$, so that attraction dominates (in fact the net Coulomb effect is attractive for all $Z \geq 1$).

5. Minimize the variational energy over a, and express it in terms of the Bohr radius $a_0 = 1/(me^2)$.

Optimizing the energy over a, we find the atomic radius

$$a = \frac{16}{11Z+5} a_0 \sim_{Z\gg 1} \frac{16}{11Z} a_0, \tag{10}$$

where $a_0 = 1/me^2$ is the Bohr radius.

6. Does the $a(Z)$ (the atomic radius as a function of the atomic number) you calculated reproduce the behavior of that in *real* atoms?

We see that the size of the atom decreases linearly with the atomic number. *Real atoms do not do this!!!!* In real atoms, the atomic radius actually has a complicated evolution and is much larger than Eq. (10) for large Z.

Exercise 3: Second quantization of the Coulomb potential. As we have seen, in second quantized notation, the non-interacting Hamiltonian of a three-dimensional system of electrons subject to a lattice potential is given by

$$\hat{H}^{(0)} = \int dx \sum_\sigma c_\sigma^\dagger(x) \left[\frac{\hat{p}^2}{2m} + V(x)\right] c_\sigma(x), \tag{11}$$

where the fermionic electron field operators obey the anticommutation relations $\{c_\sigma(\mathbf{x}), c_{\sigma'}^\dagger(\mathbf{x}')\} = \delta(\mathbf{x}-\mathbf{x}')\delta_{\sigma\sigma'}$. Applying a two-body Coulomb interaction potential, $\frac{1}{2}\sum_{i\neq j} \frac{e^2}{|x_i - x_j|}$, where x_i denotes the position of the ith electron, the total many-body Hamiltonian takes the second quantized form

$$\hat{H} = \hat{H}^{(0)} + \frac{1}{2}\int dx \int dx' \sum_{\sigma\sigma'} c_\sigma^\dagger(x) c_{\sigma'}^\dagger(x') \frac{e^2}{|x-x'|} c_{\sigma'}(x') c_\sigma(x). \tag{12}$$

Setting $V(x) = 0$ and switching to the Fourier basis, reexpress the Coulomb interaction. Show that the latter is non-diagonal, and scatters electrons between different quasimomentum states.

The creation/annihilation operators become in Fourier space:

$$c_\sigma(x) = \int \frac{\mathrm{d}p}{(2\pi)^3} c_\sigma(p) e^{ipx}, \qquad c_\sigma^\dagger(x) = \int \frac{\mathrm{d}p}{(2\pi)^3} c_\sigma(p)^\dagger e^{-ipx} \tag{13}$$

while the Coulomb potential $\phi(x) = \frac{e^2}{|x|^2}$ becomes $\phi(p) = \frac{4\pi e^2}{p^2}$. To prove the last point it is useful to consider the Yukawa potential $\phi_m(x) = \frac{e^2 e^{-m|x|}}{|x|^2}$ and then to take $m \to 0$. Developing each term and simplifying the Dirac distributions $\delta(x) = \int \frac{\mathrm{d}p}{(2\pi)^3} e^{ipx}$ we find:

$$\hat{H}_{\text{int}} = \frac{1}{2}\int dx \int dx' \sum_{\sigma\sigma'} c_\sigma^\dagger(x) c_{\sigma'}^\dagger(x') \frac{e^2}{|x-x'|} c_{\sigma'}(x') c_\sigma(x) \tag{14}$$

$$= \frac{1}{2}\int \frac{\mathrm{d}p_1 \mathrm{d}p_2 \mathrm{d}p}{(2\pi)^9} \sum_{\sigma\sigma'} c_\sigma^\dagger(p_1) c_{\sigma'}^\dagger(p_1) \frac{4\pi e^2}{p^2} c_{\sigma'}(p_2+p) c_\sigma(p_1-p). \tag{15}$$

We see that an exchange of momentum p between the electron label σ and the electron label σ'. In particular, the Hamiltonian is non-diagonal.

Exercise 4: About time-reversal symmetry.

1. Assuming that the Hamiltonian is invariant under time reversal, prove that the wave function for the corresponding spinless nondegenerate system at any given instant of time can always be chosen to be real.

Let $|n\rangle$ be an eigenstate of the Hamiltonian $\hat{H}$: $\hat{H}|n\rangle = E_n|n\rangle$. Applying the time reversal operator θ we have $\hat{H}\theta|n\rangle = \theta\hat{H}|n\rangle = E_n|n\rangle$ *i.e.* $\theta|n\rangle = e^{i\delta}|n\rangle$ using that the Hamiltonian is nondegenerate. Here, δ is arbitrary bu redefinition of θ. Letting the dynamics happen we have

$$\theta|n,t\rangle = \theta e^{-iE_nt}|n\rangle = e^{iE_nt}\theta|n\rangle = e^{iE_nt+\delta}|n\rangle = e^{2iE_nt+i\delta}|n,t\rangle \tag{16}$$

Now introducing the identity $\int \mathrm{d}x|x\rangle\langle x|$ and using that θ is anti-linear, we find

$$\theta\int \mathrm{d}x|x\rangle\langle x|n,t\rangle = \int \mathrm{d}x|x\rangle\langle x|n,t\rangle^* = e^{2iE_nt+i\delta}\int \mathrm{d}x|x\rangle\langle x||n,t\rangle \tag{17}$$

Then the eigenstate fulfil $\phi_n(x,t)^* = e^{2iE_nt+i\delta}\phi_n(x,t)$. At each time t there exists a phase δ such that ϕ_n is real.

2. The wave function for a plane-wave state at $t = 0$ is given by a complex function $e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}$. Why does this not violate time-reversal invariance?

To understand this, let us consider a simple case: $\hat{H} = \frac{p^2}{2m}$. The Schrdinger equation then writes $\frac{\hbar^2}{2m}\Delta\phi_n = E_n\phi_n$. Therefore, $\phi_n(x) = Ae^{ipx/\hbar} + Be^{-ipx/\hbar}$. There is a degeneracy with the two states $|\pm p\rangle$ which have the same energy. In particular, the previous question does not apply and real combinations could be chosen.

3. Let $\phi(\mathbf{p}')$ be the momentum-space wave function for a state $|\alpha\rangle$, that is, $\phi(\mathbf{p}') = \langle\mathbf{p}'|\alpha\rangle$. Is the momentum-space wave function for the time-reversed state $\Theta|\alpha\rangle$ given by $\phi(\mathbf{p}'), \phi(-\mathbf{p}'), \phi^*(\mathbf{p}')$, or $\phi^*(-\mathbf{p}')$? Justify your answer.

First, we must have $\theta|p\rangle = |-p\rangle$ as a time reversal with invert the momentum. We can decompose $|\alpha\rangle = \int \mathrm{d}p\phi(p)|p\rangle$. Therefore,

$$\langle p|\theta|\alpha\rangle = \langle p|\theta\int \mathrm{d}p'\phi(p')|p'\rangle = \langle p|\int \mathrm{d}p'\phi(p')^*|-p'\rangle = \phi(-p)^* \tag{18}$$

4. *(Hard)* Consider a spin-1 system whose Hamiltonian is given by

$$H = AS_z^2 + B(S_x^2 - S_y^2). \tag{19}$$

Find the normalized energy eigenstates and eigenvalues. (A spin-dependent Hamiltonian of this kind actually appears in crystal physics.) Is this Hamiltonian invariant under time reversal? How do the normalized eigenstates you obtained transform under time reversal?

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