Homework 4

Due: February 23 at 11:59 PM. Submit on Canvas.

Problem 1 (Benzene): The benzene molecule, shown in Figure 1, consists of 6 carbon atoms arranged in a ring. Each carbon atom contributes one mobile electron which will be delocalized around the entire molecule. A toy model describing a single such electron is as follows: let $|n\rangle$ denote the state where the electron is localized around carbon atom $n = 1, \ldots, 6$. There are 6 mobile electrons, assumed to be non-interacting, each of which is described by the Hamiltonian

$$H = -\alpha \sum_{n=1}^{6} \left(|n+1\rangle\langle n| + |n\rangle\langle n+1|\right). \tag{1}$$

where we interpret $|6+1\rangle = |1\rangle$: namely the chain closes on itself!

10 **A:** This problem has a $\mathbb{Z}_6$ symmetry which we can use to exactly solve it.

A1. Define the operator

$$R = \sum_{n=1}^{6} |n+1\rangle\langle n|. \tag{2}$$

Show that $R^6 = 1$.

A2. Show that $[H, R] = 0$.

A3. Find the eigenvectors/values of H.

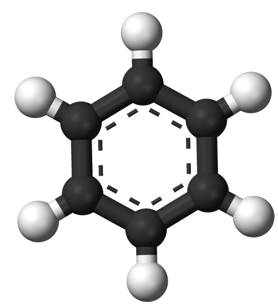

Figure 1: The molecule benzene, with carbon atoms in black and hydrogen atoms in white (from Wikipedia). This problem is about the electronic states on the central carbon ring.

10 **B:** Now return to the 6 electron problem. While you do not need to write the wave function explicitly, qualitatively describe the configuration of the electrons in the ground state of benzene.

20 **Problem 2:** Consider a Hamiltonian H describing a particle hopping in a one-dimensional lattice:

$$H = \sum_{n=-\infty}^{\infty} \left[4a\left(|n+1\rangle\langle n| + |n\rangle\langle n+1|\right) - a\left(|n+2\rangle\langle n| + |n\rangle\langle n+2|\right)\right]. \tag{3}$$

1. Write out $H|n\rangle$ (as in Lectures 10 and 11).
2. Show that $[H, R] = 0$. Here R is defined as in Lecture 11.
3. Find the eigenvalues of H, and describe the resulting dispersion relation $E(k)$.
4. Are the low energy states well approximated by a particle of some effective mass? Why or why not?

20 **Problem 3 (White dwarf):** A **white dwarf** is a star in which the quantum mechanical "degeneracy pressure" arising from a Fermi gas of mobile electrons prevents gravitational collapse. In this problem, we consider a white dwarf to be a star of radius r, containing a density n of nucleons of mass m_{nuc}. Assume that every nucleon contributes one mobile electron of mass m to a Fermi gas. The gravitational potential energy of a white dwarf of N total nucleons can be approximated as

$$V_{\text{grav}} = -\frac{3GM^2N^2}{5r}. \tag{4}$$

1. What is the number density of mobile electrons, and the corresponding energy density of the Fermi gas?[1] Conclude that the total energy of the white dwarf is given by

$$E_{\text{tot}} = -\frac{3GM^2N^2}{5r} + \left(\frac{3}{2\pi}\right)^{7/3} \frac{\pi^3\hbar^2N^{5/3}}{5mr^2} \tag{5}$$

2. Find the radius R of the white dwarf by minimizing E_{tot}:

$$r = \left(\frac{9\pi}{4}\right)^{2/3} \frac{\hbar^2}{GmM^2N^{1/3}}. \tag{6}$$

3. Numerically determine the radius of a white dwarf with a total mass comparable to our sun, 10^{30} kg. Estimate that the nucleon mass $M \approx 10^{-27}$ kg and the electron mass $m \approx 10^{-30}$ kg in your calculation.

Problem 4: Consider the following model of a single electron moving in a one-dimensional solid:

$$H = -\sum_{n=-\infty}^{\infty} (\beta + (-1)^n\gamma)\left(|n\rangle\langle n+1| + |n+1\rangle\langle n|\right). \tag{7}$$

This Hamiltonian is similar to, but distinct from, the one studied in Lecture 12.

10 **A:** Show explicitly that if $\gamma \neq 0$, $[H, R] \neq 0$ (where R was defined in Lecture 11); however, $[H, R^2] = 0$ does hold.

20 **B:** Show that the eigenvalues of H are

$$E(k) = \pm 2\sqrt{\beta^2\cos^2 k + \gamma^2\sin^2 k}, \tag{8}$$

where k is the dimensionless wave number discussed in Lectures 11 and 12. Explain in this formula (or the one you find) the range of k that correspond to distinct quantum states, and why.

10 **C:** Suppose that in a chain of length $L \gg 1$, a fraction νL ($0 \leq \nu \leq 1$ of the atoms in the chain contribute a mobile electron that can move throughout the metal. For what values of ν do we find a metal, and for what ν an insulator? Explain your answer.

[1] *Hint:* The answer is given in Lecture 9 – scan through the recorded lecture if you need to!

Problem 5 (Space group): The symmetry group of a crystal lattice, called the **space group**, generally combines both a discrete rotational group (called a point group - as it leaves one point fixed!) and a spatial translation. In this problem we will think about the simplest such "interesting" space group, which describes the Hamiltonian model from Lectures 10 and 11:

$$H = -\beta \sum_{n\in\mathbb{Z}} \left[|n+1\rangle\langle n| + |n\rangle\langle n+1|\right]. \tag{9}$$

5 **A:** Let us define the parity transformation

$$P|n\rangle = |-n\rangle. \tag{10}$$

Note that this leaves the origin $|0\rangle$ fixed. Show that $[H, P] = 0$ and that $P^2 = 1$; hence H has a parity symmetry.

10 **B:** Let R be the discrete translation defined in Lectures 10 and 11. Show that H has a *symmetry group* consisting of $\{R^n, R^nP\}$ for any $n \in \mathbb{Z}$. You should justify both of the emphasized words.

5 **C:** Why does H have a degenerate spectrum?