Quantum Mechanics

Lecture #2: Ch. 2: One-dimensional eigenvalue problems

Fa Wang[1]

[1]International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China

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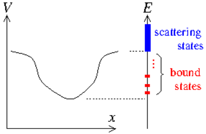
Outline

Goals and Requirements: Lecture #2

- This lecture deals with non-relativistic particle in 1D static potential, $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$.
- The goal of this lecture is for you to become familiar with the following items:
  - some qualitative features about bound states in 1D.
  - eigenvalues and eigenstates(standing waves) for infinite square well.
  - ladder operators, eigenvalues and eigenstates for harmonic oscillator.
  - how to deal with δ-function potential.
  - how to set up equations for finite square well (and similar) problems.
  - the basic idea about wave packet, group velocity.
  - the basic idea about reflection/transmission coefficients in 1D.
- By the end of this lecture, you should master the following skills:
  - directly writing down eigenvalues and eigenstates of an infinite square well problem.
  - using ladder operators to do calculations for a harmonic oscillator problem.
  - setting up boundary condition equations for eigenstates at δ-potentials and discontinuous points of potentials.
  - determining number of bound states from transcendental equations related to finite square well (and similar) problems
- "Side remark"'s are NOT required.
- References:
  D.J. Griffiths, *Introduction to Quantum Mechanics*, Chapter 2.

Qualitative features of 1D eigenvalue problems

- The eigenvalue problem, $[-\frac{\hbar^2}{2m}\partial_x^2 + V(x)]\psi(x) = E\cdot\psi(x)$, has the following features (may not be proved here, check Sturm-Liouville theory):
  - *Bound states* (normalizable eigenstates) $\psi(x)$ energy eigenvalue $E \geq \min_x V(x)$ (Homework #2).
    Proof: if eigenstate ψ has $\langle\psi|\psi\rangle = 1$, then $E = \langle\psi|\hat{H}|\psi\rangle = \langle\psi|\frac{\hat{p}^2}{2m}|\psi\rangle + \int_{-\infty}^{\infty}|\psi(x)|^2 V(x)\,\mathrm{d}x$,
    $\langle\psi|\frac{\hat{p}^2}{2m}|\psi\rangle = \frac{1}{2m}\langle\hat{p}\psi|\hat{p}\psi\rangle \geq 0$, $\int_{-\infty}^{\infty}|\psi(x)|^2 V(x)\,\mathrm{d}x \geq [\min_x V(x)]\cdot\int_{-\infty}^{\infty}|\psi(x)|^2\,\mathrm{d}x = \min_x V(x)$.
    Exercise: think about where the normalizable property is really used.
  - *Bound states* energies are discrete, and $E \leq \underline{\lim}_{x\to\pm\infty} V(x)$, $\underline{\lim}$ is lower limit.
  - *Scattering states* (non-normalizable) energies are continuous, and $E > \underline{\lim}_{x\to\pm\infty} V(x)$.
  - Side remark: for $E < \min_x V(x)$ we can have "evanescent states", whose eigenstates $\psi(x)$ are exponentially growing/decaying as $x \to \pm\infty$, we will not consider these states in this course.
  - Schematic picture of the *energy spectrum* (collection of energy eigenvalues, shown on the right):



  - Eigenstates $\psi(x)$ can be chosen real.
    - Proof: if ψ is eigenstate, take complex conjugate of the eigenvalue equation above, then ψ^* is also eigenstate with the same eigenvalue E, then real functions $\psi + \psi^*$ and $\mathrm{i}(\psi^* - \psi)$ are also eigenstates.
  - If $V(x) = +\infty$ in a neighborhood of x_0, then eigenstate ψ vanishes at this point, $\psi(x_0) = 0$.
  - If $V(x)$ is finite in a neighborhood of x_0, then eigenstate ψ is smooth at x_0.
  - Eigenstates ψ are continuous, otherwise $\hat{p}\psi$ contains δ-function, $E = \frac{\langle\hat{p}\psi|\hat{p}\psi\rangle}{2m} + \langle\psi|\hat{V}|\psi\rangle$ diverges.

