8.322: Quantum Theory II

Problem Set #4 Solutions
March 12, 2007

1. **A linear potential**

   The exact solution is described by the Airy function. From Sakurai the energy is

   $$E_n = \lambda_n \left(\frac{k^2\hbar^2}{2m}\right)^{1/3}$$

   where λ_n is the n$^{\text{th}}$ zero of the Airy function. In particular, $\lambda_1 = 2.338$. The Airy function blows up exponentially, therefore the best ansätze contain an exponential factor.

   Interestingly the best guess anyone turned in was just $\psi \sim e^{-\alpha r^2}$, which was turned in by a lot of people. This gives

   $$E_0 \leq \left(\frac{81k^2\hbar^2}{4\pi m}\right)^{1/3} \approx 2.3448 \left(\frac{k^2\hbar^2}{2m}\right)^{1/3}$$

   One other good trial wavefunction was $\psi \sim e^{-\alpha r^{3/2}}$ giving a bound of $\approx 2.35 \left(\frac{k^2\hbar^2}{2m}\right)^{1/3}$.

2. **Constraints**

   Let $|\psi\rangle$ be the ground state of the constrained system. Then,

   $$|\psi\rangle = \sum c_i |\psi_i\rangle$$

   where $\{|\psi_i\rangle\}$ is a complete set of energy eigenstates.

   $$H[\psi] = \sum |c_i|^2 E_i \geq E_0$$

   An equivalent solution is given by using the variational method. The original ground state is obtained by minimizing the energy over all possible states. If one restricts the space of states by introducing a constraint, then the new minimal energy will necessarily be greater or equal than the old minimum.

3. **Adding a basis state**

   (a) The best variational upper limit is the lowest energy of all states in $\mathfrak{h}_n$. Such states can be written as linear combinations of energy eigenstates $|\psi_i^{(n)}\rangle$

   $$|\psi\rangle = \sum c_i |\psi_i^{(n)}\rangle$$

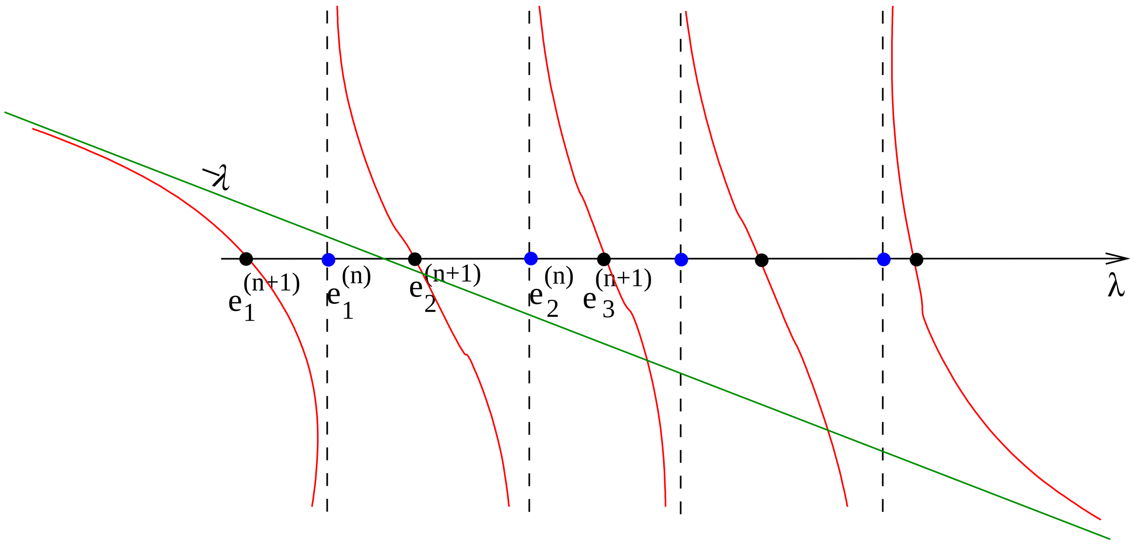

Figure 1: Graphical solution.

$$\langle\psi|H|\psi\rangle = \sum |c_i|^2 e_i^{(n)} \geq e_1^{(n)}$$

(b) Let

$$|\psi\rangle = \sum_{i=1}^{n+1} c_i |\phi_i\rangle$$

where $\{|\phi_i^{(n+1)}\rangle\} = \{|\psi_i^{(n)}\rangle, |\phi_{n+1}\rangle\}$. Hence,

$$\langle\psi|H|\psi\rangle = \sum_{i=1}^{n} |c_n|^2 e_i^{(n)} + \sum_{i=1}^{n} c_{n+1}^* c_n H_{n+1,n} + \text{h.c.} + c_{n+1}^* c_{n+1} H_{n+1,n+1}$$

