

18.303 Fall 2009, Problem Set 4 Solutions

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The one-dimensional Schrödinger equation:

$$i\frac{\partial\Psi}{\partial t} = -\frac{1}{2}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi$$

where $V(x) = \begin{cases} 0, & -a \leq x \leq a \\ V_0, & |x| > a \end{cases}$

Boundary conditions are $|\Psi| \rightarrow 0$ as $x \rightarrow \infty$. We use separation of variables:

$$\begin{aligned}\Psi(x, t) &= \phi(x)T(t) \\ i\phi\dot{T} &= -\frac{1}{2}\phi''T + V(x)\phi T \\ i\frac{\dot{T}}{T} &= -\frac{1}{2}\frac{\phi''}{\phi} + V(x) = E\end{aligned}$$

We then have

$$\begin{aligned}\frac{\dot{T}}{T} &= -iE \\ T(t) &= e^{-iEt} \\ -\frac{1}{2}\phi'' + V(x)\phi &= E\phi \\ \phi'' - 2(V - E)\phi &= 0\end{aligned}\tag{1}$$

We only consider solutions for which the energies satisfy $0 < E < V_0$. For $|x| > a$, we have $\phi = C \exp(\lambda x) + D \exp(-\lambda x)$, where $\lambda = \sqrt{2(V_0 - E)}$. Applying the boundary conditions, we need $\phi \rightarrow 0$ as $|x| \rightarrow \infty$. So we have

$$\phi(x) = \begin{cases} De^{-\lambda x}, & x > a \\ Ce^{\lambda x}, & x < -a \end{cases}$$

For $|x| \leq a$, $V(x) = 0$, thus we have $\phi = A \cos kx + B \sin kx$, where $k = \sqrt{2E}$. Note that a symmetric potential $V(x)$ allows the solution to be classified into two symmetric classes: either even or odd parity.

Consider ϕ even, then $\phi = A \cos kx$, for $|x| \leq a$. For $|x| > a$, we have $C = D$ (even function). We require ϕ and ϕ' to be continuous at $|x| = a$:

$$\begin{aligned}A \cos ka &= Ce^{-\lambda a} \\ -Ak \sin ka &= -C\lambda e^{-\lambda a} \\ \Rightarrow \lambda &= k \tan ka, \quad C = Ae^{\lambda a} \cos ka\end{aligned}$$

Thus for even parity,

$$\phi_n(x) = \begin{cases} A_n e^{\lambda_n a} \cos(k_n a) e^{-\lambda_n x}, & x > a \\ A_n \cos(k_n x), & -a \leq x \leq a \\ A_n e^{\lambda_n a} \cos(k_n a) e^{\lambda_n x}, & x < -a \end{cases} \quad (2)$$

where $k_n = \sqrt{2E_n}$, $\lambda_n = \sqrt{2(V_0 - E_n)}$, and E_n satisfies the equation

$$\sqrt{2(V_0 - E_n)} = \sqrt{2E_n} \tan(\sqrt{2E_n}a)$$

Consider ϕ odd, then $\phi = B \sin kx$, for $|x| \leq a$. For $|x| > a$, we have $C = -D$ (odd function). We require ϕ and ϕ' to be continuous at $|x| = a$:

$$\begin{aligned} B \sin ka &= D e^{-\lambda a} \\ B k \cos ka &= -D \lambda e^{-\lambda a} \\ \Rightarrow \quad \lambda &= -k \cot ka, \quad D = B e^{\lambda a} \sin ka \end{aligned}$$

Thus for odd parity,

$$\phi_m(x) = \begin{cases} B_m e^{\lambda_m a} \sin(k_m a) e^{-\lambda_m x}, & x > a \\ B_m \sin(k_m x), & -a \leq x \leq a \\ -B_m e^{\lambda_m a} \sin(k_m a) e^{\lambda_m x}, & x < -a \end{cases} \quad (3)$$

where $k_m = \sqrt{2E_m}$, $\lambda_m = \sqrt{2(V_0 - E_m)}$, and E_m satisfies the equation

$$\sqrt{2(V_0 - E_m)} = -\sqrt{2E_m} \cot(\sqrt{2E_m}a)$$

Combining equations (4), (5) and (6), we get the solution of the Schrödinger equation:

$$\boxed{\Psi(x, t) = \sum_{E_n} \phi_n(x) e^{-iE_n t} + \sum_{E_m} \phi_m(x) e^{-iE_m t}} \quad (4)$$

Note that the summations are over finite number of terms, i.e. there are finite number of E_n and E_m satisfying

$$\begin{aligned} \sqrt{2(V_0 - E_n)} &= \sqrt{2E_n} \tan(\sqrt{2E_n}a) \\ \sqrt{2(V_0 - E_m)} &= -\sqrt{2E_m} \cot(\sqrt{2E_m}a) \end{aligned}$$

For larger values of V_0 , the number of intersections increases, but the number of intersections will remain finite.

