Physics 731 Lecture Notes 3

Summary: One-dimensional Energy Eigenvalue Problems

Here we review examples of one-dimensional energy eigenvalue problems for a particle of mass m moving in a one-dimensional potential. This material is covered briefly in Sakurai, 1st Ed., Revised (**S1r**), Appendix A, (see also Chapter 2, sections 2.3 and 2.4), as well as Sakurai, 2nd Ed. (**S2**), Section 2.5, and Sakurai, 3rd Ed. (**S3**), Appendix B. More comprehensive discussions can be found in Merzbacher, Chapters 4-6; Schiff, Chapter 2; and Shankar, Chapters 5 and 7, Merzbacher 4-6, and Schiff 2, among many other references.

The starting point is the eigenvalue problem:

$$H|n\rangle = \left(\frac{p^2}{2m} + V(x)\right)|n\rangle = E_n|n\rangle \tag{1}$$

Mostly, we will work in position space:

$$\langle x|H|n\rangle = -\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} + V(x)\psi_n(x) = E_n\psi_n(x). \tag{2}$$

This equation is known as the time-independent Schrödinger equation. The possible solutions can be broadly classified in two categories:

- *Bound states.* These are states for which E is less than the asymptotic value of the potential. They are normalizable states, by definition. The requirement of normalizability generally results in the quantization of the allowed energy eigenvalues.
- *Scattering or continuum states.* These are states for which E is greater than the asymptotic value of the potential. These states are normalizable only in the delta-function sense, and thus constitute improper basis states. Physical (normalizable) propagating states, often known as wavepacket states, must be formed from appropriate linear combinations of these states. This class of states are associated with a continuum of energy eigenvalues.

It is useful to exploit symmetries of the potential, when present. A simple example is the case of symmetric potentials:

$$V(x) = V(-x). \tag{3}$$

For symmetric potentials, without loss of generality, it is straightforward to show that the eigenstates can be classified by their parities:

- *Even parity*: $\psi(-x) = \psi(x)$.
- *Odd parity*: $\psi(-x) = -\psi(x)$.

This property emerges automatically in one-dimensional bound state problems with symmetric potentials, because there is no degeneracy. In cases where there is degeneracy, it is still possible to classify states according to their parities without loss of generality, because we can always form linear combinations of degenerate states that are even or odd:

$$\psi_\pm(x) = \psi(x) \pm \psi(-x). \tag{4}$$

In general, for bound state problems involving symmetric potentials, it is useful to treat even and odd parity states separately.

Free Particle. For $V(x) = 0$, the energy eigenstates are momentum eigenstates:

$$\langle x|k\rangle = \psi_k(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\pm ikx}, \quad E_k = \frac{\hbar^2 k^2}{2m}, \tag{5}$$

where $k = p/\hbar$. These states are of course delta-function normalized (with respect to momentum), such that

$$\langle k|k'\rangle = \int_{-\infty}^{\infty} \psi_k^*(x)\psi_{k'}(x)\,dx = \delta(p - p'), \tag{6}$$

as we know from our general consideration of the p eigenstates. Another procedure, designed for allowing these states to become proper basis states by restricting the allowed values of k, is box normalization. A discussion of this procedure can be found for example in **S2**, Section 2.5, among other sources). We will generally avoid box normalization in this course, and instead deal directly with the improper basis states.