We must solve

$$\det(H - \lambda \mathbb{1}) = 0$$

that is

$$\begin{vmatrix} e_1^{(n)} - \lambda & 0 & 0 & \cdots & H_{n+1,1} \\ 0 & e_2^{(n)} - \lambda & 0 & \cdots & H_{n+1,2} \\ \vdots & 0 & \ddots & 0 & \vdots \\ H_{1,n+1} & H_{2,n+1} & H_{3,n+1} & \cdots & H_{n+1,n+1} - \lambda \end{vmatrix} = 0.$$

Expanding the above determinant gives

$$(H_{n+1,n+1} - \lambda) \prod_{i=1}^{n} (e_i^{(n)} - \lambda) - \sum_{i=1}^{n} H_{i,n+1} H_{n+1,i} \prod_{j \neq i}^{n} (e_j^{(n)} - \lambda) = 0$$

After dividing out the $\prod_{i=1}^{n}(e_i^{(n)} - \lambda)$ factor, we obtain

$$H_{n+1,n+1} - \sum_{i=1}^{n} \frac{|H_{n+1,i}|^2}{e_i^{(n)} - \lambda} = \lambda$$

The graphical solution is shown in Figure 1.

This gives

$$e_1^{(n+1)} < e_1^{(n)} < e_2^{(n+1)} < e_2^{(n)} \cdots < e_n^{(n)} < e_{n+1}^{(n+1)}.$$

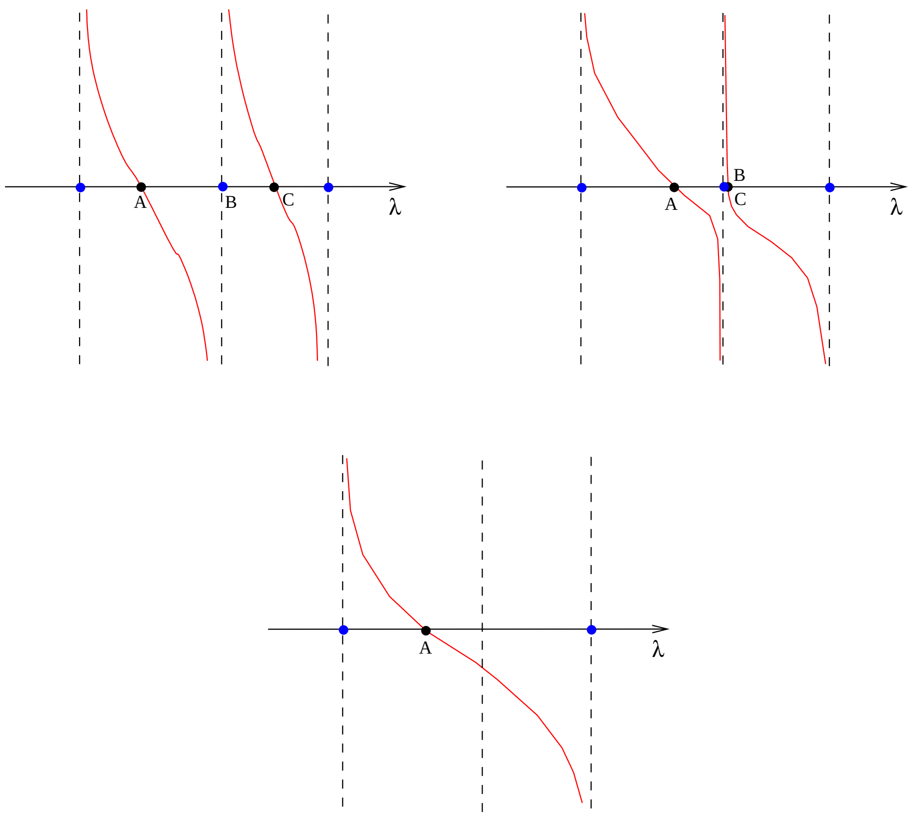

Figure 2: Vanishing $H_{n+1,i}$ matrix elements. The first figure shows the non–vanishing case. In the second figure, the corresponding matrix element is set to a small value. We see that C approaches the lower order root B. The third picture shows the case where the matrix element is zero.

4. **The minimax principle**

Let $\mathcal{H}_\phi$ denote the space spanned by $\{|\phi_i\rangle\}$. According to the variational principle, $E_n[\phi_1, \phi_2, \ldots]$ is just the ground state in $\mathcal{H}_\phi^\perp$. Let $|0\rangle, |1\rangle, \ldots$ denote the energy eigenstates. Clearly,

$$E_n[\ |0\rangle, |1\rangle, \ldots, |n-1\rangle\ ] = \langle n|H|n\rangle = E_n$$

