130B Quantum Physics

Part 2. Piecewise Potentials

Basic Piecewise Potentials

■ General Setup

■ Schrödinger Equation

Consider a single quantum particle moving along a *one-dimensional line* under a *time-independent* potential $V(x)$. The system is described by the **Hamiltonian** operator

$$\hat{H} = \frac{\hat{p}^2}{2\,m} + V(\hat{x}). \tag{1}$$

- $\hat{x}$: **position** operator,
- $\hat{p} = -i\,\hbar\,\partial_x$: **momentum** operator.

For *time-independent* $\hat{H}$, we look for **stationary state** solution by solving the **stationary Schrödinger equation**

$$\hat{H}\,\psi(x) = E\,\psi(x), \tag{2}$$

explicitly:

$$\boxed{\left(-\frac{\hbar^2}{2\,m}\,\partial_x^2 + V(x)\right)\psi(x) = E\,\psi(x).} \tag{3}$$

- This is an **eigen equation** for the Hamiltonian operator $\hat{H}$.
- Each solution $\psi(x)$ is an **energy eigenstate** with eigen energy E.

■ Stationary State

The full wavefunction $\psi(x,\,t)$ in the spacetime separates into the *spatial* and *temporal* parts:

$$\psi(x,\,t) = \psi(x)\,e^{-i\,E\,t/\hbar}. \tag{4}$$

- The time dependence is only a global *phase rotation*.
- The **probability density** $\rho(x)$ and the **probability current density** $j(x)$ both remain time-independent:

$$\rho(x) = |\psi(x,\, t)|^2 = |\psi(x)|^2,$$
$$j(x) = \frac{1}{2\,m}\,(\psi(x)^*\,\hat{p}\,\psi(x) - \psi(x)\,\hat{p}\,\psi(x)^*). \tag{5}$$

- For any physical observable $\hat{O}$ that does not explicitly depend on time,
  - its **expectation value** $\langle O \rangle$ will be *invariant* on stationary state,
  - its measurement outcome **probability distribution** will be *invariant* on stationary state.
- Stationary states are **energy eigenstates**.

■ Free Particle (Flat Potential)

■ Wave Function

Hamiltonian (for $V(x) = 0$)

$$\hat{H} = \frac{\hat{p}^2}{2\,m} = -\frac{\hbar^2}{2\,m}\,\partial_x^2. \tag{6}$$

In this case, the Schrödinger equation Eq. (3) simply admits **plane wave** solution

$$\boxed{\psi(x) = e^{i\,k\,x},} \tag{7}$$

where k is determined from

$$\boxed{E = \frac{p^2}{2\,m} = \frac{\hbar^2\,k^2}{2\,m} \Rightarrow k = \pm\frac{1}{\hbar}\,\sqrt{2\,m\,E}\,.} \tag{8}$$

■ Energy Spectrum

- **Energy spectrum** is *continuous*. ($\because$ k takes continuous value, $\therefore$ E is also continuous)
- **Level degeneracy** = 2 (except for the $k = 0$ state).

■ Travelling and Standing Wave

- **Travelling wave** (*momentum* eigenstate, $\psi(x) = e^{i\,k\,x}$)
  - $k > 0$: right-moving, i.e. $k = +\hbar^{-1}\,\sqrt{2\,m\,E}\,.$
  - $k < 0$: left-moving, i.e. $k = -\hbar^{-1}\,\sqrt{2\,m\,E}\,.$
- They are *orthogonal* states, related by the **reflection symmetry** $x \to -x$.
  - If two states are related by **symmetry**, their energy must be the same. ⇒ They are **degenerated**.

- For 1D free particle with reflection symmetry, every energy level is *two-fold* degenerated (except for $k = 0$).

- **Sanding wave** (equal weight superposition of travelling wave)

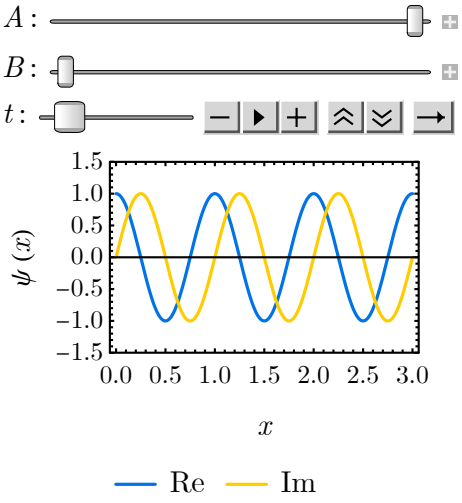
$$\begin{aligned} &\textbf{even}\ \text{parity}: \frac{1}{2}\left(e^{i\,k\,x} + e^{-i\,k\,x}\right) = \cos k\,x, \\ &\textbf{odd}\ \text{parity}: \frac{1}{2\,i}\left(e^{i\,k\,x} - e^{-i\,k\,x}\right) = \sin k\,x. \end{aligned} \tag{9}$$

  - Linear superposition of *degenerated* eigenstates are still eigenstates.

- Generic superposition of travelling waves

$$\begin{aligned} &\Psi(x,\,t) = \psi(x)\,e^{-i\,\omega\,t}, \\ &\psi(x) = A\,e^{i\,k\,x} + B\,e^{-i\,k\,x}, \end{aligned} \tag{10}$$

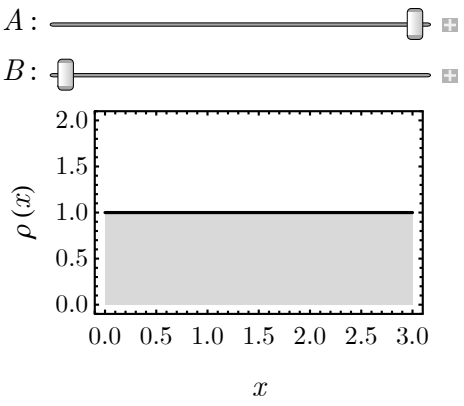
  - Normalization condition: $|A|^2 + |B|^2 = 1$.



  - Wave **node** and **antinode**.

  - Probability distribution

$$\rho(x) = |\psi(x)|^2 = \left|A\,e^{i\,k\,x} + B\,e^{-i\,k\,x}\right|^2. \tag{11}$$



■ Hard-Wall Potential

■ Wave Function

Potential profile

$$V(x) = \begin{cases} 0 & x > 0, \\ \infty & x < 0. \end{cases} \tag{12}$$

- Particle *can not enter* the negative half-space ($x < 0$) ⇒ *no probability* to appear in the negative half-space ⇒ wavefunction must *vanish* for $x \le 0$ ⇒ the **hard-wall condition**

$$\psi(x \le 0) = 0. \tag{13}$$

- In the positive half-space ($x > 0$), Hamiltonian still looks like Eq. (6) ⇒ general solution is given by Eq. (10)

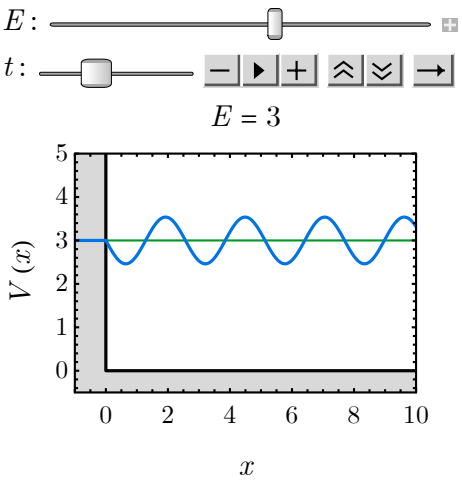
$$\psi(x \ge 0) = A\, e^{i\,k\,x} + B\, e^{-i\,k\,x}. \tag{14}$$

Eq. (13) and Eq. (14) must match at $x = 0$ ⇒ $A + B = 0$, so

$$\boxed{\psi(x) = \begin{cases} \sin k\,x & x > 0, \\ 0 & x \le 0. \end{cases}} \tag{15}$$

■ Energy Spectrum

- **Energy spectrum** is still *continuous*. $E = \hbar^2\, k^2 \,/\, (2\, m)$
- **Level degeneracy** = 1 ⇒ only $\sin k\,x$ states survives. $\cos k\,x$ states are not consistent with the hard-wall condition $\psi(x \le 0) = 0$.



