

## Homework 7

**Due:** March 16 at 11:59 PM. Submit on Canvas.

**Problem 1:** Consider the following Hamiltonian, which describes a particle attracted to the origin by a force of constant strength  $F$ :

$$H = \frac{p^2}{2m} + F|x|, \quad (1)$$

10 **A:** Consider the trial wave function

$$\psi_{\text{trial}}(x) = A \times \begin{cases} \ell - |x| & |x| \leq \ell \\ 0 & \text{otherwise} \end{cases}. \quad (2)$$

By requiring that the wave function is normalized, show that

$$A = \sqrt{\frac{3}{2\ell^3}}. \quad (3)$$

20 **B:** Using the variational principle, conclude that the ground state energy of this Hamiltonian obeys

$$E_0 \leq \left( \frac{81\hbar^2 F^2}{128m} \right)^{1/3}. \quad (4)$$

**Problem 2 (Yukawa potential):** The binding of two nucleons (with reduced mass  $m$ ) is reasonably described by the following Hamiltonian for an effective single particle problem:

$$H = \frac{\mathbf{p}^2}{2m} - A\xi \frac{e^{-|\mathbf{r}|/\xi}}{|\mathbf{r}|}. \quad (5)$$

The last term, which is similar to the Coulomb potential, but with an exponential decay, is the **Yukawa potential**. This binding is mediated by the nuclear strong forces and is responsible for the existence of more complicated atoms (and ultimately, us!).<sup>1</sup>

20 **A:** Consider the following variational ansatz, already normalized for you:

$$\psi_{\text{trial}}(r; \alpha) = \sqrt{\frac{\alpha^3}{\pi}} e^{-\alpha r}. \quad (6)$$

**A1.** Show that for this problem, with a spherically symmetric trial wave function,

$$E_{\text{trial}}(\alpha) = \langle \psi_{\text{trial}}(\alpha) | H | \psi_{\text{trial}}(\alpha) \rangle = \int dr \, 4\pi r^2 \left( \frac{\hbar^2}{2m} \left| \frac{\partial \psi_{\text{trial}}}{\partial r} \right|^2 - A\xi \frac{e^{-|\mathbf{r}|/\xi}}{|\mathbf{r}|} |\psi_{\text{trial}}(\alpha)|^2 \right). \quad (7)$$

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<sup>1</sup> *Hint:* This problem is discussed in Tong's notes, if you want a few intermediate results! (But you'll need to show more steps of the calculation than he does.) Also I have switched up notation a bit, so make sure to be careful when comparing your answer to Tong.

A2. Evaluate this integral (feel free to use **Mathematica**) and show that

$$E_{\text{trial}}(\alpha) = \frac{\hbar^2 \alpha^2}{2m} - \frac{4A\xi^3 \alpha^3}{(1 + 2\alpha\xi)^2}. \quad (8)$$

15 **B:** Now let us analyze (8).

B1. Argue that there is a finite length  $\xi_c$  for which if  $\xi > \xi_c$ , a bound state must exist (i.e. the ground state energy  $E_0 < 0$ ).<sup>2</sup>

B2. For realistic nucleons,  $m \approx 8 \times 10^{-28}$  kg, and  $\xi \approx 2 \times 10^{-15}$  m. Using the fact that non-trivial atoms (nuclear bound states) exist, estimate a lower bound (numerical value, with units) on  $A$ .

**Problem 3 (Ferromagnetism):** As a toy model for how electrons in a metal interact, consider a one-dimensional infinite square well of side length  $L$  in each direction. Inside of this well, we consider two spin- $\frac{1}{2}$  electrons of charge  $-e$  and mass  $m$ .

15 **A:** As in Lecture 8, consider the problem of two non-interacting electrons in the box; namely, begin with the Hamiltonian

$$H_0 = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V_{\text{well}}(x_1) + V_{\text{well}}(x_2), \quad (9)$$

where  $V_{\text{well}}$  is the infinite square well potential.

A1. What is the ground state wave function? Why is it unique? Call it  $|0\rangle$ .

A2. Show that  $H_0$  has four degenerate first-excited states: what are they?

A3. Show that these degenerate excited states are naturally organized into a spin triplet and spin singlet state. Call a representative of the triplet (e.g. the  $J_z = \hbar$  state)  $|t\rangle$ , and call a representative of the singlet state  $|s\rangle$ .

20 **B:** Now, let us consider the electrostatic interactions of the two electrons. If this metal were truly one-dimensional, the electrostatic potential energy between them would be<sup>3</sup>

$$V_{\text{int}} = -\frac{e^2}{4\pi\epsilon} |x_1 - x_2|. \quad (10)$$

In what follows, consider the true Hamiltonian to be  $H = H_0 + V_{\text{int}}$ .