Infinite Square Well. Here we consider the idealized potential

$$V(x) = \begin{cases} 0, & |x| < a \\ \infty, & |x| > a, \end{cases} \tag{7}$$

with $a > 0$. For $x > a$ and $x < -a$, the wavefunction vanishes. For $-a < x < a$, the wavefunction is that of a free particle:

$$\psi(x) = A' e^{ikx} + B' e^{-ikx} = A\cos kx + B\sin kx, \tag{8}$$

subject to the boundary conditions $\psi(a) = \psi(-a) = 0$. There are two classes of solutions:

- *Even parity*: $A \neq 0$, $B = 0$, $\cos ka = 0$, such that $k \equiv k_n = n\pi/(2a)$ for odd n. The normalized wavefunctions and energy levels are given by

$$\psi_n(x) = \sqrt{\frac{1}{a}}\cos k_n x, \quad E_n = \frac{\hbar^2 n^2 \pi^2}{8ma^2}, \quad n = 1, 3, 5, \ldots \tag{9}$$

- *Odd parity*: $A = 0$, $B \neq 0$, $\sin ka = 0$, such that $k = k_n = n\pi/(2a)$ for even n. The normalized wavefunctions and energy levels are given by

$$\psi_n(x) = \sqrt{\frac{1}{a}}\sin k_n x, \quad E_n = \frac{\hbar^2 n^2 \pi^2}{8ma^2}, \quad n = 2, 4, 6, \ldots \tag{10}$$

Here the coordinate system was chosen to exploit the symmetry of the potential. However, for this simple example, it is also common to see the the case in which the axes are instead chosen such that one side of the box is at $x' = 0$, and the other at $x' = 2a$. The reason is that the wavefunctions in this case can be expressed in the following compact form (in terms of the variable $x = x' - a$):

$$\psi_n(x) = \frac{1}{\sqrt{a}}\sin\frac{n\pi(x + a)}{2a}, \quad E_n = \frac{\hbar^2 n^2 \pi^2}{8ma^2}, \quad n = 1, 2, 3, \ldots \tag{11}$$

The energy eigenstates, of course, are unaffected by the choice of coordinates.

Finite Square Well. Here we consider the symmetric potential

$$V(x) = \begin{cases} 0, & |x| < a \\ V_0, & |x| > a, \end{cases} \tag{12}$$

with $a > 0$. This potential allows for both bound and continuum states; here we will seek only the bound states, *i.e.*, the states with $E < V_0$. For the bound states, the boundary conditions are that $\psi(x) \to 0$ as $\to \pm\infty$, and that $\psi(x)$ and $d\psi(x)/dx$ are continuous at $x = \pm a$. Let us label region I as $x < -a$, region II as $-a < x < a$, and region III as $x > a$. In region II, the wavefunction is that of a free particle:

$$\psi_{\mathrm{II}}(x) = A' e^{ikx} + B' e^{-ikx} = A \cos kx + B \sin kx, \tag{13}$$

with $k = \sqrt{2mE}/\hbar$. In regions I and III, define the variable $\kappa = \sqrt{2m(V_0 - E)}/\hbar$. The wavefunctions are

$$\psi_{\mathrm{I}}(x) = De^{\kappa x}, \quad \psi_{\mathrm{I}}(x) = Fe^{-\kappa x}, \tag{14}$$

in which we have imposed the boundary conditions at $x = \pm\infty$. We classify solutions in terms of parities:

- *Even parity*: $B = 0$, $D = F$. The boundary conditions at $x = a$ can be applied to the above states directly, or the continuity of the wavefunction at $x = a$ can be built in explicitly, such that

  $$\psi_{\mathrm{I}}(x) = A' \cos ka \, e^{\kappa x}, \quad \psi_{\mathrm{II}}(x) = A' \cos kx \, e^{-\kappa a}, \quad \psi_{\mathrm{III}}(x) = A' \cos ka \, e^{-\kappa x}, \tag{15}$$

  such that the continuity of ψ' at $x = a$ results in the condition

  $$ka \tan ka = \kappa a. \tag{16}$$

  Defining $\xi = ka$ and $\eta = \kappa a$, this can be recast as

  $$\xi \tan \xi = \eta. \tag{17}$$

  Note that ξ and η are not independent:

  $$\xi^2 + \eta^2 = \frac{2mV_0 a^2}{\hbar^2}. \tag{18}$$

  These equations can be solved numerically or graphically. You should be familiar with both methods. For $V_0 \to \infty$, $\xi \to \xi_n^\infty = n\pi/2$, as expected. A finite V_0 reduces the number of bound states to a finite number depending on the precise value of V_0, which makes sense because the finite well has a reduced strength to bind states than the infinite well. However, for the even parity solutions, it is straightforward to show that there is at least one bound state for any nonzero value of V_0.

