Homework 8

Due: 11:59 PM, Tuesday, October 27. Submit your homework via Canvas.

Grading: 30 points required for full credit. 40 points are possible. You can score over 100%.

5 points **Problem 1 (Variational principle for excited states):** Construct a variational principle to bound the eigenvalue of a Hamiltonian H which lies closest to energy level ϵ, for any ϵ.[1]

Problem 2 (Ground state wave functions): The variational principle is valuable not only for bounding ground state energies, but can also give us other meaningful results. Consider a particle of mass m in a one-dimensional potential $V(x)$; assume $|V(x)| < \infty$, and also assume that there is a well-defined ground state wave function, $\psi_0(x)$, which vanishes as $x \to \pm\infty$.

5 points (a) Prove that $\psi_0(x)$ can be chosen to be real.[2]

5 points (b) Explain why we may also choose $\psi_0(x) > 0$. Proceed as follows: suppose $\psi_0(x)$ has a zero: $\psi_0(x) = c(x - x_0) + \cdots$ near $x = x_0$. Estimate the energy of a properly chosen trial wave function which "removes" the zero, as schematically shown in Figure 1. (Imagine starting with the trial function $|\psi_0(x)|$, then smooth out the kink at x_0.) You do not need to be mathematically rigorous.

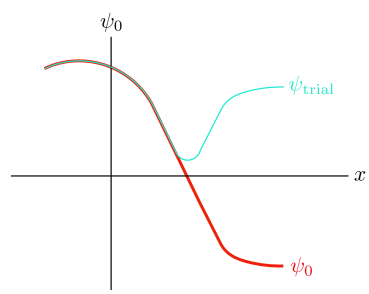

Figure 1: If the ground state wave function ψ_0 had a zero, one can design a trial function ψ_{trial} with no zeros with lower energy, leading to a contradiction.

Problem 3 (Yukawa potential): The binding of two nucleons (with reduced mass m) is reasonably described by the following Hamiltonian for an effective single particle problem:

$$H = \frac{\mathbf{p}^2}{2m} - A\xi \frac{e^{-|\mathbf{r}|/\xi}}{|\mathbf{r}|}. \tag{1}$$

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!).[3]

[1] *Hint:* What are the eigenvalues of $(H - \epsilon)^2$?

[2] *Hint:* Consider the trial function $\psi_0(x) = f(x)\exp[i\theta(x)]$, and evaluate $\langle\psi|H|\psi\rangle$. Use the variational principle to reach a contradiction if $\theta(x)$ is not a constant.

[3] *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.

5 points (a) Use the following normalized variational ansatz:

$$\psi_{\text{trial}}(r;\alpha) = \sqrt{\frac{\alpha^3}{\pi}}\mathrm{e}^{-\alpha r} \tag{2}$$

to estimate the ground state energy. Remember, this is a wave function in spherical coordinates in three dimensional space! Evaluate $E_{\text{trial}}(\alpha) = \langle\psi_{\text{trial}}(\alpha)|H|\psi_{\text{trial}}(\alpha)\rangle$.

5 points (b) Argue that there is a finite length ξ_{c} for which if $\xi > \xi_{\text{c}}$, a bound state must exist (i.e. the ground state energy $E_0 < 0$).[4]

(c) 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) do exist, estimate a lower bound (numerical value, with units) on A.

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

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + u\sin\frac{\pi x}{L}, \tag{3}$$

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

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}, \tag{4}$$

with energy levels

$$E_n = n^2\epsilon, \text{ where } \epsilon = \frac{\hbar^2\pi^2}{2mL^2}. \tag{5}$$

5 points (a) Consider the trial function $c_1\psi_1(x) + c_3\psi_3(x)$, with $c_{1,3}$ real numbers obeying $c_1^2 + c_3^2 = 1$. Is this normalized? Evaluate $\langle H\rangle$ in this trial wave function, and show that

$$\langle H\rangle = \begin{pmatrix} c_1 & c_3 \end{pmatrix}\begin{pmatrix} \epsilon + \frac{8}{3\pi}u & -\frac{8}{15\pi}u \\ -\frac{8}{15\pi}u & 9\epsilon + \frac{72}{35\pi}u \end{pmatrix}\begin{pmatrix} c_1 \\ c_3 \end{pmatrix} \tag{6}$$

You may take as given the following integral:

$$\int_0^L \mathrm{d}x\, \psi_n(x)\psi_m(x)\sin\frac{\pi x}{L} = -\frac{4mn(1+(-1)^{m+n})}{\pi((m+n)^2-1)((m-n)^2-1)}. \tag{7}$$

5 points (b) Parameterize $c_1 = \cos\theta$ and $c_3 = \sin\theta$. Then optimize the value of θ to find your variational bound on the ground state energy.[5] (The answer is ugly...you do not need to simplify it, so long as you are clear about how to obtain it.) Explain why the answer is the smallest eigenvalue of the 2×2 matrix from part (a).

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[4] *Hint:* Begin by looking for values of α 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?

[5] *Hint:* Express $\langle H\rangle$ as a function of $\cos(2\theta)$ and $\sin(2\theta)$ first. A few useful trig identities: $2\sin^2\theta = 1-\cos(2\theta)$. $2\cos^2\theta = 1+\cos(2\theta)$. $\sin(2\theta) = 2\sin\theta\cos\theta$. If $\tan\theta = x/y$, then $\cos\theta = \pm x/\sqrt{x^2+y^2}$ and $\sin\theta = \pm y/\sqrt{x^2+y^2}$.

5 points **(c)** Generalize the variational calculation, using the ansatz

$$\psi(x) = \sum_{n=1,3,5,\ldots}^{2N-1} c_n \psi_n(x) \tag{8}$$

for some integer $N > 2$. Explain why: (*1*) the ground state energy is upper bounded by the minimal eigenvalue of the $N \times N$ matrix that generalizes (6), and (*2*) this eigenvalue decreases with increasing N. Argue that in the limit $N \to \infty$, you should obtain the true ground state.

(d) Using a sufficiently large value of N, make a numerical plot of the ground state energy as a function of u.

(e) Estimate the rate of convergence of your calculation as a function of N. You should find that it is pretty rapid! What you have just implemented is (up to a change of basis) a **spectral method** for numerically finding eigenvalues of the differential operator H. What makes these spectral methods very elegant is that they "discretize" the infinite dimensional space of all functions in the domain $0 \le x \le L$ into a convenient set of *basis functions* – i.e., rather than approximating $\psi(x)$ by a pointwise "interpolation" of values $\psi(x_j)$ at a discrete set of grid points x_j ($j = 1, \ldots, N$), you have specified a set of N numbers $c_1, c_3, \ldots, c_{2N-1}$ which specify a smooth Fourier series representation of the unknown ground state wave function.