Qualitative features of 1D eigenvalue problems (cont'd)

- The eigenvalue problem, $[-\frac{\hbar^2}{2m}\partial_x^2 + V(x)]\psi(x) = E\cdot\psi(x)$,
  has the following features (may not be proved here, check Sturm-Liouville theory):
  - *Bound states* ψ are non-degenerate.
    - Proof: if ψ_1, ψ_2 are both eigenstates for eigenvalue E, then $0 = \psi_2\cdot E\psi_1 - \psi_1\cdot E\psi_2$
      $= \psi_2\cdot(-\frac{\hbar^2}{2m}\partial_x^2 + V)\psi_1 - \psi_1\cdot(-\frac{\hbar^2}{2m}\partial_x^2 + V)\psi_2 = -\frac{\hbar^2}{2m}\partial_x(\psi_2\partial_x\psi_1 - \psi_1\partial_x\psi_2)$, therefore
      $\psi_2\partial_x\psi_1 - \psi_1\partial_x\psi_2 = \mathrm{Const.}$ independent of x;
      for bound states, $\psi_{1,2}\to 0$ as $x\to\pm\infty$, then $\psi_2\partial_x\psi_1 - \psi_1\partial_x\psi_2 = 0$; divide by $\psi_1\cdot\psi_2$, then
      $\partial_x(\log\psi_1 - \log\psi_2) = 0$, then $\psi_1(x) = e^{\mathrm{Const.}}\psi_2(x)$, so $\psi_{1,2}$ are the same state.
  - Terminology: sort the bound state energies in ascending order, $E_0 \le E_1 \le E_2 \dots$.
    E_0 is the lowest energy eigenvalue, the "ground state energy". E_n is the "nth excited state energy".
    NOTE: here the label $n = 0, 1, \dots$ may not match the "quantum numbers" used later to label states.
  - Nodes of eigenstates [points where $\psi(x) = 0$, excluding $V(x) = +\infty$ cases] are "simple".
    Simple nodes: where $\psi(x) = 0$, $\partial_x\psi(x) \neq 0$ [otherwise the solution would be $\psi(x) = 0,\ \forall x$].
  - The ground state wave function $\psi_0(x)$ has NO node, can be non-negative, $\psi_0(x) \ge 0$. (*c.f.* Chapter 7)
  - The nth excited state wave function $\psi_n(x)$ has n nodes, $x_1^{(n)} < x_2^{(n)} < \cdots < x_n^{(n)}$, $\psi_n(x_n^{(n)}) = 0$.
    Nodes of adjacent levels are interpenetrating, $x_1^{(n+1)} < x_1^{(n)} < x_2^{(n+1)} < \cdots < x_n^{(n+1)} < x_n^{(n)} < x_{n+1}^{(n+1)}$.
  - Inversion symmetry: if $V(x) = V(-x)$, then eigenstates can be chosen as either even or odd functions of x.

    Proof: in this case, if $\psi(x)$ is eigenstate, then $\psi(-x)$ is also eigenstate with the same eigenvalue, then even

    function $\psi(x) + \psi(-x)$ and odd function $\psi(x) - \psi(-x)$ are also eigenstates.
    - In this case, *bound states* are either even or odd, $\psi_n(-x) = (-1)^n\psi_n(x)$, $n = 0, 1, \dots$ (see above).
      In particular, the ground state ($n = 0$) is even.
    - The inversion center may be at $x_0 \neq 0$, $V(x_0 + x) = V(x_0 - x)$.