Infinite Square Well

Wave Function

Potential profile

$$V(x) = \begin{cases} 0 & 0 < x < a, \\ \infty & \text{elsewhere.} \end{cases} \tag{16}$$

Hard-wall conditions at

$$\psi(x = 0) = \psi(x = a) = 0. \tag{17}$$

Wave nodes at both walls ⇒ the well width a sets the wave length ⇒ **momentum quantization**

$$k = \frac{n\,\pi}{a} \quad (n = 1, 2, 3 \ldots \in \mathbb{Z}_+). \tag{18}$$

Each positive integer n labels an eigenstate, whose wavefunction is given by

$$\psi_n(x) = \begin{cases} \left(\frac{2}{a}\right)^{1/2} \sin \frac{n\pi}{a}\, x & 0 < x < a, \\ \infty & \text{elsewhere.} \end{cases} \tag{19}$$

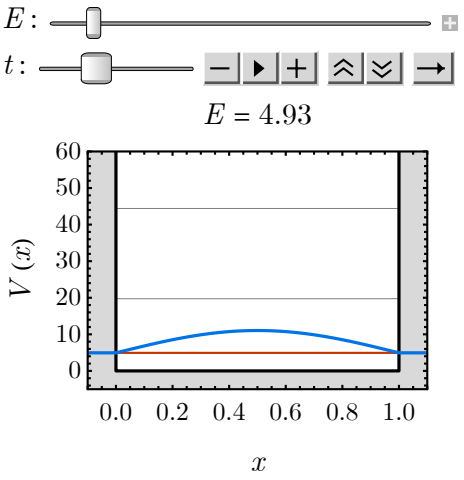
Energy Spectrum

- **Energy spectrum** becomes *discrete*

$$E_n = \frac{\hbar^2\, k^2}{2\, m} = \frac{\pi^2\, \hbar^2}{2\, m\, a^2}\, n^2 \quad (n \in \mathbb{Z}_+). \tag{20}$$

- n labels the **energy level**, so it is also called the **level index**.

- **Level degeneracy** = 1 (non-degenerated).



- As we squeeze the potential (a smaller), energy will increase. ⇒ an example of the **uncertainty principle**. The particle exerts a pressure to the walls.

■ Probability Distribution

Probability to find the particle at position x: $\rho(x) = |\psi(x)|^2$,

$$\rho(x) = \begin{cases} \frac{2}{a} \sin^2 \frac{n\pi}{a} x & 0 < x < a, \\ 0 & \text{elsewhere.} \end{cases} \tag{21}$$

- Probability must add up to 1 ⇒ **normalization condition**:

$$\int_{-\infty}^{+\infty} \rho(x)\, dx = 1. \tag{22}$$

Exc 1 Check the normalization condition Eq. (22).

- The prefactor in the wavefunction is called the **normalization factor**.
- **Bound state** wavefunctions are *normalizable*.

■ Time Evolution of Generic States

- The initial state can be decomposed on the energy eigen basis.

$$\psi(x, 0) = \sum_n c_n \psi_n(x). \tag{23}$$

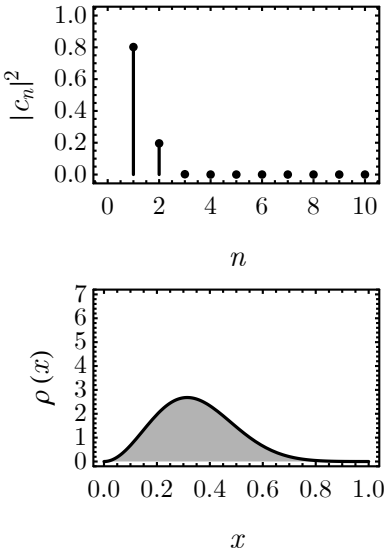
- Coefficient is given by the inner product (calculated as integral)

$$c_n = \int dx\, \psi_n^*(x)\, \psi(x, 0). \tag{24}$$

- Each energy eigen state evolves independently (phase angle rotates according to the energy)

$$\psi(x,\, t) = \sum_n c_n\, \psi_n(x)\, e^{-i\, E_n\, t}. \tag{25}$$

Example: a particle bouncing in the potential well. How is the quantum motion different from or similar to the classical analog?



■ Step Potential

■ Wave Function

Step potential at $x = 0$

$$V(x) = V_0\, \Theta(x) = \begin{cases} 0 & x < 0, \\ V_0 & x > 0. \end{cases} \tag{26}$$

Let E be the eigen energy,

$$E = \frac{p^2}{2\, m} + V(x) = \frac{\hbar^2\, k^2}{2\, m} + \begin{cases} 0 & x < 0, \\ V_0 & x > 0. \end{cases} \tag{27}$$

In different regions, different potential energies ⇒ different momentum

$$k_1^2 = \frac{2\, m\, E}{\hbar^2},\ k_2^2 = \frac{2\, m\, (E - V_0)}{\hbar^2}. \tag{28}$$

Piecewise form of the wavefunction

$$\psi(x) = \begin{cases} e^{i\, k_1\, x} + r\, e^{-i\, k_1\, x} & x < 0, \\ t\, e^{i\, k_2\, x} & x > 0. \end{cases} \tag{29}$$

Boundary condition: wavefunction and its first order derivative must match at the region boundary ($x = 0$)

$$\psi(0_+) = \psi(0_-),$$
$$\partial_x \psi(0_+) = \partial_x \psi(0_-). \tag{30}$$

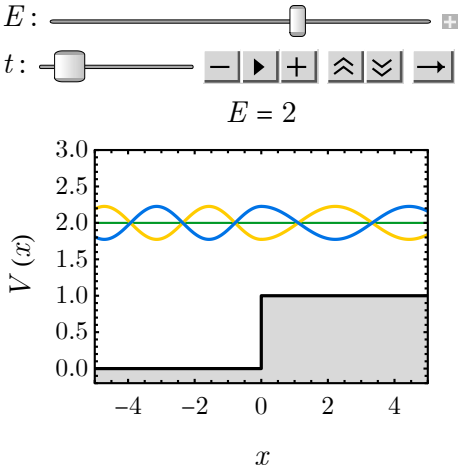
Solution for the amplitudes r and t

$$r = \frac{k_2 - k_1}{k_1 + k_2}, \quad t = \frac{2\,k_1}{k_1 + k_2}. \tag{31}$$

■ Scattering State ($E > V_0$)

According to Eq. (28), both k_1 and k_2 are real.

- Travelling wave
- Level degeneracy = 2 (left- and right-moving)



- **Reflection coefficient**

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}, \tag{32}$$

- **Transmission coefficient**

$$T = \frac{4\,k_1\,k_2}{(k_1 + k_2)^2}, \tag{33}$$

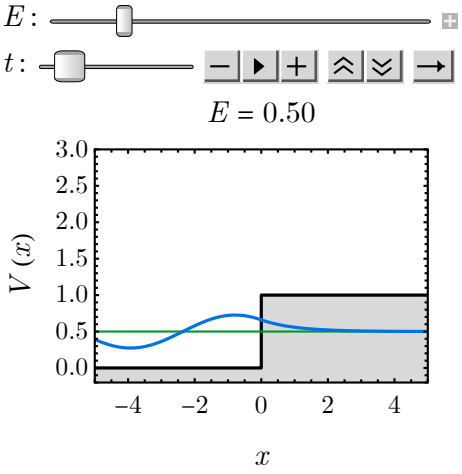
- Conservation of probability implies that $R + T = 1$.

■ Total Reflection State ($0 < E < V_0$)

According to Eq. (28), k_1 is real, but $k_2 = i\,\kappa_2$ is imaginary.

- Standing wave

- Level degeneracy = 1



In terms of the imaginary momentum κ_2

$$\psi(x) = \begin{cases} e^{i\,k_1\,x} + r\,e^{-i\,k_1\,x} & x < 0, \\ t\,e^{-\kappa_2\,x} & x > 0. \end{cases} \tag{34}$$

- The particle can penetrate into the potential barrier, but is wave amplitude decays exponentially. **Penetration depth** (a length scale)

$$\xi = \frac{1}{\kappa_2} = \frac{\hbar}{\sqrt{2\,m\,(V_0 - E)}}. \tag{35}$$

- Solution for amplitudes r and t

$$r = \frac{i\,\kappa_2 - k_1}{k_1 + i\,\kappa_2}, \quad t = \frac{2\,k_1}{k_1 + i\,\kappa_2}. \tag{36}$$

- Phase shift of the reflection wave

$$\delta = \arg r = 2\,\operatorname{arccot}\frac{\kappa_2}{k_1}. \tag{37}$$

- Reflection and transmission coefficients

$$\boxed{R = 1,\ T = 0.} \tag{38}$$

Total reflection (no transmission).

■ Square Potential

■ General Discussion

Potential profile ($a > 0$)

$$V(x) = \begin{cases} V_0 & |x| < a/2, \\ 0 & |x| > a/2. \end{cases} \tag{39}$$

Let E be the energy,

$$E = \frac{\hbar^2 k^2}{2m} + \begin{cases} V_0 & |x| < a/2, \\ 0 & |x| > a/2. \end{cases} \tag{40}$$

Two different momenta: k_1 for $|x| > a/2$, k_2 for $|x| < a/2$.

$$k_1^2 = \frac{2mE}{\hbar^2},\ k_2^2 = \frac{2m(E - V_0)}{\hbar^2}, \tag{41}$$

which are related by

$$k_1^2 - k_2^2 = \frac{2m\,V_0}{\hbar^2}. \tag{42}$$

- The potential is *symmetric* under **reflection**: $V(x) = V(-x)$, so every eigenstate has a definite **parity** quantum number (this is a $\mathbb{Z}_2$ symmetry).
  - *Even* parity $\psi(-x) = \psi(x)$

$$\psi_e(x) = \begin{cases} A_e\, e^{i k_1 x} + B_e\, e^{-i k_1 x} & x > a/2 \\ \cos k_2 x & |x| < a/2 \\ A_e\, e^{-i k_1 x} + B_e\, e^{i k_1 x} & x < -a/2 \end{cases}. \tag{43}$$