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In the Midterm exam, we know that $\int H_m(x) H_n(x) e^{-x} dx = 0$ if $m \neq n$. Thus we assume that $w(x) = e^{-x}$. First, plugging $H_0(x) = 1$ into the equation (1), we get $\lambda_0 = 0$. Next, plugging $H_1(x) = 1 - x$ into the equation (1), we get

$$-p'(x) = -\lambda_1 e^{-x} (1 - x).$$

Therefore,

$$p(x) = \lambda_1 x e^{-x}.$$

Finally, plugging $H_2(x) = 1 - 2x + \frac{x^2}{2}$ into the equation (1), we get

$$\lambda_1 e^{-x}(1-x)(x-2) + \lambda_1 x e^{-x} = -\lambda_2 e^{-x}(1-2x + \frac{x^2}{2}).$$

Hence, $\lambda_2 = 2\lambda_1$. We set $\lambda_1 = 1$ and thus $\lambda_2 = 2$.

Suppose that $H_3(x) = 1 + b_3x + c_2x^2 + d_1x^3$ is the eigenfunction of eigenvalue λ_3 and $d_1 \neq 0$. Then

$$e^{-x}(1-x)(b_3 + 2c_2x + 3d_1x^2) + e^{-x}x(2c_2 + 6d_1x) = -\lambda_3 e^{-x}(1 + b_3x + c_2x^2 + d_1x^3).$$

Simplifying both sides of the equation above and comparing the coefficients, one get

$$\begin{aligned} b_3 &= -\lambda_3 \\ -b_3 + 4c_2 &= -\lambda_3 b_3 \\ -2c_2 + 9d_1 &= -\lambda_3 c_2 \\ -3d_1 &= -\lambda_3 d_1. \end{aligned}$$

Therefore, $\lambda_3 = 3$, $b_3 = -3$, $c_2 = \frac{3}{2}$ and $d_1 = -\frac{1}{6}$.

Verify that $\int H_m(x)H_n(x)e^{-x}dx = 0$ if $m \neq n$, assuming that the eigenfunction grows no faster than a power of x at large x and are non-singular at $x = 0$. In fact, using integration by parts,

$$\begin{aligned} -\int \lambda_m H_m(x)H_n(x)e^{-x}dx &= -\int p(x)\frac{dH_m}{dx} \cdot \frac{dH_n}{dx}e^{-x}dx, \\ -\int \lambda_n H_m(x)H_n(x)e^{-x}dx &= -\int p(x)\frac{dH_m}{dx} \cdot \frac{dH_n}{dx}e^{-x}dx. \end{aligned}$$

If $m \neq n$, then $\lambda_m \neq \lambda_n$ and thus

$$\int H_m(x)H_n(x)e^{-x}dx = 0.$$

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Let u_1 and u_2 be non-trivial solutions of the Laplace equation in a finite region Ω with the boundary condition $\hat{n} \cdot \nabla u_i + h(x)u_i = \Phi(x)$, $i = 1, 2$. Define $U = u_1 - u_2$, then

$$\begin{aligned} \Delta U &= 0 & \text{in } \Omega, \\ \hat{n} \cdot \nabla U + h(x)U &= 0 & \text{on } \partial\Omega. \end{aligned}$$

Thus

$$\begin{aligned} \int_{\Omega} |\nabla U|^2 dx &= -\int_{\Omega} U \Delta U dx + \int_{\partial\Omega} U \hat{n} \cdot \nabla U \\ &= -\int_{\Omega} U \Delta U dx - \int_{\partial\Omega} h(x)U^2. \end{aligned}$$

Since $h(x) > 0$, thus $|\nabla U| = 0$ in Ω and $U = 0$ on $\partial\Omega$. Therefore, $U = 0$ in Ω . In other word, $u_1 = u_2$ and the solution is unique. $\square$