Quantum Physics II (8.05) Fall 2013
Assignment 2

Massachusetts Institute of Technology
Physics Department
September 13, 2013

Due Friday September 20, 2013
3:00 pm

Suggested Reading

- Continued from last week:
  1. Griffiths section 7.1.
  2. Introduction to linear algebra, Griffith's Appendix and Shankar Ch. 1.
- Basic foundations of quantum mechanics:
  1. Griffiths Ch.3. Griffiths does not go into as much depth with Dirac notation as we do in lecture.

Problem Set 2

1. **Square well with delta function** [10 points]

   Consider the one-dimensional infinite square well $0 \leq x \leq a$. We add a delta function at the middle of the well

   $$V(x) \;=\; V_0 a \,\delta\Big(x - \frac{a}{2}\Big)\,, \quad V_0 > 0\,, \tag{1}$$

   with V_0 a large value with units of energy. In fact, V_0 is large compared to the natural energy scale of the well:

   $$\frac{V_0}{\left(\frac{\hbar^2}{ma^2}\right)} \;\equiv\; \gamma \gg 1\,. \tag{2}$$

   The dimensionless number γ is taken to be large. The delta function is creating a barrier between the left-side and the right-side of the well. As the delta function intensity V_0 becomes infinite we can get a singular situation.

   Calculate the ground state energy, including corrections of order $1/\gamma$ but ignoring higher order ones. Compare with the energy of the first excited state. What is happening to the energy difference between these two levels?

2. **Nodes in wavefunctions** [10 points]

   We have written the Schrödinger equation in the form

   $$\psi'' + (\mathcal{E} - U(x))\psi = 0\,.$$

Let ψ_k be the energy eigenstate with energy $\mathcal{E}_k$ and ψ_{k+1} be the energy eigenstate with energy $\mathcal{E}_{k+1}$ greater than $\mathcal{E}_k$.

(a) Show that

$$\Big(\psi_{k+1}\psi_k' - \psi_k\psi_{k+1}'\Big)\Big|_a^b = (\mathcal{E}_{k+1} - \mathcal{E}_k)\int_a^b dx\,\psi_k\psi_{k+1}\,. \tag{1}$$

(b) Let now a, b with $a < b$ be two successive zeroes of $\psi_k(x)$ and assume, for convenience that $\psi_k(x) > 0$ for $a < x < b$. By making use of (1) show that ψ_{k+1} must change sign in the interval (a, b). That is, ψ_{k+1} must have at least one zero in between each pair of zeroes of ψ_k. Hint: consider the sign of each side of equation (1) under the assumption that ψ_{k+1} does not change sign in (a, b).

3. **Developing the variational principle** [10 points]

(a) Consider normalized trial wavefunctions $\psi(x)$ that are orthogonal to the ground state wavefunction ψ_1: $\int dx\,\psi_1^*(x)\psi(x) = 0$. Show that the first excited energy E_2 is bounded as:

$$E_2 \leq \int dx\;\psi^*(x)H\psi(x)\,.$$

This result has a clear generalization (that you need not prove): trial wavefunctions orthogonal to the lowest n energy eigenstates give an upper bound for the energy of the $(n+1)$-th state.

(b) Assume we can use real wavefunctions and consider the functional

$$\mathcal{F}(\psi) \;=\; \frac{\int dx\;\psi(x)H\psi(x)}{\int dx\;\psi(x)\psi(x)}\,.$$

This functional has a remarkable property: it is stationary at the energy eigenstates! You will do a computation that confirms this for a special case, while giving you insight into the nature of the critical point. Let us take

$$\psi(x) = \psi_2(x) + \sum_{n=1}\epsilon_n\psi_n(x)\,, \tag{3}$$

This is the first excited state perturbed by small additions of the other energy eigenstates: the ϵ's are all taken to be small. Evaluate the functional $\mathcal{F}$ for this wavefunction including terms quadratic in the ϵ's but ignoring terms cubic or higher order. Confirm that all linear terms in ϵ's cancel, showing that the functional is indeed stationary at $\psi_2(x)$. Does any ϵ drop out to quadratic order? Discuss the nature of the critical point (maximum, minimum, flat directions, saddle).