Free particle & wave packet

- "Free particle" has constant potential $V(x) = V_0$. Without loss of generality(w.l.o.g.), assume $V_0 = 0$, otherwise redefine E by $E - V_0$. Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m}$.
  - $[\hat{H}, \hat{p}] = 0$. We can choose simultaneous eigenstates of $\hat{H}$ and $\hat{p}$. System has translation symmetry. If $\psi(x)$ is eigenstate, then $\phi(x) \equiv \psi(x + a)$ is also eigenstate with the same energy, for any real a.
  - Eigenstates $|p\rangle$ are *planewaves* $\psi_p(x) = \frac{e^{\mathrm{i}px/\hbar}}{\sqrt{2\pi\hbar}}$, with eigenvalues $E_p = \frac{p^2}{2m}$.
  - We can also use real eigenbasis, *standing waves*, $\propto \cos(px/\hbar)$ and $\propto \sin(px/\hbar)$ (for $p \neq 0$).
  - Generic free particle state $\psi(x, t) = \int \tilde{\psi}(p, t = 0) \cdot e^{-\mathrm{i}E_p t/\hbar} \cdot \frac{e^{\mathrm{i}px/\hbar}}{\sqrt{2\pi\hbar}} \,\mathrm{d}p$. (see Lecture #1).
    Here $\tilde{\psi}(p, t)$ is the "momentum representation" of wave function, $\langle p|\psi\rangle$ at time t.
- Real particles are described by "wave packet", $\psi(x, t) = f(x, t) \cdot \frac{e^{\mathrm{i}(p_0 x - E_{p_0} t)/\hbar}}{\sqrt{2\pi\hbar}}$.
  $f(x, t)$ is a normalizable "envelop" function, with a single "broad" peak(width $\gg \frac{h}{p_0}$).
  - $\tilde{\psi}(p, t = 0) = \tilde{f}(p - p_0, t = 0)$, here $\tilde{f}(\delta p, t) \equiv \int f(x, t) \frac{e^{-\mathrm{i}\cdot\delta p\cdot x/\hbar}}{\sqrt{2\pi\hbar}} \,\mathrm{d}x$ is the Fourier transform of f.
    Therefore the momentum representation of wave function has a "narrow" peak around $p \sim p_0$.
  - Assume w.l.o.g. that $f(x, t = 0)$ peaks at $x = 0$ (otherwise redefine x). At time t,
    $f(x, t) = \int \tilde{f}(\delta p, t = 0) \cdot \exp\{\frac{\mathrm{i}}{\hbar}[\delta p \cdot x - (E_{p_0+\delta p} - E_{p_0}) \cdot t]\} \frac{1}{\sqrt{2\pi\hbar}} \,\mathrm{d}(\delta p)$. Because relevant range of δp is small, we can approximate $E_{p_0+\delta p} - E_{p_0} \approx v_g \cdot \delta p$, where $v_g = \left.\frac{\partial E}{\partial p}\right|_{p=p_0} = \frac{p_0}{m}$ is the group velocity.
    $f(x, t) \approx \int \tilde{f}(\delta p, t = 0) \cdot \exp[\frac{\mathrm{i}}{\hbar}\delta p \cdot (x - v_g \cdot t)] \frac{1}{\sqrt{2\pi\hbar}} \mathrm{d}(\delta p) = f(x - v_g \cdot t, 0)$.
    So the peak of envelop function moves by the *group velocity*.
    Nonlinear dispersion will cause broadening of the wave packet.

Infinite square well potential: bound states

- $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$, $V(x) = \begin{cases} +\infty, & x < 0 \text{ or } x > a; \\ 0, & 0 < x < a. \end{cases}$
  - Good approximation for "deep" (depth$\gg$energy level measured from bottom) potential well with "narrow walls" (width of "walls"$\ll$relevant wave length).
  - According to [2.1]: there are bound states with energy $E \geq 0$; eigenstates $\psi(x) = 0$ for $x < 0$ or $x > a$. For $0 < x < a$, the Hamiltonian is the same as free particle, so $\psi(x)$ is linear superposition of $e^{\mathbb{i}kx}$ in this region.
  - Boundary condition: eigenstates $\psi(x)$ are continuous at $x = 0$ and a, so $\psi(x=0) = \psi(x=a) = 0$. This leads to the "quantization" of wavevector k, and therefore the "quantization" of energy eigenvalues.
  - Energy eigenvalues: $E_n = \frac{\hbar^2}{2m}(\frac{n\pi}{a})^2$, here $n = 1, 2, \ldots$;
    eigenstates are standing waves: $\psi_n(x) = \begin{cases} 0, & x < 0 \text{ or } x > a; \\ \sqrt{\frac{2}{a}}\sin(\frac{n\pi}{a}x), & 0 < x < a. \end{cases}$. (see textbook Figure 2.2)
    NOTE: here the ground state is labeled by $n = 1$; 1^{st}-excited state is $n = 2$; ....
    Exercise: check that the nodes of ψ_n inside $(0, a)$ satisfy the interpenetrating property in [2.1])
  - These standing waves ψ_n form complete orthonormal basis for the Hilbert space of wave functions satisfying $\psi(x) = 0$ for $x \leq 0$ or $x \geq a$.
  - Generalization: $V(x) = \begin{cases} +\infty, & x < a \text{ or } x > b; \\ V_0, & a < x < b. \end{cases}$, then
    $E_n = V_0 + \frac{\hbar^2}{2m}(\frac{n\pi}{b-a})^2$, $\psi_n(x) = \begin{cases} 0, & x < a \text{ or } x > b; \\ \sqrt{\frac{2}{b-a}}\sin(\frac{n\pi}{b-a}(x-a)), & a < x < b. \end{cases}$, $n = 1, 2, \ldots$.