  - *Odd* parity $\psi(-x) = -\psi(x)$

$$\psi_o(x) = \begin{cases} A_o\, e^{i k_1 x} + B_o\, e^{-i k_1 x} & x > a/2 \\ \sin k_2 x & |x| < a/2 \\ -A_o\, e^{-i k_1 x} - B_o\, e^{i k_1 x} & x < -a/2 \end{cases}. \tag{44}$$

■ Bound State in Potential Well ($V_0 < E < 0$)

▫ The Logarithmic Trick

According to Eq. (41), $k_1 = i\kappa_1$ is imaginary, k_2 is real. In this case, we require $B_e = B_o = 0$, otherwise the wavefunction is not normalizable. So Eq. (43) and Eq. (44) becomes:

- *Even* parity $\psi(-x) = \psi(x)$

$$\psi_e(x) = \begin{cases} A_e\, e^{-\kappa_1 x} & x > a/2 \\ \cos k_2 x & |x| < a/2 \\ A_e\, e^{\kappa_1 x} & x < -a/2 \end{cases}. \tag{45}$$

- *Odd* parity $\psi(-x) = -\psi(x)$

$$\psi_o(x) = \begin{cases} A_o\, e^{-\kappa_1 x} & x > a/2 \\ \sin k_2 x & |x| < a/2 \\ -A_o\, e^{\kappa_1 x} & x < -a/2 \end{cases}. \tag{46}$$

Both $\psi(x)$ and $\partial_x\psi(x)$ are required to be continuous at the region boundaries, this implies $\partial_x \ln\psi(x) = \partial_x\psi(x)/\psi(x)$ to also be continuous (as long as $\psi(x)$ does not vanish at the region

boundary):

$$\begin{aligned}\partial_x \ln \psi_e(a/2+0_+) &= \partial_x \ln \psi_e(a/2-0_+),\\ \partial_x \ln \psi_o(a/2+0_+) &= \partial_x \ln \psi_o(a/2-0_+).\end{aligned} \tag{47}$$

Plugging in the wavefunctions in Eq. (45) and Eq. (46), and combine with Eq. (42),

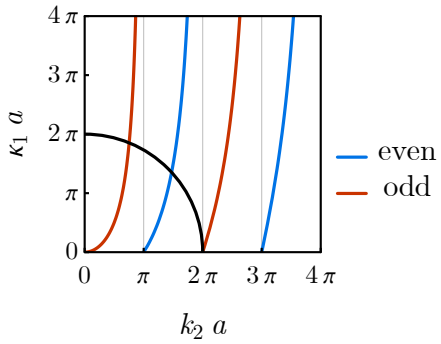
$$\begin{aligned}&\text{even}: \kappa_1 = k_2 \tan\frac{k_2\, a}{2},\\ &\text{odd}: \kappa_1 = -k_2 \cot\frac{k_2\, a}{2},\\ &\kappa_1^2 + k_2^2 = -\frac{2\, m\, V_0}{\hbar^2} \equiv k^2.\end{aligned} \tag{48}$$

From Eq. (48), we can solve for (κ_1, k_2). Then the amplitudes A_e and A_o follow from

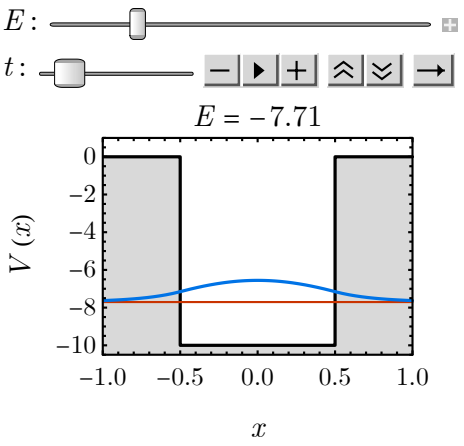
$$A_e = e^{\kappa_1\, a/2} \cos\frac{k_2\, a}{2},\ A_o = e^{\kappa_1\, a/2} \sin\frac{k_2\, a}{2}. \tag{49}$$

Pictorial Solutions

The solution of (κ_1, k_2) can be found pictorially by intersecting a circle (of radius k) with the curves of $\kappa_1(k_2)$.



- The $k\, a \to 0$ limit (meaning $V_0\, a^2 \to 0$), physically it can be
  - a *shallow* well: $V_0 \to 0$ with a fixed,
  - a *narrow* well: $a \to 0$ with V_0 fixed,
  - a *sharp* well: $a \to 0,\ V_0 \to -\infty$, with $V_0\, a = \gamma$ fixed.
- In either cases, there is one (and only one) *bound state* solution remaining in the *even* parity sector. All the higher energy bound states are pushed out of the well.



- *Bound state* energy levels are *discrete* and *non-degenerated*

$$E_n = -\frac{\hbar^2}{2\,m}\,\kappa_{1,n}^2. \tag{50}$$

- The number of bound states are given by

$$n_{\max} = \left\lfloor \frac{(2\,m\,V_0)^{1/2}\,a}{\pi\,\hbar} \right\rfloor + 1. \tag{51}$$

- In the *sharp* well limit ($a \to 0$ with $V_0\,a = \gamma$ fixed), the bound state is *unique* and its energy is given by

$$E_1 = -\frac{m}{2\,\hbar^2}\,(V_0\,a)^2 = -\frac{m\gamma^2}{2\,\hbar^2}. \tag{52}$$

HW 1

In the sharp well limit, (i) is the bound state of even parity of odd parity? (ii) Analyze the behavior of Eq. (48) in this limit to find the solution of κ_1. (iii) Use the solution to show the bound state energy is given by Eq. (52).

Solution (HW 1)

▪ Scattering State ($E > 0$ regardless of V_0)

According to Eq. (41), k_1 is real as long as $E > 0$, k_2 could be real or imaginary depending on the sign of $E - V_0$.

- The energy levels should be *continuous* for *scattering* states, so any $E > 0$ is admissible (there is no need to solve for k_1 and k_2).
- Every level is *doubly degenerated* (degeneracy = 2), corresponding to ψ_e and ψ_o.

From the boundary condition at $a/2$, we can determine A_e and B_e in Eq. (43) as well as A_o and B_o in Eq. (44). By combining ψ_e and ψ_o it is possible to eliminate $e^{-i\,k_1\,x}$ in the $x > a/2$ region, such that the wavefunction takes the form of

$$\psi(x) = \begin{cases} t\, e^{i\, k_1\, x} & x > a/2 \\ \ldots & |x| < a/2\,, \\ r\, e^{-i\, k_1\, x} + e^{i\, k_1\, x} & x < -a/2 \end{cases} \tag{56}$$

where the *reflection* and *transmission* amplitudes are

$$\begin{aligned} r &= \frac{1}{2}\left(\frac{A_e}{B_e} + \frac{A_o}{B_o}\right), \\ t &= \frac{1}{2}\left(\frac{A_e}{B_e} - \frac{A_o}{B_o}\right). \end{aligned} \tag{57}$$

- The transmission coefficient

$$\boxed{T = |t|^2 = \left(1 + \frac{V_0^2}{4\, E(E - V_0)}\, \sin^2 k_2\, a\right)^{-1},} \tag{58}$$

Exc 2 Derive Eq. (58).

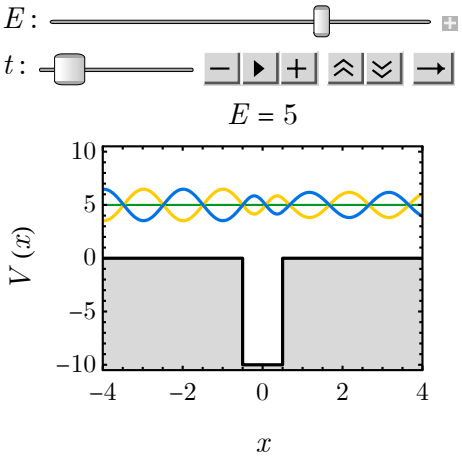
where k_2 is set by $(E - V_0)$ according to Eq. (41).

- In the *sharp* well limit ($a \to 0$ with $V_0\, a = \gamma$ fixed), Eq. (58) becomes

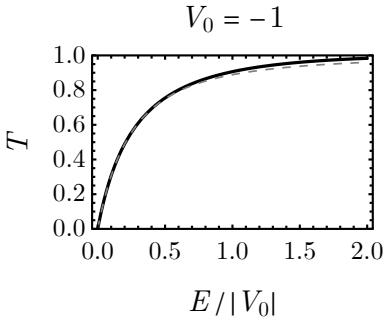
$$T = \left(1 + \frac{m\, \gamma^2}{2\, \hbar^2\, E}\right)^{-1}. \tag{59}$$

Exc 3 Prove Eq. (59).

▫ Scattered by a Potential Well ($V_0 < 0$)



- **Resonant transmission**: perfect transmission due the the cancelation (by *interference*) of reflection waves form the front and back interfaces.