- *Odd parity*: $A = 0$, $D = -F$. The procedure is similar to that of the even parity states (homework).

The nonvanishing wavefunction in regions I and III is an example of quantum mechanical tunneling (*i.e.*, nonzero probability in classically forbidden regions). The *penetration depth* $d \sim 1/\kappa = \hbar/(2m(V_0 - E))^{1/2}$ is a characteristic distance over which the particle can have a nontrivial presence in the classically forbidden region. This is a purely quantum mechanical effect, as $d \to 0$ as $\hbar \to 0$.

Attractive delta-function potential: Here we consider another idealized potential, the attractive delta-function potential:

$$V(x) = -\lambda \delta(x), \tag{19}$$

with $\lambda > 0$. This potential again allows for continuum states (with $E > 0$), and bound states (with $E < 0$). Here we will focus on bound states, and defer the discussion of the continuum states for later.

For the bound states, we require that $\psi(x) \to 0$ as $\to \pm\infty$, for normalizability. Due to the singular nature of the potential, the boundary conditions are that $\psi(x)$ is continuous at $x = 0$, but $d\psi(x)/dx$ is discontinuous. Denoting $x < 0$ as region I and $x > 0$ as region II, the boundary condition on the derivative of the wavefunction can be obtained by integrating the Schrödinger equation in a small interval about the δ function:

$$
\begin{aligned}
-\frac{\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\frac{d^2\psi(x)}{dx^2}dx - \lambda\int_{-\epsilon}^{\epsilon}\delta(x)\psi(x)dx &= E\int_{-\epsilon}^{\epsilon}\psi(x)dx \\
-\frac{\hbar^2}{2m}\left[\frac{d\psi}{dx}\right]_{-\epsilon}^{\epsilon} - \lambda\psi(x=0) &= 0. \qquad (20)
\end{aligned}
$$

This leads to the condition

$$\left[\frac{d\psi_{\rm II}}{dx} - \frac{d\psi_{\rm I}}{dx}\right]_{x=0} = -\frac{2m\lambda}{\hbar^2}\psi(x=0). \tag{21}$$

The wavefunction takes the form

$$\psi_{\rm I}(x) = Ae^{\kappa x}, \quad \psi_{\rm II}(x) = Ae^{-\kappa x}, \tag{22}$$

with $\kappa = \sqrt{-2mE}/\hbar$. Eq. (21) leads to the condition that there is only one allowed value of E:

$$E = -\frac{m\lambda^2}{2\hbar^2}. \tag{23}$$

Hence, the attractive delta-function potential in one dimension admits one and only one bound state, independent of the size of the parameter λ.

Simple Harmonic Oscillator. The harmonic oscillator Hamiltonian is

$$\frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2. \tag{24}$$

This potential admits bound states only. We will solve the eigenvalue problem $H|n\rangle = E_n|n\rangle$ in three bases: position space, momentum space, and the "energy" basis (*i.e.*, using the operator method).

First, there is a basis-independent proof that all the $E_n \geq 0$. Consider the expectation value of H with respect to an arbitrary state $|\psi\rangle$:

$$\langle H\rangle = \langle\psi|H|\psi\rangle = \frac{1}{2m}\langle\psi|p^2|\psi\rangle + \frac{1}{2}m\omega^2\langle\psi|x^2|\psi\rangle = \frac{1}{2m}\langle p\psi|p\psi\rangle + \frac{1}{2}m\omega^2\langle x\psi|x\psi\rangle \geq 0 \tag{25}$$

For $|\psi\rangle = |n\rangle$, $\langle H\rangle = E_n$, and hence $E_n \geq 0$. The only way that E_n could be zero is if the state $|n\rangle$ is the null vector (a trivial solution, which we will ignore). Hence, without loss of generality, we can take $E_n > 0$.