Harmonic oscillator: algebraic method

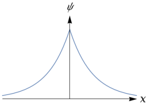
- $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$, $V(x) = \frac{m\omega^2}{2}x^2$ (harmonic potential). $\omega > 0$ is the "angular frequency".
  - Good approximation for "small" oscillation about the minimum of a smooth potential well.
- Ladder operators: $\hat{a}_\mp = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} \pm \frac{\mathrm{i}}{m\omega}\hat{p})$, "lowering" / "raising" operators respectively.
  - $(\hat{a}_\mp)^\dagger = \hat{a}_\pm$, commutator $[\hat{a}_-, \hat{a}_+] = 1$, and $\hat{H} = \hbar\omega \cdot (\hat{a}_+\hat{a}_- + \frac{1}{2})$. Exercise: check these.
  - Useful fact: if $[\hat{A}, \hat{B}] = c \cdot \hat{B}$, then $\hat{B}|\hat{A} = \lambda\rangle$ will either be proportional to $|\hat{A} = \lambda + c\rangle$, or vanish($= 0$). Proof: $\hat{A}(\hat{B}|\hat{A} = \lambda\rangle) = (\hat{B}\hat{A} + [\hat{A}, \hat{B}])|\hat{A} = \lambda\rangle = (\hat{B} \cdot \lambda + c \cdot \hat{B})|\hat{A} = \lambda\rangle = (\lambda + c)(\hat{B}|\hat{A} = \lambda\rangle)$.
  - Useful fact: $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$. Proof: expand the commutations. Generalization: $[\hat{A}, \hat{B}_1\hat{B}_2 \ldots \hat{B}_n] = [\hat{A}, \hat{B}_1]\hat{B}_2 \ldots \hat{B}_n + \cdots + \hat{B}_1 \ldots \hat{B}_{i-1}[\hat{A}, \hat{B}_i]\hat{B}_{i+1} \ldots \hat{B}_n + \cdots + \hat{B}_1 \ldots \hat{B}_{n-1}[\hat{A}, \hat{B}_n]$.
  - $[\hat{a}_+\hat{a}_-, \hat{a}_\pm] = \pm\hat{a}_\pm$, (these two formulas are related by hermitian conjugation). Namely $\hat{a}_\pm$ changes eigenvalue of $\hat{a}_+\hat{a}_-$ by ± 1. Therefore eigenvalues of $\hat{a}_+\hat{a}_-$ form "ladder(s)" $(\ldots, \lambda - 1, \lambda, \lambda + 1, \ldots)$.