B1. Using the variational principle, and following Lecture 21, calculate the energies

$$E_0 = \langle 0 | H | 0 \rangle, \quad (11a)$$

$$E_s = \langle s | H | s \rangle, \quad (11b)$$

$$E_t = \langle t | H | t \rangle. \quad (11c)$$

You are encouraged to use **Mathematica** to do symbolic integration, rather than evaluate two-dimensional integrals that arise by hand. Argue that  $E_0 < E_s$  always, whereas  $E_t$  can either be larger or smaller than  $E_0$ , depending on the strength of interactions.

B2. Take  $m \sim 10^{-30}$  kg,  $L \sim 4 \times 10^{-10}$  m, and  $e^2/4\pi\epsilon \sim 2 \times 10^{-8}$  J/m. For these numbers, deduce that the triplet state is the lowest energy state.

<sup>2</sup>Hint: Begin by looking for values of  $\alpha$  where  $E_{\text{trial}}(\alpha) = 0$ . Can you then argue that if there two of these points, then  $E_{\text{trial}}(\alpha)$  has to be negative somewhere?

<sup>3</sup>Here,  $\epsilon$  would have different SI units than in our three-dimensional world!

When the triplet state is the lowest energy state, there is an effective interaction that prioritizes nearby electronic spins in the metal to *align*. If this happens between many electron spins, then there is a macroscopic magnetization, since each electron spin has a small magnetic moment. This leads to a **ferromagnet**: a phase of matter where magnetization will spontaneously arise.

While this is of course a toy model, the physical conclusion you should reach is actually quite reasonable. In ordinary metals such as iron, the origin of ferromagnetism (spontaneous magnetization) arises from these “exchange interactions”, and not from the dipole-dipole interactions between the electron spins themselves.

**Problem 4 (Spectral methods):** Consider an infinite square well (particle constrained to the domain  $0 \leq x \leq L$ ). Inside of this well, the Hamiltonian is

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + u \sin \frac{\pi x}{L}, \quad (12)$$

where  $u > 0$  is some positive constant. In this problem, let  $\psi_n(x)$  denote the normalized eigenstates of this Hamiltonian with  $u = 0$ :

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}, \quad (13)$$

with energy levels

$$E_n = n^2 \epsilon, \text{ where } \epsilon = \frac{\hbar^2 \pi^2}{2mL^2}. \quad (14)$$

- 10 **A:** We will attempt to find the ground state of  $H$  numerically, using a variational calculation with trial wave function

$$\psi_{\text{trial}}(x) = \sum_{n=1,3,5,\dots}^{2N-1} c_n \psi_n(x) \quad (15)$$

for some integer  $N \geq 1$ . This wave function should be normalized.

**A1.** Find the matrix  $M$  such that

$$\langle \psi_{\text{trial}} | H | \psi_{\text{trial}} \rangle = \begin{pmatrix} c_1 & \cdots & c_{2N-1} \end{pmatrix} M \begin{pmatrix} c_1 \\ \vdots \\ c_{2N-1} \end{pmatrix}. \quad (16)$$

You may take as given the following integral:

$$\int_0^L dx \psi_n(x) \psi_m(x) \sin \frac{\pi x}{L} = -\frac{4mn(1 + (-1)^{m+n})}{\pi((m+n)^2 - 1)((m-n)^2 - 1)}. \quad (17)$$

- A2.** If you were to apply the variational principle to upper bound the ground state energy of  $H$ , what would you need to calculate about the matrix  $M$ ?
- A3.** Explain why your estimate of the ground state energy  $E_0$  can only improve as  $N$  increases.
- A4.** Explain why your estimate of  $E_0$  converges to the correct answer as  $N \rightarrow \infty$ .

- 10 **B:** Now, implement this algorithm numerically.

**B1.** Pick a fixed value of  $u \neq 0$ . Estimate how quickly your estimate of  $E_0$  is converging as  $N$  gets sufficiently large.<sup>4</sup>

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<sup>4</sup>For  $u/\epsilon \sim 1$ , you should be able to deduce the answer without going beyond  $N = 100$ .

- B2. Using a sufficiently large value of  $N$ , make a numerical plot of the ground state energy as a function of  $u$  for, e.g.,  $|u|/\epsilon \lesssim 10$ .

What you have just implemented is a kind of **spectral method** for numerically finding eigenvalues of the differential operator  $H$ . Namely, rather than approximating derivatives a la

$$\frac{d\psi(x_j)}{dx} \approx \frac{\psi(x_j) - \psi(x_{j-1})}{x_j - x_{j-1}}, \quad (18)$$

and numerically implementing  $H$  in this fashion, we are instead “discretizing” the function  $\psi(x)$  by expanding it into a convenient basis of functions! While these spectral methods can be harder to scale to ultra-large scale computations, for most other problems, (pseudo)spectral methods are the gold standard for numerical solutions of differential equations.