- Resonance happens at $k_2\, a = n\,\pi$ ($n \in \mathbb{Z}$), where $\sin k_2\, a = 0$ and hence $T = 1$.
- Energy associated to the resonance forms *discrete* level

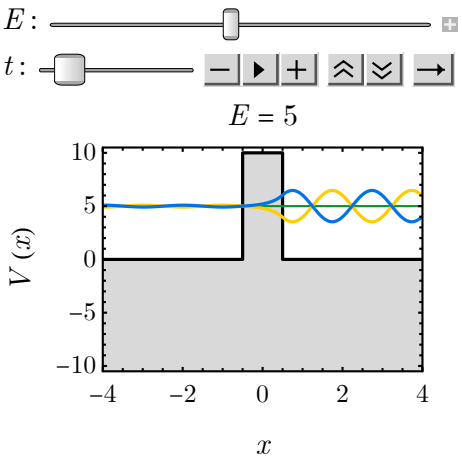
$$E_n = \frac{\pi^2\,\hbar^2}{2\,m\,a^2}\,n^2 + V_0, \tag{60}$$

for $n \geq n_{\max}$, where $n_{\max}$ is the number of bound states given in Eq. (51). Compare with Eq. (20), these levels locate at the same energy as the bound state level of a infinite depth well of the same width.

- Lower bound of the transmission coefficient is set by

$$T_{\text{low}} = \frac{4\,E(E - V_0)}{(2\,E - V_0)^2}. \tag{61}$$

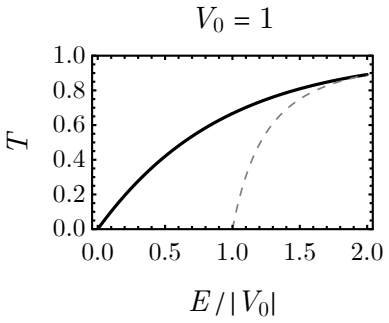
▫ Scattered by a Potential Barrier ($V_0 > 0$)



- **Quantum tunnelling**: Even if the energy is bellow the barrier ($0 < E < V_0$), wave can still tunnel through.
  - But the **tunneling rate** is *exponentially* suppressed.

$$T = \frac{16\,E(V_0 - E)}{V_0^2}\exp\left(-\frac{2\,a}{\hbar}\sqrt{2\,m\,(V_0 - E)}\right). \tag{62}$$

- *Heavier* particles (larger m) are harder to tunnel.
- The *wider* and *higher* the barrier is, the harder to tunnel.



- Above the barrier ($E > V_0$): **resonant tunneling** happens at

$$E_n = \frac{\pi^2 \hbar^2}{2\, m\, a^2}\, n^2 + V_0, \tag{63}$$

for $n = 1, 2, 3, \ldots$.

■ Dirac Potential

■ General Discussion

Dirac δ-function potential at $x = 0$ (a model for a single **impurity**)

$$V(x) = \gamma\, \delta(x). \tag{64}$$

Schrödinger equation Eq. (3) implies

$$\partial_x^2\, \psi(x) = \frac{2\, m}{\hbar^2}\, (\gamma\, \delta(x) - E)\, \psi(x). \tag{65}$$

Integrating both sides of Eq. (65) across $x = 0 \Rightarrow$ first-order derivative of the wavefunction jumps

$$\partial_x\, \psi(0_+) - \partial_x\, \psi(0_-) = \frac{2\, m}{\hbar^2} \int_{0_-}^{0_+} dx\, (\gamma\, \delta(x) - E)\, \psi(x) = \frac{2\, m\, \gamma}{\hbar^2}\, \psi(0). \tag{66}$$

Dimensional analysis: the γ sets a typical length scale - the **scattering length**

$$\boxed{a_s = \frac{\hbar^2}{m\, \gamma}.} \tag{67}$$

- **Matching Condition**: Eq. (66) requires the first-order derivative to jump by

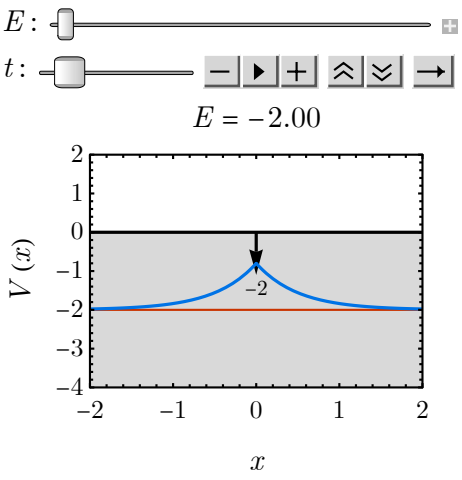
$$\boxed{\partial_x\, \psi(0_+) - \partial_x\, \psi(0_-) = \frac{2}{a_s}\, \psi(0).} \tag{68}$$

- **Continuity Condition**: Wavefunction must be continuous

$$\psi(0_+) = \psi(0_-). \tag{69}$$

■ Bound State ($\gamma < 0$, $E < 0$)

- *Attractive* impurity traps *bound* states.



- There is a *unique* bound state trapped by the Dirac potential

$$\psi(x) = \frac{1}{\sqrt{|a_s|}}\, e^{-|x|/|a_s|}. \tag{70}$$

Note that because $\gamma < 0$, the scattering length a_s is *negative*.

- The bound state is of *even* parity. There is no odd parity state that can be trapped by Dirac potential.
- The corresponding eigen energy is

$$E = -\frac{m\,\gamma^2}{2\,\hbar^2} = -\frac{\hbar^2}{2\,m\,a_s^2}, \tag{71}$$

which is consistent with Eq. (52).

HW 2

(i) Verify that $\psi(x)$ in Eq. (70) is a normalized wavefunction.
(ii) Apply the Dirac potential Hamiltonian (with $\gamma < 0$) to $\psi(x)$ in Eq. (70) to show that it is an eigenstate with eigen energy given by Eq. (71).
(iii) Show that the expectation value of the kinetic energy is $\langle E_K \rangle = -E$ and the expectation value of the potential energy $\langle E_V \rangle = 2\,E$.

▪ Scattering State ($E > 0$)

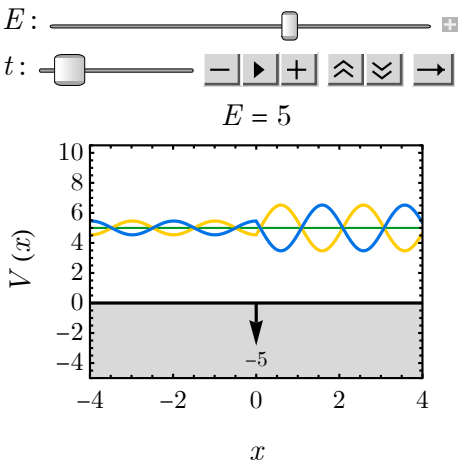
- Both *attractive* and *repulsive* impurity *scatters* the particle around.

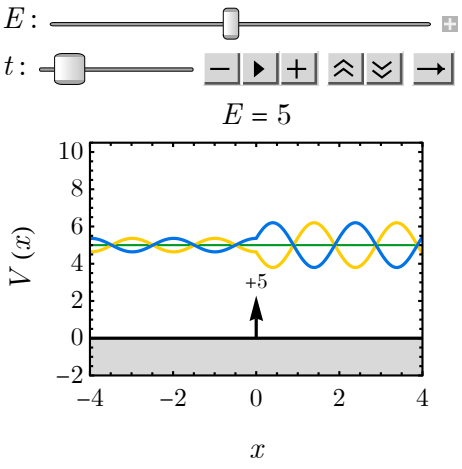
  For $E > 0$, let us take the *scattering state* wavefunction ansatz,

$$\psi(x) = \begin{cases} e^{i k x} + r\, e^{-i k x} & x < 0, \\ t\, e^{i k x} & x > 0, \end{cases} \tag{72}$$

where the momentum is determined by $k^2 = 2\, m\, E \,/\, \hbar^2$. By Eq. (68) and Eq. (69),

$$\begin{aligned} r &= -\frac{1}{1 - i\, k\, a_s}, \\ t &= \frac{1}{1 + i\, /(k\, a_s)}. \end{aligned} \tag{73}$$





- The reflection and transmission coefficients

$$R = \frac{1}{1 + k^2\, a_s^2} = \left(1 + \frac{2\, \hbar^2\, E}{m\, \gamma^2}\right)^{-1}, \tag{74}$$

$$T = \frac{k^2\, a_s^2}{1 + k^2\, a_s^2} = \left(1 + \frac{m\,\gamma^2}{2\,\hbar^2\, E}\right)^{-1}.$$

They sum up to unity $R + T = 1$. This is consistent with Eq. (59) for the sharp square potential. The *reflection* is *enhanced* (or the *transmission* is *reduced*)if

- the Dirac potential is strong ($|\gamma|$ large),
- the energy is low (E small),
- the particle is massive (m large). Intuitive argument: heavy particle ⇒ large momentum ⇒ short wave length ⇒ hard to diffract through the impurity, scatters strongly.

- **Scattering phase shift**: the reflected and transmitted wave are phase shifted from the incident wave.

$$\begin{aligned} \Delta\varphi_r &\equiv \arg r = \arctan k\, a_s - \pi \operatorname{sgn} a_s, \\ \Delta\varphi_t &\equiv \arg t = \arctan k\, a_s - (\pi/2) \operatorname{sgn} a_s. \end{aligned} \tag{75}$$

  - Weak potential limit ($\gamma \to 0,\ a_s \to \infty$): $\Delta\varphi_t = 0$, plane wave transmitted through the potential without phase shift (as if nothing happened).
  - Strong potential ($\gamma \to \infty,\ a_s \to 0$): $\Delta\varphi_r = \pi$, all incident wave are reflected with **half-wave loss**.