  - $\hat{a}_+\hat{a}_-$ is positive semi-definite, $\langle\psi|\hat{a}_+\hat{a}_-|\psi\rangle = \langle\hat{a}_-\psi|\hat{a}_-\psi\rangle \geq 0$. So eigenvalues of $\hat{a}_+\hat{a}_-$ must ≥ 0. Then there is a minimal eigenvalue $\lambda_{\min}$ in a "ladder", and $\hat{a}_-|\hat{a}_+\hat{a}_- = \lambda_{\min}\rangle = 0$ [if this does not vanish, we would have eigenstate for eigenvalue $(\lambda_{\min} - 1)$ contradicting the assumption of minimal eigenvalue $\lambda_{\min}$]. Then $\hat{a}_+\hat{a}_-|\hat{a}_+\hat{a}_- = \lambda_{\min}\rangle = 0$, so $\lambda_{\min} = 0$, there is only one "ladder" of eigenvalues $n = 0, 1, 2, \ldots$.
  - Label the $|\hat{a}_+\hat{a}_- = n\rangle$ state by $|\psi_n\rangle$, it is eigenstate of $\hat{H}$ for eigenvalue $E_n = \hbar\omega \cdot (n + \frac{1}{2})$.
  - Ground state ψ_0 satisfies $\hat{a}_-\psi_0 = 0$, or $(x + \frac{\hbar}{m\omega}\partial_x)\psi_0(x) = 0$. So $\psi_0(x) = (\frac{m\omega}{\pi\hbar})^{1/4}e^{-\frac{m\omega}{2\hbar}x^2}$.
  - nth excited state $\psi_n \propto (\hat{a}_+)^n\psi_0$. For normalization, consider $\langle(\hat{a}_+)^n\psi_0|(\hat{a}_+)^n\psi_0\rangle = \langle\psi_0|(\hat{a}_-)^n(\hat{a}_+)^n|\psi_0\rangle$ $= \langle\psi_0|(\hat{a}_-)^{n-1}\left((\hat{a}_+)^n\hat{a}_- + [\hat{a}_-, (\hat{a}_+)^n]\right)|\psi_0\rangle = \langle\psi_0|(\hat{a}_-)^{n-1}\left(0 + n(\hat{a}_+)^{n-1}\right)|\psi_0\rangle$ (useful fact above) $= n \cdot \langle\psi_0|(\hat{a}_-)^{n-1}(\hat{a}_+)^{n-1}|\psi_0\rangle = n!$ (mathematical induction). So $\psi_n = \frac{1}{\sqrt{n!}}(\hat{a}_+)^n\psi_0$.
  - $\hat{a}_+|\psi_n\rangle = \sqrt{n+1}|\psi_{n+1}\rangle$, $\hat{a}_-|\psi_n\rangle = \sqrt{n}|\psi_{n-1}\rangle$.
    Exercise: check the matrices $(a_\pm)_{m,n} \equiv \langle\psi_m|\hat{a}_\pm|\psi_n\rangle$ are hermitian conjugate to each other
  - Example: $\langle\psi_0|\hat{x}^2|\psi_0\rangle = \langle\hat{x}\psi_0|\hat{x}\psi_0\rangle$, and $\hat{x}\psi_0 = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_- + \hat{a}_+)\psi_0 = \sqrt{\frac{\hbar}{2m\omega}}(0 + \psi_1)$, so $\langle\psi_0|\hat{x}^2|\psi_0\rangle = \frac{\hbar}{2m\omega}\langle\psi_1|\psi_1\rangle = \frac{\hbar}{2m\omega}$. Or use $\hat{x}^2 = \frac{\hbar}{2m\omega}(\hat{a}_-^2 + \hat{a}_+^2 + 2\hat{a}_+\hat{a}_- + 1)$.