- *Position space*. The Schrödinger equation takes the form

  $$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_n(x) + \frac{1}{2}m\omega^2x^2\psi_n(x) = E_n\psi_n(x). \tag{26}$$

  It is useful to recast this equation in terms of the following dimensionless variables: $y = x/b$ (in which $b = \sqrt{\hbar/(m\omega)}$) and $\xi = E/(\hbar\omega)$:

  $$\psi'' + (2\xi - y^2)\psi = 0. \tag{27}$$

  By considering limits of this equation as $y \to 0$ and $y \to \infty$, we can extract out the asymptotic form of the desired solution, which must be finite as $y \to \pm\infty$ due to the requirement of normalizability. The appropriate form is

  $$\psi(y) = u(y)e^{-y^2/2}, \tag{28}$$

in which $u(y)$ is of polynomial form, with $u(y) = A + By$ as $y \to 0$. The differential equation for $u(y)$ is

$$u'' - 2yu' + (2\xi - 1)u = 0, \tag{29}$$

otherwise known as the Hermite equation. Inserting a power series expansion for $u(y) = \sum_{k=0}^{\infty} c_k y^k$, we obtain the recursion equation

$$c_{k+2} = c_k \frac{2k + 1 - 2\xi}{(k+1)(k+2)}. \tag{30}$$

The series is divergent except for particular values of ξ, namely $\xi = (2n+1)/2$, with n a nonnegative integer. The divergent solutions must be discarded, as they do not obey the normalizability requirement. Eliminating these solutions and keeping only those with $\xi = (2n+1)/2$ for nonnegative integer n, leads to the well-known energy quantization condition for the simple harmonic oscillator:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega. \tag{31}$$

The $u_n(y)$ are the Hermite polynomials, $H_n(y)$. As the potential is symmetric, we expect the eigenstates to be classified by parity, and indeed they are: the even n solutions have even parities, and the odd n solutions have odd parities ($H_n(-y) = (-)^n H_n(y)$).

The Hermite polynomials obey the relations:

$$H_n(y) = \sum_{s=0}^{[n/2]} (-1)^s (2y)^{n-2s} \frac{n!}{(n-2s)!s!} = e^{y^2/2}\left(y - \frac{d}{dy}\right)^n e^{-y^2/2}, \tag{32}$$

in which $[n/2]$ is the largest integer less than $n/2$, and

$$\begin{aligned} H_n'(y) &= 2nH_{n-1}(y) && (33) \\ H_{n+1}(y) &= 2yH_n(y) - 2nH_{n-1}(y). && (34) \end{aligned}$$

The generating function is

$$g(y,t) = e^{-t^2+2ty} = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(y), \tag{35}$$

such that

$$H_n(y) = \left(\frac{\partial^n}{\partial t^n} g(y,t)\right)_{t=0}. \tag{36}$$

Including normalization factors, the wavefunctions $\psi_n(x)$ for the simple harmonic oscillator in one dimension are

$$\psi_n(x) = \left[\frac{m\omega}{\pi\hbar 2^{2n}(n!)^2}\right]^{1/4} e^{-m\omega x^2/(2\hbar)} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right). \tag{37}$$

These functions form a complete orthonormal set, as expected as they are eigenstates of a self-adjoint differential operator.