■ Double Dirac Potential

■ General Discussion

Double Dirac potential of strength γ, separated by distance a

$$V(x) = \gamma\,(\delta(x - a/2) + \delta(x + a/2)). \tag{76}$$

- Define momentum k and scattering length a_s

$$k^2 = \frac{2\,m\,E}{\hbar^2},\ a_s = \frac{\hbar^2}{m\,\gamma}. \tag{77}$$

- Bound state ($E < 0$) wavefunction ($k = i\,\kappa$ in this case)
  - Even parity

$$\psi(x) = \begin{cases} A\, e^{\kappa\, x} & x < -a/2, \\ \cosh \kappa\, x & -a/2 < x < a/2, \\ A\, e^{-\kappa\, x} & x > a/2. \end{cases} \tag{78}$$

  - Odd parity

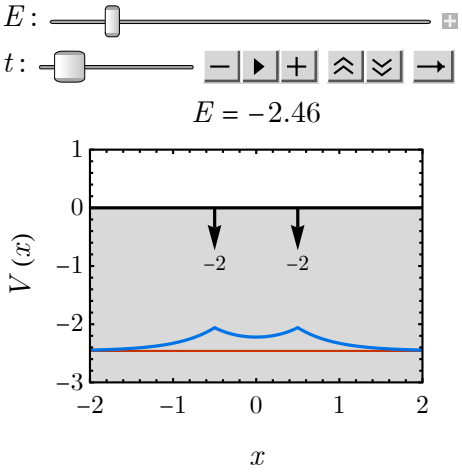
$$\psi(x) = \begin{cases} -A\, e^{\kappa x} & x < -a/2, \\ \sinh \kappa x & -a/2 < x < a/2, \\ A\, e^{-\kappa x} & x > a/2. \end{cases} \tag{79}$$

- Scattering state $(E > 0)$ wavefunction

$$\psi(x) = \begin{cases} e^{i k x} + r\, e^{-i k x} & x < -a/2, \\ A\, e^{i k x} + B\, e^{-i k x} & -a/2 < x < a/2, \\ t\, e^{i k x} & x > a/2. \end{cases} \tag{80}$$

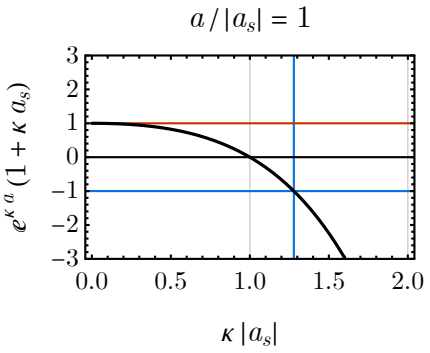
■ Bound State ($E < 0$)

- Depending on the scattering length $a_s = \hbar^2 (m\gamma)^{-1}$:
  - $a_s > 0$: no bound state,
  - $-a < a_s < 0$: *one* bound state of *even* parity,
  - $a_s < -a < 0$: *two* bound states of both parities.



- By matching wavefunction, κ can be determined from

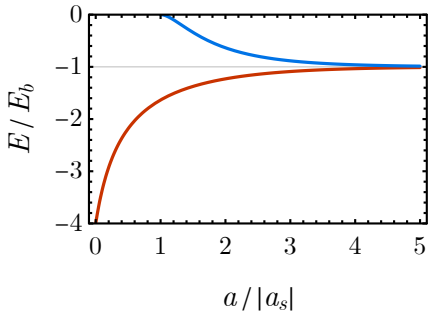
$$e^{\kappa a}(1 + \kappa\, a_s) = \begin{cases} -1 & \text{even parity}, \\ +1 & \text{odd parity}. \end{cases} \tag{81}$$



- Even parity: ■, odd parity: ■.
- When $a < |a_s|$, impurities are too close to host the odd parity solution.
- When $a = 0$, two impurities merge to one with *doubled* strength, so $\kappa = 2\,|a_s|$.

- The bounding energies are given by

$$E = -\frac{\hbar^2\,\kappa^2}{2\,m}. \tag{82}$$



- The energy E is in unit of the bound state energy $-E_b$ of a single Dirac well, with

$$E_b := \frac{\hbar^2}{2\,m\,a_s^2}, \tag{83}$$

as given in Eq. (71).

- As the impurities binds together ($a \to 0$), the **binding energy** $E_b = 3\,|E_0|$ will be released.

- **Force** between impurities are given by

$$F = -\frac{\partial\,E}{\partial\,a} \tag{84}$$

- Force can be *mediated* by *exchanging* particles.
- **Bonding orbital**: impurity *attracts* by exchanging particles in *even* parity state.

- **Anti-bounding orbital**: impurity *repels* by exchanging particles in *odd* parity state.

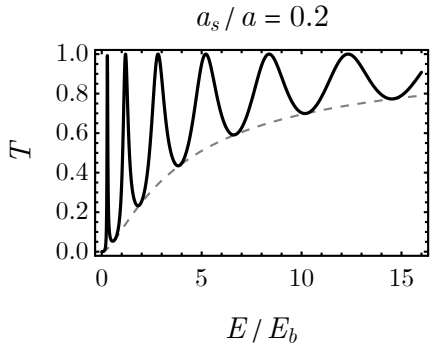
■ Scattering State ($E > 0$)

Transmission coefficient ($T = |t|^2$)

$$T = \left(1 + \frac{4\left(1 + k^2\, a_s^2\right)}{k^4\, a_s^4} \sin^2(k\, a + \varphi)\right)^{-1}, \tag{85}$$

$\varphi = \arctan k\, a_s$.

Exc 4 Solve the scattering state wavefunction and show Eq. (85).



- **Resonant tunneling** ($T = 1$) when ($k\, a + \varphi$) vanishes, which happens at

$$k_n\, a + \arctan k_n\, a_s = n\,\pi, \tag{86}$$

with $n = (0), 1, 2, \ldots$. (n can take 0 only if $\gamma < 0$ and $a < |a_s|$), and the corresponding energy is

$$E_n = \frac{\hbar^2\, k_n^2}{2\, m}. \tag{87}$$

- Weak potential limit $\gamma \to 0$ (or $a_s \to \pm\infty$)
  - Weak well limit $\gamma \to 0_-$

$$E_n = \frac{\pi^2\, \hbar^2}{2\, m\, a^2}\left(n + \frac{1}{2}\right)^2,\ (n = 0, 1, 2, \ldots). \tag{88}$$

  - Weak barrier limit $\gamma \to 0_+$

$$E_n = \frac{\pi^2\, \hbar^2}{2\, m\, a^2}\left(n - \frac{1}{2}\right)^2,\ (n = 1, 2, \ldots). \tag{89}$$

- Strong potential limit $\gamma \to \infty$ (or $a_s \to 0$)

$$E_n = \frac{\pi^2\, \hbar^2}{2\, m\, (a + a_s)^2}\, n^2,\ (n = 1, 2, \ldots). \tag{90}$$

- **Quasi-bound states** formed at these levels, when

$$n \ll \left| \frac{a}{\pi\, a_s} \right|. \tag{91}$$

(Such that the resonance is sharp).

- Note that quasi-bound state are still *scattering* state. The resonant levels are still *doubly degenerated* (left- and right-moving).
- When $a_s = 0$, one of the quasi-bound states becomes the *bound state* inside a pair of *infinite walls*, and the other becomes a resonant state outside the walls.

HW 3

Consider a quantum particle confined in a one-dimensional infinite square well of width a, with an additional Dirac potential at the center of strength γ:
$V(x) = \begin{cases} \gamma\,\delta(x) & |x| < a/2, \\ +\infty & |x| > a/2. \end{cases}$
(a) Show that the energy levels are given by
$E_n = \frac{\hbar^2}{2\,m}\, k_n^2$, $(n = 1, 2, 3, \ ...)$,
where for even n, $k_n = n\,\pi/a$; and for odd n, k_n is determined by the equation $\tan(k_n\, a/2) = -k_n\, a_s$ (with $a_s = \hbar^2 (m\,\gamma)^{-1}$ being the scattering length).
(b) Discuss how the energy levels behave in the limits $\gamma \to +\infty$ (strong repulsive) and $\gamma \to -\infty$ (strong attractive). In particular, describe the level degeneracies in each case.
(c) For attractive impurity $\gamma < 0$, show that the impurity bound state forms only when infinite square well is sufficiently wide: $a > 2\,|a_s|$.

■ Periodic Dirac Potential

■ General Discussion

1D **periodic potential** formed by an infinite array of Dirac delta functions

$$V(x) = \sum_{l=-\infty}^{\infty} \gamma\,\delta(x - l\,a), \tag{92}$$

where

- γ - the strength of each Dirac potential, which defines the scattering length a_s

$$a_s = \frac{\hbar^2}{m\,\gamma}, \tag{93}$$

- a - **lattice spacing** (periodicity in space),
- $l \in \mathbb{Z}$ - lattice index.