Harmonic oscillator: analytic method

- Consider the eigenvalue problem, $(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{m\omega^2}{2}x^2)\psi(x)=E\cdot\psi(x)$.
  Define dimensionless $\xi=\sqrt{\frac{m\omega}{\hbar}}x$, $K=\frac{2E}{\hbar\omega}$, this equation becomes $\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}\psi=(\xi^2-K)\cdot\psi$.
  - Asymptotic behavior: the ξ^2 term dominates as $\xi\to\pm\infty$; assume $\psi=e^{f(\xi)}$, $\frac{\mathrm{d}^2\psi}{\mathrm{d}\xi^2}=[(\frac{\mathrm{d}f}{\mathrm{d}\xi})^2+\frac{\mathrm{d}^2f}{\mathrm{d}\xi^2}]\cdot\psi$,
    (i) assume $\frac{\mathrm{d}^2f}{\mathrm{d}\xi^2}\sim\xi^2$, then $f\sim\frac{\xi^4}{12}$, $(\frac{\mathrm{d}f}{\mathrm{d}\xi})^2\sim\frac{\xi^6}{9}$ is the dominant term, so this is not self-consistent;
    (ii) assume $(\frac{\mathrm{d}f}{\mathrm{d}\xi})^2\sim\xi^2$, then $f\sim\pm\frac{\xi^2}{2}$, $\frac{\mathrm{d}^2f}{\mathrm{d}\xi^2}\sim\pm1$, self-consistent. Normalizable $\psi\sim e^{-\frac{\xi^2}{2}}$, $\xi\to\pm\infty$.
  - Assume $\psi(\xi)=h(\xi)\cdot e^{-\frac{\xi^2}{2}}$, then $\frac{\mathrm{d}^2h}{\mathrm{d}\xi^2}-2\xi\frac{\mathrm{d}h}{\mathrm{d}\xi}+(K-1)h=0$. Assume $h(\xi)=\sum_{j=0}^{\infty}a_j\xi^j$, we have the recursion relation $a_{j+2}=\frac{2j+1-K}{(j+1)(j+2)}\cdot a_j$. If all $a_j\neq0$, for large j, $a_{j+2}\sim\frac{2}{j+1}a_j\sim\frac{1}{(j/2)!}\cdot$ Const., then $h\sim e^{\xi^2}$, contradicts with normalizable ψ (there are loopholes in this argument). Normalizable ψ requires h being truncated to finite order, $a_n\neq0$ but $a_j=0$ for $j>n$. Then $2n+1-K=0$ (otherwise $a_{n+2}\neq0$).
  - Bound state energies are $E_n=(n+\frac{1}{2})\cdot\hbar\omega$. Corresponding $h_n(\xi)$ has only $\xi^n,\xi^{n-2},\xi^{n-4},\ldots$ terms (if it has ξ^{n-1} term, it will have all $\xi^{n+(\text{odd integer})}$ terms). h_n and ψ_n are even/odd functions for n even/odd.
  - $\psi_n=(\frac{m\omega}{\pi\hbar})^{1/4}\frac{1}{\sqrt{2^n n!}}H_n(\xi)e^{-\frac{\xi^2}{2}}$. H_n is Hermite polynomial. $H_n(x)=(-1)^n e^{x^2}\frac{\mathrm{d}^n}{\mathrm{d}x^n}e^{-x^2}=2^nx^n+\ldots$.
  - Generating function: $e^{-(x-t)^2}=\sum_{n=0}^{\infty}\frac{t^n}{n!}H_n(x)e^{-x^2}$ (related to “coherent state”, textbook Problem 3.35).
  - Recursion relation: $H_{n+1}(x)=2x\cdot H_n(x)-2n\cdot H_{n-1}(x)$. Exercise: “derive” this from the above ψ_n formula, and $2\sqrt{\frac{m\omega}{\hbar}}\hat{x}\psi_n=\sqrt{2}(\hat{a}_-+\hat{a}_+)\psi_n=\sqrt{2n}\psi_{n-1}+\sqrt{2(n+1)}\psi_{n+1}$.
  - ψ_n form complete orthonormal basis for the Hilbert space of normalizable wave functions in 1D.

