ICFP M1 - QUANTUM MATTER - TD n°1 - Exercises
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?
2. Write down an "effective" Hamiltonian which describes two of the bands at and near their crossing (i.e. a 2×2 matrix).
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.
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?
5. What are the consequences on the band "crossing"?

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

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

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. (1) 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 $|\Psi\rangle$.

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

   $$\psi(r) = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{r}{a}}, \tag{2}$$

   where a will determine the "size" of the atom and is a variational parameter.
2. Check that this is a normalized wavefunction.
3. What is the form of the variational energy for this specific wavefunction? Identify the physical origin of each term.
4. What does this predict when $Z \gg 1$ (and in fact for any $Z \geq 1$)?
5. Minimize the variational energy over a, and express it in terms of the Bohr radius $a_0 = 1/(me^2)$.
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?

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

$$\hat{H}^{(0)} = \int dx \sum_{\sigma} c_{\sigma}^{\dagger}(x) \left[\frac{\hat{p}^2}{2m} + V(x) \right] c_{\sigma}(x), \tag{3}$$

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

$$\hat{H} = \hat{H}^{(0)} + \frac{1}{2} \int dx \int dx' \sum_{\sigma\sigma'} c_{\sigma}^{\dagger}(x) c_{\sigma'}^{\dagger}(x') \frac{e^2}{|x - x'|} c_{\sigma'}(x') c_{\sigma}(x). \tag{4}$$

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.

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.

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?

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.

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

$$H = AS_z^2 + B(S_x^2 - S_y^2). \tag{5}$$

   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?