Introduce the **itinerant momentum** K (assuming $E > 0$),

$$K^2 = \frac{2\,m\,E}{\hbar^2}, \tag{94}$$

In each region, the wave function takes the form of

$$\psi(x) = \begin{cases} \vdots & \vdots \\ A_l\, e^{i\,K\,x} + B_l\, e^{-i\,K\,x} & l\,a < x < (l+1)\,a, \\ \vdots & \vdots \end{cases} \tag{95}$$

■ Bloch's Theorem

For any **periodic potential** $V(x+a) = V(x)$, the eigenstate $\psi(x)$ of the Schrödinger equation must take the form of **Bloch function**

$$\boxed{\psi(x) = e^{i\,k\,x}\,u_k(x),} \tag{96}$$

where

- $u_k(x)$ is **periodic**: $u_k(x+a) = u_k(x)$ (of the same periodicity)
- $k \in [-\pi/a, \pi/a)$ is the **quasi-momentum**.

Proof: The key is to notice that the system has a **lattice translation symmetry**, which can be implemented by a *unitary* operator $\hat{T}_a$,

$$\boxed{\hat{T}_a = e^{i\,\hat{p}\,a/\hbar},} \tag{97}$$

such that

$$\begin{aligned} \hat{T}_a^\dagger\,\hat{p}\,\hat{T}_a &= \hat{p}, \\ \hat{T}_a^\dagger\,\hat{x}\,\hat{T}_a &= \hat{x} - a. \end{aligned} \tag{98}$$

Exc 5 Show Eq. (98) based on the definition Eq. (97).

Given $\hat{H} = \frac{1}{2\,m}\,\hat{p}^2 + V(\hat{x})$ with $V(x-a) = V(x)$, Eq. (98) implies

$$\hat{T}_a^\dagger\,\hat{H}\,\hat{T}_a = \hat{H}, \tag{99}$$

or equivalently, $\left[\hat{H},\,\hat{T}\right] = 0$. Therefore, the eigenstates of $\hat{H}$ can be organized as joint eigenstates of $\hat{H}$ and $\hat{T}$. Let $|\psi\rangle$ be a *common* eigenstate of $\hat{H}$ and $\hat{T}$. Because $\hat{T}$ is *unitary*, its eigenvalue can only be a *phase factor*, might as well be denoted as $e^{i\,k\,a}$ (introducing $k \in [-\pi/a, \pi/a)$ to parametrize the phase),

$$\hat{T}\,|\psi\rangle = e^{i\,k\,a}\,|\psi\rangle. \tag{100}$$

In terms of the wave function, Eq. (100) means

$$\psi(x+a) = e^{i\,k\,a}\,\psi(x). \tag{101}$$

If we define $u_k(x) = e^{-i\,k\,x}\,\psi(x)$, it can be shown that

$$u_k(x+a) = e^{-i\,k\,(x+a)}\,\psi(x+a) = e^{-i\,k\,x}\,\psi(x) = u_k(x) \tag{102}$$

is a *periodic* function of the same periodicity as the lattice. So the Bloch function in Eq. (96) is indeed a generic form for $\psi(x)$ to take in order to satisfy the requirement Eq. (101) for it to be an eigenstate of $\hat{T}_a$.

■ Kronig-Penney Relation

Applying the Bloch theorem to the wavefunction Eq. (95), it can be casted into

$$\begin{aligned}&\psi(x) = e^{i\,k\,x}\,u_k(x),\\&u_k(x) = A\;e^{i\;(K-k)\,(x \bmod a)} + B\,e^{-i\,(K+k)\,(x \bmod a)}.\end{aligned} \tag{103}$$

- $x \bmod a$ ensures the function $u_k(x+a) = u_k(x)$ to be periodic.
- The momentum $K \pm k$ ensures that in the region between Dirac potentials, the wave momentum should match the *itinerant momentum* K set by the energy E in Eq. (94).

Substitute Eq. (103) to the **continuity** and **matching** conditions

$$\begin{aligned}&\psi(l\,a+0_+) = \psi(l\,a+0_-),\\&\partial_x\,\psi(l\,a+0_+) - \partial_x\,\psi(l\,a+0_-) = 2\,/\,a_s\,\psi(l\,a),\end{aligned} \tag{104}$$

the coefficients A, B need to satisfy

$$e^{i\,k\,l\,a}\begin{pmatrix} 1-e^{i\,(K-k)\,a} & 1-e^{-i\,(K+k)\,a} \\ -2\,a_s^{-1}+i\,K\left(1-e^{i\,(K-k)\,a}\right) & -2\,a_s^{-1}-i\,K\left(1-e^{-i\,(K+k)\,a}\right)\end{pmatrix}\begin{pmatrix}A\\B\end{pmatrix} = \begin{pmatrix}0\\0\end{pmatrix}. \tag{105}$$

To ensure that the linear equation has a nontrivial solution, the determinant of the coefficient matrix must be zero, which leads to the **Kronig-Penney relation**:

$$\cos k\,a = \cos K\,a + \frac{1}{K\,a_s}\sin K\,a. \tag{106}$$

Exc 6 Derive Eq. (105) and Eq. (106).

This equation relates the **energy** $E = \hbar^2\,K^2\,/\,(2\,m)$ (or the **itinerant momentum** K) to the **quasi-momentum** k, and defines the allowed energy bands.

- **Bound states**: For $E < 0$, the itinerant momentum becomes *imaginary* $K = i\,Q$, i.e.

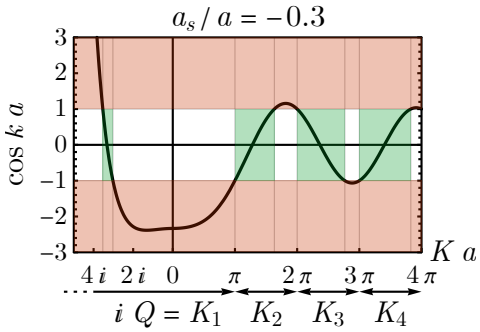
$$Q^2 = -\frac{2\,m\,E}{\hbar^2}, \tag{107}$$

the Kronig-Penney relation for Q reads

$$\cos k\,a = \cosh Q\,a + \frac{1}{Q\,a_s}\sinh Q\,a. \tag{108}$$

▪ Energy Bands and Gaps

In both Eq. (106) and Eq. (108), the left-hand-side — $\cos k\,a$ — is bounded by $[-1, 1]$, so only certain value of K or Q (and thus E) are allowed. Follow plot shows the right-hand-side of the Kronig-Penney relation, which suppose to match $\cos k\,a$.



- Horizontal axis:
  - To the right: *real* K, corresponding to $E > 0$ **scattering states**.
  - To the left: *imaginary* $K = i\,Q$, corresponding to $E < 0$ **bound states**.
- Vertical axis:
  - White zone: *feasible* region $[-1, 1]$
  - Red zone: *infeasible* region
- **Energy bands**: energy values corresponding to the *allowed solutions* that fall in the green bands, where the right-hand-side function fall in the *feasible* region $[-1, 1]$, such that *real* solutions of k exist for $\cos k\,a$.
- **Energy gaps**: energy values that are *forbidden*, as they result in the right-hand-side function to enter the *infeasible* region where no real solutions of k exist for $\cos k\,a$ (an imaginary solution of k would indicate a decaying wave that can not propagate into the lattice bulk).

▪ Band Structure

Given any k, there are *multiple* solutions for K. Let $K_n(k)$ be the nth solution (including $K_1 = i\,Q$ if necessary).

- The index $n = 1, 2, 3, \ldots$ labels the energy bands, and is called the **band index**.
- $K_n\left(k + \frac{2\pi}{a}\right) = K_n(k)$ is a *periodic* function of k with $2\pi / a$ periodicity, because k only enters the Kronig-Penney relation through $\cos k\,a$, which has that periodicity. Therefore, it is sufficient to restrict k within the **first Brillouin zone**:

$$k \in [\pi / a, -\pi / a). \tag{109}$$

- Each **band index** n and **quasi-momentum** k jointly labels a state, with

- **Energy**:

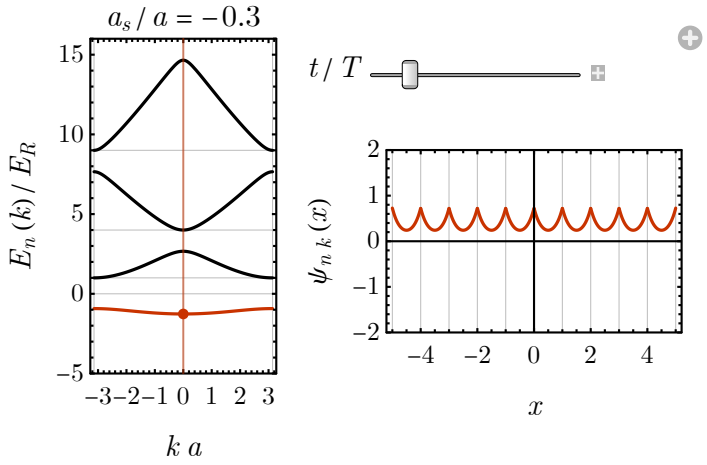
$$E_n(k) = \frac{\hbar^2}{2\,m}\,K_n(k)^2. \tag{110}$$

It is often measured in unit of the **recoil energy** $E_R := \hbar^2(\pi/a)^2/(2\,m)$.