δ-function potential: bound states

- $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$, $V(x) = \alpha \cdot \delta(x)$. Note: α has unit of (energy·length).
  The sign of α here is opposite to that in textbook.
  - Good approximation for "narrow" (width≪relevant "wavelength") potential barrier/well $V(x)$, and $\alpha = \int \mathrm{d}x\, V(x)$.
  - For $[-\frac{\hbar^2}{2m}\partial_x^2 + \alpha \cdot \delta(x)]\psi = E \cdot \psi$, integrate over $x \in [-\epsilon, \epsilon]$ and take $\epsilon \to +0$ limit,
    $-\frac{\hbar^2}{2m}\partial_x \psi\Big|_{x=0-}^{0+} + \alpha\psi(x=0) = 0$. So derivative of eigenstate ψ may have discontinuity at the δ-potential.
    This "boundary condition" works also for $V(x)$ containing other terms finite at $x = 0$.
  - According to [2.1], if $\alpha < 0$, there may be bound states with $E < 0$; if $\alpha > 0$, there is no bound state.
  - For $\alpha < 0$, suppose the bound state energy is $E < 0$, define "imaginary wavevector" $\kappa = \sqrt{-2mE}/\hbar$. For regions $x > 0$ and $x < 0$ away from δ-potential, the problem is the same as free particle, $-\frac{\hbar^2}{2m}\partial_x^2\psi = E\psi$.
    Therefore the eigenstate is a linear combination of $e^{\pm\kappa x}$ in each region. Normalizable ψ must be $Ae^{-\kappa x}$ for $x > 0$, and $Be^{\kappa x}$ for $x < 0$.
  - Boundary condition at $x = 0$: ψ is continuous, $\psi(x = 0+) = \psi(x = 0-)$, or $A = B$;
    for $\partial_x\psi$, $-\frac{\hbar^2}{2m}[\partial_x\psi(x = 0+) - \partial_x\psi(x = 0-)] + \alpha\psi(x = 0) = 0$, or $A \cdot \frac{\hbar^2}{m}\kappa + \alpha \cdot A = 0$ (used $A = B$).
    Then $\kappa = \frac{m\cdot(-\alpha)}{\hbar^2}$.
  - There is only one bound state for δ-function potential well ($\alpha < 0$), with
    $E_0 = -\frac{m\alpha^2}{2\hbar^2}$, $\psi_0(x) = \sqrt{\kappa}e^{-\kappa|x|}$, $\kappa = \frac{m\cdot(-\alpha)}{\hbar^2}$. (see schematic picture of wave function below)

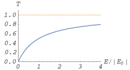


δ-function potential: scattering states

- $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$, $V(x) = \alpha \cdot \delta(x)$.
  - For $E > 0$, define wavevector $k = \sqrt{2mE}/\hbar$. For regions $x > 0$ and $x < 0$ away from δ-potential, the problem is the same as free particle, $-\frac{\hbar^2}{2m}\partial_x^2\psi = E\psi$. Therefore the eigenstate is a linear combination of planewaves $e^{\pm \mathbb{i}kx}$ in each region. $\psi = Ae^{\mathbb{i}kx} + Be^{-\mathbb{i}kx}$ for $x < 0$; and $\psi = Fe^{\mathbb{i}kx} + Ge^{-\mathbb{i}kx}$ for $x > 0$.
  - Boundary condition at $x = 0$: ψ is continuous, $\psi(x = 0+) = \psi(x = 0-)$, or $A + B = F + G$; for $\partial_x\psi$, $-\frac{\hbar^2}{2m}[\partial_x\psi(x = 0+) - \partial_x\psi(x = 0-)] + \alpha\psi(x = 0) = 0$, or $-\frac{\hbar^2}{2m}(\mathbb{i}k)(F - G - A + B) + \alpha \cdot (A + B) = 0$. We can solve F, G in terms of A, B (textbook Problem 2.53), or solve B, F in terms of A, G (textbook Problem 2.52).
  - Transmission & reflection coefficient: consider the case with $G = 0$, view the A term as incident wave, B term as reflected wave, F term as transmitted wave. The transmission/reflection coefficient is the ratio $\frac{\text{transmitted/reflected probability current}}{\text{incident probability current}}$.
  - For planewave $Ae^{\mathbb{i}kx}$, the probability current is $J = \mathrm{Re}[\psi^* \frac{\hat{p}}{m}\psi] = |A|^2 \frac{\hbar k}{m}$.
  - Define $\beta \equiv -\frac{m\alpha}{\hbar^2 k}$, and $E_0 = -\frac{m\alpha^2}{2\hbar^2}$ for the bound state energy (for $\alpha < 0$ case, see last page).

    Reflection coefficient $R \equiv \left(\frac{|B|^2}{|A|^2}\right)_{G=0} = \frac{\beta^2}{1+\beta^2} = \frac{|E_0|}{|E_0|+E}$.

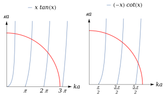
    Transmission coefficient $T \equiv \left(\frac{|F|^2}{|A|^2}\right)_{G=0} = \frac{1}{1+\beta^2} = \frac{E}{|E_0|+E}$.



  - Note that for low energy $E \ll |E_0|$, the incident wave is almost completely reflected; for high energy $E \gg |E_0|$, the potential is “transparent”, the incident wave is almost completely transmitted.