4. **One-dimensional attractive potentials have a bound state** [10 points]

   (Based on Exercise 5.2.2 of Shankar (p.163) part (b).) Use the variational principle to prove that any attractive potential in one dimension must have at least one bound state. We take an attractive potential to be one where the potential goes to zero at plus and minus infinity: $\lim_{x\to\pm\infty}|V(x)| = 0$, it is piecewise continuous, never positive, and not equal to zero. Note that it follows that $V(x) = -|V(x)|$.

   To do this, consider the trial wavefunction

$$\psi_\alpha(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2},$$

   and try to show that the expectation value $E(\alpha)$ of $\hat{H}$ on this state

$$E(\alpha) = \int dx\, \psi_\alpha(x)\hat{H}\psi_\alpha(x), \quad \hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - |V(x)|.$$

   can be made negative for a suitable choice of α. Finding the contribution of the potential term to $E(\alpha)$ is challenging. For arbitrary attractive $V(x)$ it can't be calculated explicitly, but finding a bound for it suffices.

   A bound can be obtained by finding a point x_0 where the potential is continuous and takes a negative value (such point must exist). Suppose

$$|V(x_0)| = 2v_0 > 0.$$

   Since the potential goes to zero at plus and minus infinity, there is a finite interval $[x_1, x_2]$ about x_0 (with $x_1 < x_0 < x_2$, $\Delta \equiv x_2 - x_1$) for which

$$|V(x)| \geq v_0.$$

   Explain how the potential term can be bounded by replacing $V(x)$ by a potential $\tilde{V}$ that satisfies $\tilde{V}(x) = -v_0$ for $x \in [x_1, x_2]$ and zero elsewhere.

5. **Variational analysis of the potential** $V(x) = \alpha x^4$ [20 points]

   We are considering the SE

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \alpha x^4\,\psi = E\psi.$$

   (a) Perform a change of coordinates, setting $x = \beta u$ and determine the constant β so that the differential equation takes the form

$$-\frac{1}{2}\frac{d^2\psi}{du^2} + (u^4 - e)\,\psi = 0.$$

   How is E given in terms of the unit-free constant e?

(b) Use an algebraic manipulator that can handle differential equations to determine the value of the constant e for the ground state energy to six digits accuracy ($e \simeq 0.67$). For this try integrating the equation numerically starting at $u = 0$ setting $\psi(0) = 1$ and $\psi'(0) = 0$ (why is this derivative zero?). Only for discrete values of e the solution does not blow up as u becomes large. The lowest such value of e is the one you are looking for.

(c) Write a candidate wavefunction for the variational principle and determine an upper bound for the first excited energy.

(d) Use the algebraic manipulator to determine the next-to-lowest value of e (to three digits accurary) and compare with your variational estimate.

6. **A property of matrices** [5 points]

We can define a function of a matrix $\mathbf{M}$ by a power series. If $f(z)$ is a function with a Taylor series expansion $f(z) = \sum_{n=0}^{\infty} f_n z^n$, then we define $f(\mathbf{M}) \equiv \sum_{n=0}^{\infty} f_n \mathbf{M}^n$. Let $\mathbf{M}$ be the matrix

$$\mathbf{M} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Show that $e^{i\mathbf{M}\theta}$ takes the form

$$e^{i\mathbf{M}\theta} = A(\theta)\,\mathbf{1} + B(\theta)\,\mathbf{M}, \tag{4}$$

where $\mathbf{1}$ is the 2×2 identity matrix and A and B are functions you must determine. What is the algebraic property of a matrix $\mathbf{M}$ of arbitrary size that would lead to this result?