- *Momentum space*. The Schrödinger equation in momentum space takes the form

$$\frac{p^2}{2m}\varphi_n(p) - \frac{1}{2}m\omega^2\hbar^2 \frac{d^2\varphi_n(p)}{dp^2} = E_n\varphi_n(p). \tag{38}$$

The symmetry of the harmonic oscillator Hamiltonian indicates that the $\varphi_n(p)$ are given (up to an overall phase factor of $(-i)^n$) by $\psi_n(x)$ with the following replacements:

$$x \to p, \quad m\omega \to \frac{1}{m\omega}. \tag{39}$$

The phase factors of $(-i)^n$ in the momentum space wavefuntions are necessary to ensure that $\psi_n(x)$ and $\varphi_n(p)$ are Fourier transforms of each other, as they must be to maintain the form of the canonical commutation relations.

To summarize, the momentum space eigenfunctions take the form

$$\varphi_n(p) = (-i)^n \left[\frac{1}{m\omega\pi\hbar 2^{2n}(n!)^2}\right]^{1/4} e^{-p^2/(2\hbar m\omega)} H_n\left(\frac{p}{\sqrt{m\omega\hbar}}\right). \tag{40}$$

These also form a complete orthonormal set.

- In the operator method, the following non-Hermitian operators are introduced:

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left[x + i\frac{p}{m\omega}\right] = \frac{1}{\sqrt{2}}\left[y + \frac{d}{dy}\right] \tag{41}$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left[x - i\frac{p}{m\omega}\right] = \frac{1}{\sqrt{2}}\left[y - \frac{d}{dy}\right], \tag{42}$$

using the definition of y given above. The operators a and $a^\dagger$, which are known as the annihilation and creation operators, respectively, satisfy the following commutation relation:

$$[a, a^\dagger] = 1. \tag{43}$$

The Hermitian number operator $N = a^\dagger a$ is related to the Hamiltonian, as follows:

$$N = a^\dagger a = \frac{H}{\hbar\omega} - \frac{1}{2}. \tag{44}$$

Therefore, if we find the eigenstates of N, *i.e.* the states $|n\rangle$ such that $N|n\rangle = n|n\rangle$, we have solved the energy eigenvalue problem. Note that

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega. \tag{45}$$

The states $|n\rangle$ can be found by noticing that if $|n\rangle$ is an eigenvector of N with eigenvalue n, the state $a|n\rangle$ is either an eigenvector of N with eigenvalue $n-1$ or $a|n\rangle = 0$. Therefore, since $E_n > 0$, n must be a nonnegative integer, resulting in the energy quantization condition. The operators $a^\dagger$ and a are raising and lowering operators, respectively:

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \quad a|n\rangle = \sqrt{n}|n-1\rangle. \tag{46}$$

We can also write x and p in terms of the creation and annihilation operators as follows:

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \tag{47}$$

$$p = i\sqrt{\frac{m\omega\hbar}{2}}(a^\dagger - a). \tag{48}$$

Hence, it is straightforward to show that

$$\begin{aligned} \langle n'|x|n\rangle &= \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}) && (49) \\ \langle n'|p|n\rangle &= i\sqrt{\frac{m\omega\hbar}{2}}(\sqrt{n+1}\delta_{n',n+1} - \sqrt{n}\delta_{n',n-1}). && (50) \end{aligned}$$

The ground state $|0\rangle$ (not the null vector) satisfies $a|0\rangle = 0$. In position space, this results in

$$\langle x|a|0\rangle = \left(y + \frac{d}{dy}\right)\psi_0 = 0, \quad (51)$$

which has the solution $\psi_0(y) = A_0 e^{-y^2/2}$. The remaining states can be obtained from $|0\rangle$ by acting with the creation operator:

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle. \quad (52)$$

In position space, this results in the following expression for the eigenstates, as expected:

$$\begin{aligned} \psi_n(x) = \langle x|n\rangle &= \langle x|\frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle \\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{(\sqrt{2})^n\sqrt{n!}}\left[y - \frac{d}{dy}\right]^n e^{-y^2/2} \\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{(\sqrt{2})^n\sqrt{n!}} e^{-y^2/2} H_n(y). && (53) \end{aligned}$$