If we do not exclude all the eigenstates up to the $(n-1)$-th excited state, then $E_n[\phi_1, \phi_2, \ldots]$ will be less than E_n and the corresponding state will have a component in the $\{|0\rangle, |1\rangle, \ldots, |n-1\rangle\}$ subspace. Thus,

$$E_n[\phi_1, \phi_2, \ldots] \leq E_n[\ |0\rangle, |1\rangle, \ldots, |n-1\rangle\ ]$$

and

$$E_n = \max_{\{\phi_i\}} E_n[\phi_1, \phi_2, \ldots].$$

5. **The quantum crossroads prize**

(a) The Schrödinger equation is

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V(x,y)\right]\psi = E\psi$$

where $V(x,y) = 0$ inside and $V = \infty$ outside. Far from the crossroads the only constraint is coming from the width d. Hence we expect that for large y

$$\psi \propto \sin\left(\frac{n\pi x}{d}\right)\left(c_1 e^{iky} + c_2 e^{-iky}\right) \qquad (n = 1, 2, \ldots)$$

and the same with $x \leftrightarrow y$ for large x. Therefore the energy threshold is

$$E_t = \frac{\hbar^2}{2m}\left(\frac{\pi}{d}\right)^2$$

(b) The above argument shows that there is a sequence of thresholds

$$E_t^n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{d}\right)^2$$

where the density of states jumps and four new modes become available.

(c) We need to construct a trial wavefunction whose energy is less than the threshold for continuum states. This is done in part (d).

(d) The best variational wavefunction was (d=1)

$$\psi \propto \begin{cases} (1-b)\left(\cos(\pi x) + \cos(\pi y)\right) + b\cos\left(\pi\sqrt{x^2 + y^2 - \frac{1}{4}}\right) & \text{for } -\frac{1}{2} \leq x \leq \frac{1}{2},\ -\frac{1}{2} \leq y \leq \frac{1}{2} \\ \cos(\pi x) e^{-a(y-1/2)} & \text{for } -\frac{1}{2} \leq x \leq \frac{1}{2},\ y > \frac{1}{2} \\ \text{Similar for other legs} & \end{cases}$$

with $a = 1.77367$ and $b = -1.17683$. This wavefunction gives ($\frac{\hbar^2}{2md^2} = 1$)

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = 0.68125 \cdot \pi^2$$

6. **WKB approximation to the transition amplitude**

(a) The particle is classically allowed everywhere. Thus, there are no turning points and we can use a single WKB wavefunction

$$\psi(x) \propto \frac{1}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int dx p(x)}$$

At $x \to -\infty$,

$$\psi(x) \propto e^{ikx}$$

At $x \to +\infty$,

$$\psi(x) \propto e^{ikx+i\delta(E)}$$

Hence,

$$2\delta(E) = \frac{1}{\hbar}\int_{-\infty}^{\infty} dx\,(p(x) - k)$$

(b) The potential is

$$V(x) = -\frac{\hbar^2}{ma^2}\text{sech}^2(x/a)$$

We need to compute the following function

$$2\delta(E) = \frac{1}{\hbar}\int_{-\infty}^{\infty} dx\,(p(x) - k)$$

where

$$p(x) = \sqrt{2m(E - V(x))} = \sqrt{\hbar^2 k^2 + \frac{2\hbar^2}{a^2}\text{sech}^2(x/a)}$$

So

$$2\delta(E) = \frac{1}{a}\int_{-\infty}^{\infty} dx \left[\sqrt{k^2a^2 + 2\ \text{sech}^2(x/a)} - ka\right]$$

Let $z = x/a$,

$$2\delta(E) = \int_{-\infty}^{\infty} dz \left[\sqrt{(ka)^2 + 2\ \text{sech}^2(z)} - ka\right]$$

Numerical integration shows that

$$\lim_{ka\to\infty} \delta(E) = \frac{1}{ka}$$

which precisely equals to the exact $\delta = \frac{1}{ka}$ value.

7. **WKB approximation to the density of states**

The Bohr–Sommerfeld quantization reads

$$\int_{x_1(E)}^{x_2(E)} dx \sqrt{2m(E - V(x))} = \hbar\pi(N(E) + \frac{1}{2})$$

Hence, differentiating w.r.t. E gives

$$\hbar\pi \frac{dN}{dE} = \sqrt{2m(E - V(x_2(E)))} - \sqrt{2m(E - V(x_1(E)))} + \frac{1}{2}\int_{x_1(E)}^{x_2(E)} dx \sqrt{\frac{2m}{E - V(x)}}$$

$$= \frac{1}{2}\int_{x_1(E)}^{x_2(E)} dx \sqrt{\frac{2m}{E - V(x)}} \tag{0.1}$$

since $V = E$ at the turning points.

Classically, the speed of the particle is given by

$$\frac{1}{2}mv(x)^2 = E - V(x)$$

$$\implies \quad |v(x)| = \sqrt{\frac{2(E - V(x))}{m}}$$

Hence, the period is

$$\tau(E) = 2\int_{x_1(E)}^{x_2(E)} dx \frac{1}{|v(x)|}$$

Comparing it with (0.1), we obtain

$$\frac{dN}{dE} = \frac{\tau(E)}{2\hbar\pi} = \frac{\tau(E)}{h}$$