PHYS 501: Mathematical Physics I

Fall 2011

Notes on Homework #2

Problem 2.4

We want to diagonalize the matrix H defined by

$$H_{nm} = \int_{-\infty}^{\infty} dx \ \psi_n^*(x) \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi_m(x) \,,$$

where the potential function is

$$V(x) = \begin{cases} 0 & (|x| < a) \,, \\ V_0 & (|x| > a) \,. \end{cases}$$

As discussed in class, we will expand the solution to the problem in terms of harmonic oscillator wavefunctions

$$\psi_n(x) = \left(\frac{\beta^2}{\pi} \right)^{1/4} \frac{1}{\sqrt{2^n n!}} \ e^{-\frac{1}{2}\beta^2 x^2} \, H_n(\beta x) \,,$$

where H_n is a Hermite polynomial and $\beta^4 = mk/\hbar^2$, where $k = 2V_0/a^2$ is the "spring constant" of the equivalent harmonic potential. The units in this calculation are such that $V_0 a^2 = 2\hbar^2/m$, so $\beta^4 = 2mV_0/\hbar^2 a^2$, or $\beta = \sqrt{2}/a$. The normalization is such that $\int |\psi_n|^2 dx = 1$, and the Hermite polynomials satisfy

$$(H_n, H_m) \equiv \int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) dx = \pi^{1/2} \, 2^n n! \, \delta_{nm} \,.$$

We write $H_{nm} = K_{nm} + V_{nm}$, where

$$K_{nm} = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \ \psi_n^*(x) \psi_m''(x)$$

and

$$V_{nm} = \int_{-\infty}^{\infty} dx \ \psi_n^*(x) V(x) \psi_m(x) \,.$$

Integrating by parts, and assuming that $\psi_n' \to 0$ as $|x| \to \infty$, we find

$$K_{nm} = \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \ \psi_n'^*(x) \psi_m'(x) \,.$$

We can evaluate this by differentiating the expression for ψ_n and using the relation $H_n'(y) = 2nH_{n-1}(y)$ (see A&W, p. 772):

$$\psi_n' = \left(\frac{\beta^2}{\pi} \right)^{1/4} \frac{1}{\sqrt{2^n n!}} \ e^{-\frac{1}{2}\beta^2 x^2} \left[-\beta^2 x H_n(\beta x) + 2n\beta H_{n-1}(\beta x) \right] \,,$$

Substituting $y = \beta x$ in the integral, we obtain

$$\begin{aligned}
K_{nm} &= A_{nm}\beta \int_{-\infty}^{\infty} dy\ [e^{-\frac{1}{2}y^2} H_n(y)]'\ [e^{-\frac{1}{2}y^2} H_m(y)]' \\
&= A_{nm}\beta \int_{-\infty}^{\infty} dy\ e^{-y^2}[nH_{n-1}(y) - \tfrac{1}{2}H_{n+1}(y)]\ [mH_{m-1}(y) - \tfrac{1}{2}H_{m+1}(y)] \\
&= A_{nm}[nm(H_{n-1}, H_{m-1}) - \tfrac{1}{2}m(H_{n+1}, H_{m-1}) - \tfrac{1}{2}n(H_{n-1}, H_{m+1}) + \tfrac{1}{4}(H_{n+1}, H_{m+1})]\,,
\end{aligned}$$

where

$$A_{nm} = \frac{\hbar^2\beta}{2m\pi^{1/2}} \frac{1}{\sqrt{2^n n!}} \frac{1}{\sqrt{2^m m!}}\,.$$

We can evaluate the above expression using the above expressions for (H_n, H_m) and a little algebra as

$$K_{nm} = \frac{\hbar^2}{ma^2}\left[(n+\tfrac{1}{2})\delta_{nm} - \tfrac{1}{2}\sqrt{(n+1)(n+2)}\ \delta_{n,m-2} - \tfrac{1}{2}\sqrt{(n-1)n}\ \delta_{n,m+2}\right]\,,$$

where we have used the fact that $\hbar^2\beta^2/2m = \hbar^2/ma^2$. The potential term may be written as

$$V_{nm} = V_0\left[\delta_{nm} - \int_{-a}^{a} dx\ \psi_n^*(x)\psi_m(x)\right]\,,$$

where $V_0 = 2\hbar^2/ma^2$ and the integral must be done numerically:

$$I_{nm} = \pi^{-1/2}\frac{1}{\sqrt{2^n n!}}\frac{1}{\sqrt{2^m m!}}\int_{-\sqrt{2}}^{\sqrt{2}} dy\ e^{-y^2} H_n(y) H_m(y)\,.$$

Collecting terms, we find

$$H_{nm} = \frac{\hbar^2}{ma^2}\left[(n+\tfrac{5}{2})\delta_{nm} - 2I_{nm} - \tfrac{1}{2}\sqrt{(n+1)(n+2)}\ \delta_{n,m-2} - \tfrac{1}{2}\sqrt{(n-1)n}\ \delta_{n,m+2}\right]\,.$$

The program `hw2.4.c` diagonalizes this matrix and hence determines the eigenvalues of the system.