- **Wavefunction**: takes the Bloch wavefunction form

$$\begin{aligned}\psi_{nk}(x) &= e^{i\,k\,x}\,u_{nk}(x),\\ u_{nk}(x) &= A_{nk}\;e^{i\,(K_n(k)-k)\,(x \bmod a)} + B_{nk}\,e^{-i\,(K_n(k)+k)\,(x \bmod a)},\end{aligned} \tag{111}$$

where A_{nk}, B_{nk} are null vector solutions of Eq. (105) (with the solution $K = K_n(k)$ plugged in).



- The **quasi-momentum** k characterizes the momentum of the *envelope wave* of the wavefunction, omitting the intricate and sharp variations in the wavefunction due to the *potential scattering*. It reflects the *large-scale coherent* propagation of a quantum particle in the lattice, capturing its *effective* momentum.
- The **energy gap** opens at $k = 0$ or $k = \pi/a$, where Bloch waves become **standing waves**, which have **nodes** (points of zero amplitude) and **anti-nodes** (points of max amplitude).
  - If the standing wave places its *anti-nodes on the potential sites*, the particle experiences the potential interaction with maximal likelihood. Depending on whether the potential is *attractive* or *repulsive*, the energy will be *lowered* or *raised*.
  - Conversely, if the standing wave places its *nodes on the potential sites*, the particle effectively avoids the potential — as if the periodic potential is invisible — and its energy remains *unaffected*.

  These two standing wave configurations share the *same quasi-momentum* but experience *different energy shifts* due to their different spatial alignment with the potential. This energy

difference defines the *energy gap*, which quantifies the *strength of potential scattering*.

General Piecewise Potentials

■ Transfer Matrix Method

■ Generic Potential Profile

Divide the 1D line into n regions, separated by $(n-1)$ points at $\{x_1, x_2, \ldots, x_{n-1}\}$.

- Within each region, the potential is constant

$$V_\Theta(x) = \begin{cases} V_1 & x \in (-\infty, x_1) \\ V_i & x \in (x_{i-1}, x_i) \\ V_n & x \in (x_{n-1}, +\infty) \end{cases}. \tag{112}$$

- At the region interface, we may have δ-function potentials

$$V_\delta(x) = \sum_{i=1}^{n-1} \gamma_i \, \delta(x - x_i). \tag{113}$$

The total potential is

$$V(x) = V_\Theta(x) + V_\delta(x). \tag{114}$$

■ Interface Conditions

Schrödinger equation (the standard form)

$$\left(-\frac{\hbar^2}{2\,m}\,\partial_x^2 + V(x)\right)\psi(x) = E\,\psi(x). \tag{115}$$

We may set $\hbar = m = 1$ by rescaling,

$$\boxed{\partial_x^2\,\psi(x) = 2\,(V(x) - E)\,\psi(x).} \tag{116}$$

The wavefunction at the transition point x_i should satisfy

$$\boxed{\begin{aligned} &\psi(x_i + 0_+) = \psi(x_i - 0_+) \equiv \psi(x_i), \\ &\partial_x\,\psi(x_i + 0_+) = \partial_x \psi(x_i - 0_+) + 2\,\gamma_i\,\psi(x_i). \end{aligned}} \tag{117}$$

Exc 7 Prove Eq. (117).

■ Matching Wave Functions

Solving the Schrödinger equation in each region ⇒ **trial wavefunction**:

$$\psi(x_{i-1} < x < x_i) = A_i\, e^{i\, k_i\, x} + B_i\, e^{-i\, k_i\, x}, \tag{122}$$

where k_i is given by (use the rescaled Schrödinger equation in Eq. (116))

$$k_i = \sqrt{2\,(E - V_i)}\,. \tag{123}$$

Matching the wavefunctions from different regions at the boundary by Eq. (117), we found

$$\begin{aligned}&\begin{pmatrix} 1 & 1 \\ i\, k_{i+1} & -i\, k_{i+1} \end{pmatrix}\begin{pmatrix} e^{i\, k_{i+1}\, x_i} & 0 \\ 0 & e^{-i\, k_{i+1}\, x_i} \end{pmatrix}\begin{pmatrix} A_{i+1} \\ B_{i+1} \end{pmatrix} \\ &= \begin{pmatrix} 1 & 1 \\ i\, k_i + 2\,\gamma_i & -i\, k_i + 2\,\gamma_i \end{pmatrix}\begin{pmatrix} e^{i\, k_i\, x_i} & 0 \\ 0 & e^{-i\, k_i\, x_i} \end{pmatrix}\begin{pmatrix} A_i \\ B_i \end{pmatrix}.\end{aligned} \tag{124}$$

The coefficients are passed down from one region to the next by the **transfer matrix**

$$\begin{pmatrix} A_{i+1} \\ B_{i+1} \end{pmatrix} = S_{i+1\leftarrow i}\begin{pmatrix} A_i \\ B_i \end{pmatrix}, \tag{125}$$

where $S_{i+1\leftarrow i}$ is given by

$$S_{i+1\leftarrow i} = \frac{1}{2\, k_{i+1}}\begin{pmatrix} (k_{i+1} + k_i - 2\, i\, \gamma_i)\, e^{i\,(k_i - k_{i+1})\, x_i} & (k_{i+1} - k_i - 2\, i\, \gamma_i)\, e^{-i\,(k_i + k_{i+1})\, x_i} \\ (k_{i+1} - k_i + 2\, i\, \gamma_i)\, e^{i\,(k_i + k_{i+1})\, x_i} & (k_{i+1} + k_i + 2\, i\, \gamma_i)\, e^{-i\,(k_i - k_{i+1})\, x_i} \end{pmatrix}. \tag{126}$$

Exc 8 Derive Eq. (126).

Conversely, the **inverse transfer matrix**,

$$\begin{pmatrix} A_{i-1} \\ B_{i-1} \end{pmatrix} = S_{i-1\leftarrow i}\begin{pmatrix} A_i \\ B_i \end{pmatrix}, \tag{127}$$

where $S_{i-1\leftarrow i} = S^{-1}_{i\leftarrow i-1}$ is given by

$$S_{i-1\leftarrow i} = \frac{1}{2\, k_{i-1}}\begin{pmatrix} (k_{i-1} + k_i + 2\, i\, \gamma_{i-1})\, e^{i\,(k_i - k_{i-1})\, x_i} & (k_{i-1} - k_i + 2\, i\, \gamma_{i-1})\, e^{-i\,(k_i + k_{i-1})\, x_i} \\ (k_{i-1} - k_i - 2\, i\, \gamma_{i-1})\, e^{i\,(k_i + k_{i-1})\, x_i} & (k_{i-1} + k_i - 2\, i\, \gamma_{i-1})\, e^{-i\,(k_i - k_{i-1})\, x_i} \end{pmatrix} \tag{128}$$

Using the transfer matrices in both directions, one can express the wave coefficient (A_i, B_i) in any region in terms of those in a **reference region**, say (A_c, B_c),

$$\begin{pmatrix} A_i \\ B_i \end{pmatrix} = S_{i\leftarrow c}\begin{pmatrix} A_c \\ B_c \end{pmatrix}, \tag{129}$$

where

$$S_{i\leftarrow c} = \begin{cases} S_{i\leftarrow i+1}\, S_{i+1\leftarrow i+2} \ldots S_{c-1\leftarrow c} & \text{if } c > i, \\ S_{i\leftarrow i-1}\, S_{i-1\leftarrow i-2} \ldots S_{c+1\leftarrow c} & \text{if } c < i. \end{cases} \tag{130}$$

■ Boundary Regions

By default, the left-most region is $l = 1$, the right-most region is $r = n$.

- If $V_1 > E$, momentum $k_1 = i\,\kappa_1 \in \mathbb{I}$ is imaginary $\Rightarrow \psi(x < x_1) = A_1\, e^{-\kappa_1\, x} + B_1\, e^{\kappa_1\, x} \Rightarrow A_1 = 0$.

$$(1\ \ 0)\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \boldsymbol{v}_l \begin{pmatrix} A_l \\ B_l \end{pmatrix} = 0, \tag{131}$$

with $\boldsymbol{v}_l = (1\ \ 0)$.

- If $V_1 = \infty \Rightarrow A_1 = B_1 = 0$; left-most region shifts to $l = 2$

$$(e^{i k_2 x_1}\ \ e^{-i k_2 x_1}) \begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \boldsymbol{v}_l \begin{pmatrix} A_l \\ B_l \end{pmatrix} = 0. \tag{132}$$

with $\boldsymbol{v}_l = (e^{i k_2 x_1}\ \ e^{-i k_2 x_1})$.

- If $V_n > E$, momentum $k_n = i \kappa_n \in \mathbb{I}$ is imaginary $\Rightarrow \psi(x > x_{n-1}) = A_n e^{-\kappa_n x} + B_n e^{\kappa_n x} \Rightarrow B_n = 0$.

$$(0\ \ 1)\begin{pmatrix} A_n \\ B_n \end{pmatrix} = \boldsymbol{v}_r \begin{pmatrix} A_r \\ B_r \end{pmatrix} = 0, \tag{133}$$

with $\boldsymbol{v}_r = (0\ \ 1)$.