Finite square well: bound states

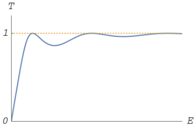
- $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$, $V(x) = \begin{cases} 0, & |x| > a; \\ -V_0, & |x| < a. \end{cases}$
  - According to [2.1], there may be bound states with $-V_0 < E < 0$.
  - For $x > a$ or $x < -a$, it is free particle $-\frac{\hbar^2}{2m}\partial_x^2\psi = E\psi$; for $-a < x < a$, it is $-\frac{\hbar^2}{2m}\partial_x^2\psi = (E+V_0)\psi$.
    Define $\kappa = \sqrt{-2mE}/\hbar$, $k = \sqrt{2m(E+V_0)}/\hbar$. The bound states must be
    $\psi = Ae^{-\kappa x}$ for $x > a$; $\psi = Be^{\kappa x}$ for $x < -a$; $\psi = C\cos(kx) + D\sin(kx)$ for $-a < x < a$.
  - The potential has inversion symmetry, $V(x) = V(-x)$, the bound states will be either even or odd functions.
  - The boundary condition is that ψ and $\partial_x\psi$ are continuous at $x = \pm a$.
  - Even solutions: $B = A$, $D = 0$. From the boundary condition at $x = a$ ($x = -a$ produces the same equations),
    $Ae^{-\kappa a} = C\cos(ka)$, $(-\kappa)Ae^{-\kappa a} = -kC\sin(ka)$. So $(\kappa a) = (ka)\cdot\tan(ka)$.
  - Odd solutions: $B = -A$, $C = 0$. From the boundary condition at $x = a$
    $Ae^{-\kappa a} = D\sin(ka)$, $(-\kappa)Ae^{-\kappa a} = kD\cos(ka)$. So $(\kappa a) = -(ka)\cdot\cot(ka)$.
  - Note that κa and ka are positive, and $(\kappa a)^2 + (ka)^2 = \frac{2mV_0a^2}{\hbar^2}$ is a constant (red circles in pictures below).
    Left picture: $(x\cdot\tan x)$ has positive-valued branches for $x \in (n\pi, n\pi + \frac{\pi}{2})$,
    monotonically increasing from 0 to $+\infty$ for x from $n\pi$ to $n\pi + \frac{\pi}{2}$.
    Right picture: $(-x\cdot\cot x)$ has positive-valued branches for $x \in (n\pi - \frac{\pi}{2}, n\pi)$,
    monotonically increasing from 0 to $+\infty$ for x from $n\pi - \frac{\pi}{2}$ to $n\pi$.



  - Number of even solutions: $\lfloor \frac{a\sqrt{2mV_0}}{\hbar\pi} \rfloor + 1$. Number of odd solutions: $\lfloor \frac{a\sqrt{2mV_0}}{\hbar\pi} + \frac{1}{2} \rfloor$.
    There is always one bound state (ground state), with even wave function, no matter how small V_0 is. This is a special property of 1D problems. In higher dimensions, shallow potential well may not have bound states.
  - Exercise: check that when $a \to 0$ and $2aV_0 = \alpha$, this becomes the δ-potential;
    check that when $V_0 \to +\infty$, this becomes the infinite square well.

Finite square well: scattering states

- $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$, $V(x) = \begin{cases} 0, & |x| > a; \\ -V_0, & |x| < a. \end{cases}$
  - For scattering state, $E > 0$, define $k = \sqrt{2mE}/\hbar$.
    The transmission coefficient $T = [1 + \frac{V_0^2}{4E(E+V_0)} \sin^2(\frac{2a}{\hbar}\sqrt{2m(E+V_0)})]^{-1}$.
    See textbook Section 2.6 for details.
  - When $E = -V_0 + \frac{\hbar^2}{2m}(\frac{n\pi}{2a})^2$ ($n = 1, 2, \ldots$), the would-be bound state energy for infinite square potential well of width $2a$, the transmission coefficient reaches unity (resonant tunneling).
    See a schematic picture of T vs. E below.



  - Exercise: check that when $a \to 0$ and $2aV_0 = \alpha$, the transmission coefficient becomes the δ-potential result.