- If $V_n = \infty \Rightarrow A_n = B_n = 0$; right-most region shifts to $r = n-1$

$$(e^{i k_{n-1} x_{n-1}}\ \ e^{-i k_{n-1} x_{n-1}}) \begin{pmatrix} A_{n-1} \\ B_{n-1} \end{pmatrix} = \boldsymbol{v}_r \begin{pmatrix} A_r \\ B_r \end{pmatrix} = 0. \tag{134}$$

with $\boldsymbol{v}_r = (e^{i k_{n-1} x_{n-1}}\ \ e^{-i k_{n-1} x_{n-1}})$.

- The boundary conditions can be in general expressed as

$$\begin{aligned} \boldsymbol{v}_l \begin{pmatrix} A_l \\ B_l \end{pmatrix} &= \boldsymbol{v}_l\, S_{l\leftarrow c} \begin{pmatrix} A_c \\ B_c \end{pmatrix} = 0, \\ \boldsymbol{v}_r \begin{pmatrix} A_r \\ B_r \end{pmatrix} &= \boldsymbol{v}_r\, S_{r\leftarrow c} \begin{pmatrix} A_c \\ B_c \end{pmatrix} = 0, \end{aligned} \tag{135}$$

which combines into a single condition $P \cdot (A_c, B_c)^{\mathsf{T}} = 0$, where P is a 2×2 matrix given by

$$\boxed{P = \begin{pmatrix} \boldsymbol{v}_l\, S_{l\leftarrow c} \\ \boldsymbol{v}_r\, S_{r\leftarrow c} \end{pmatrix}.} \tag{136}$$

- Solutions for (A_c, B_c) span the *null space* of P.
  - Once the solutions of (A_c, B_c) is found in the reference region, (A_i, B_i) in any other regions can be obtained by applying the transfer matrix, following Eq. (129). Then the wave function can be reconstructed from Eq. (122).
- If P is full rank, we will need to tune the energy E to make

$$\boxed{\det P(E) = 0,} \tag{137}$$

such that E will correspond to an *eigen energy* level, and the null vectors of $P(E)$ will form the solutions of (A_c, B_c), which can be used to construct the *eigen wave function*.

■ Applications

■ Harmonic Oscillator

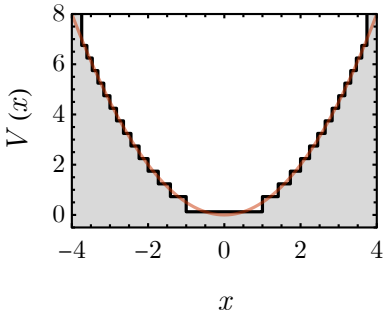
Harmonic oscillator is a particle in a quadratic potential

$$V(x) = \frac{1}{2}\, m\, \omega^2\, x^2. \tag{138}$$

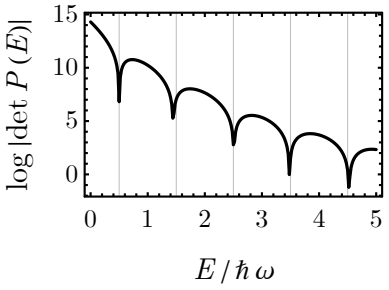
We may set $m = \omega = 1$ to simplify.

- Approximate $V(x)$ by a piecewise potential:

$$V(x) = \begin{cases} +\infty & x \in (-\infty,\, x_1) \\ \frac{1}{2}\left(\frac{x_{i-1}+x_i}{2}\right)^2 & x \in (x_{i-1},\, x_i) \\ +\infty & x \in (x_{n-1},\, +\infty) \end{cases} \tag{139}$$



- Scan |det $P(E)$| (in logarithmic scale) to find its zeros, see Eq. (137), which corresponds to the eigen energies in the potential well.

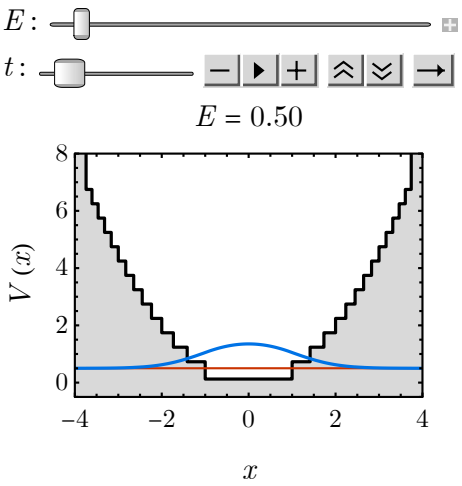


Energy levels appear approximately at

$$E_n \approx \left(n + \frac{1}{2}\right) \hbar\, \omega, \tag{140}$$

matching the expectation (with $\hbar\, \omega = 1$).

- Wave functions can be reconstructed at eigen energy levels, demonstrating how any 1D wave function can be approximated by piecing exponential functions $e^{\pm i\, k\, x}$ or $e^{\pm \kappa\, x}$ together.



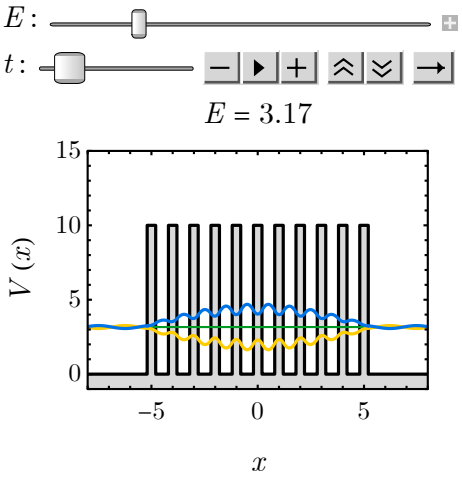
■ Crystal and Band Structure

A **crystal** is a solid composed of *atoms* arranged in *regular*, *repeating* pattern. This *long-range order* gives rise to a **lattice structure**, and the electrons inside experience a **periodic potential** due to the repeated arrangement of atomic nuclei.

The essential physics can be captured by a 1D **array of square potentials**.

$$V(x) = \begin{cases} V_0 & a\,i - b/2 < x < a\,i + b/2 \text{ for } i \in \mathbb{Z} \\ 0 & \text{otherwise} \end{cases} \tag{141}$$

- a - **lattice spacing**: distance between adjacent potentials,
- b - **potential width**: width of each single potential,
- V_0 - **potential height**: energy inside the potential region.

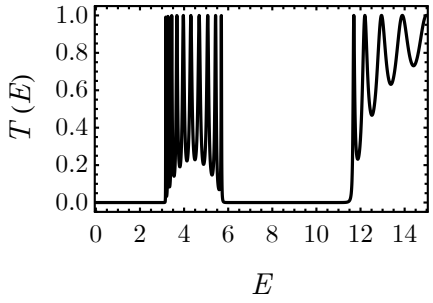


Wave propagating in periodic structures gives rise to **energy bands** and **energy gaps**.

- Incident wave energy lies in an *energy band* ⇒ wave can propagate through the crystal ⇒ the crystal appears **transparent**.

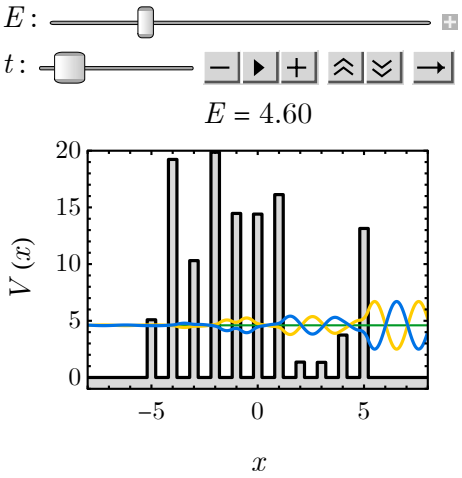
- Incident wave energy falls in an *energy gap* ⇒ wave propagation is forbidden in the crystal ⇒ the crystal becomes **opaque**.

These two distinct behaviors can be studied using the **transmission coefficient** $T(E)$ as a function of the energy E.

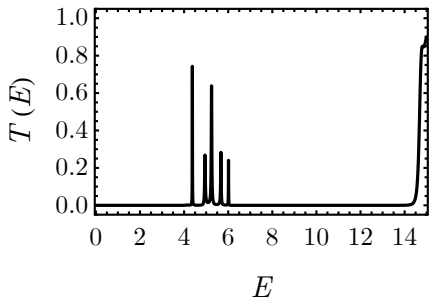


■ Disorder and Localization

In reality, no crystal is perfect. Imperfections — such as impurities, vacancies, or lattice distortions — introduce **disorder**, modeled by **random fluctuations** in the potential energy.



- Transmission coefficient is largely suppressed in the presence of disorder.



- **Localization**: A wave become **localized** if it *decays exponentially* away from some local region, rather than spreading throughout the space.

$$|\psi(x)| \sim e^{-|x-x_0|/\xi}, \tag{142}$$

where ξ is the **localization length**.

- **Disorder** and **Anderson localization**: in 1D, even *weak* disorder can dramatically affect wave propagation,
  - Every potential *scatters* part of the wave,
  - *Randomness* causes **phases** to *misalign*, suppressing constructive interference,
  - Over long distance, *scattered* waves **interfere destructively** with the *forward propagating* wave, effectively *trapping* the wave.

Code Section