

Impenetrable wall + delta function potential

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

Bound state: $E < 0$, $k = \sqrt{-E}$

Region 1:

$$\psi_1(x) = Ae^{-kx} + Be^{kx}$$

Boundary condition: $\psi_1(0) = 0$, $A = -B$

Therefore,

$$\psi_1(x) = A(e^{-kx} - e^{kx})$$

Region 2:

$$\psi_2(x) = Ce^{-kx} + De^{kx}$$

Boundary condition: $\psi_2(\infty) = 0$

Therefore,

$$\psi_2(x) = Ce^{-kx}$$

Continuity conditions:

$$\psi_1(a) = \psi_2(a)$$

$$\Delta \frac{d\psi}{dx} = -\frac{2m}{\hbar^2} \psi(a)$$

!!! Assume $\Delta \frac{d\psi}{dx} = -\psi(a)$ for simplicity

From the continuity:

$$A(e^{-ka} - e^{ka}) = Ce^{-ka}$$

$$C = A(1 - e^{2ka})$$

Derivatives:

$$\left. \frac{d\psi_1}{dx} \right|_{x=a} = A(-ke^{-ka} - ke^{ka})|_{x=a} = -kA(e^{-ka} + e^{ka})$$

$$\left. \frac{d\psi_2}{dx} \right|_{x=a} = -kCe^{-ka} = -kA(1 - e^{2ka})e^{-ka} = -kA(e^{-ka} - e^{ka})$$

$$\Delta \frac{d\psi}{dx} = 2kAe^{ka} = -A(e^{-ka} - e^{ka})$$

Assume $a = 1$ for simplicity.

$$2ke^k = e^k - e^{-k}$$

Scattering states:

$$\psi_1(x) = Ae^{-ikx} + Be^{ikx}$$

$$\psi_1(-1) = 0 = Ae^{ik} + Be^{-ik}.$$

TODO: suppose both A and B are real.

$\frac{A}{B}e^{2ik} = -1$, therefore, $A = B$ or $A = -B$ to match magnitudes. TODO is that important? We should distinguish, I suppose.

Suppose $A = -B$

$$2k = 2\pi n, k = \pi n, n \in \mathbb{Z}$$

$$\psi_1(x) = A(e^{-i\pi nx} - e^{i\pi nx})$$

$$\psi_1'(x) = -i\pi nA(e^{-i\pi nx} + e^{i\pi nx})$$

$$\psi_1'(0) = -2i\pi nA$$

$$\psi_2(x) = Ce^{-ikx} + De^{ikx}$$

$$\psi_1(0) = \psi_2(0) = 0$$

$$0 = C + D, D = -C$$

$$\psi_2(x) = C(e^{-i\pi nx} - e^{i\pi nx})$$

$$\psi_2'(x) = -i\pi nC(e^{-i\pi nx} + e^{i\pi nx})$$

$$\psi_2'(0) = -2i\pi nC$$

$$\Delta \frac{d\psi}{dx} = -\psi(0) = 0$$

So, $-C + A = 0, A = C$

Ok, what does all that mean? For energies $\pi^2 n^2$, there is no delta barrier, there is just stationary point at zero?

1 Infinite well + step

$$V(x) = \begin{cases} \infty, & x < -1 \\ 0, & -1 < x < 0 \\ -V_0, & 0 < x < 1 \\ \infty, & x > 1 \end{cases}$$

Suppose $-V_0 < E < 0$

$$k = \sqrt{-E}$$

$$\psi_1(x) = Ae^{-kx} + Be^{kx}$$

$$\psi_1(-1) = 0 = Ae^k + Be^{-k}, \text{ therefore, } B = -Ae^{2k}$$

$$\psi_1(x) = A(e^{-kx} - e^{2k}e^{kx})$$

$$\psi_1'(x) = -kA(e^{-kx} + e^{2k}e^{kx})$$

$$k' = \sqrt{E + V_0} = \sqrt{-k^2 + V_0}$$

$$\psi_2(x) = Ce^{-ik'x} + De^{ik'x}$$

$$\psi_2(1) = 0 = Ce^{-ik'} + De^{ik'}, \text{ therefore, } D = -Ce^{-2ik'}$$

$$\psi_2(x) = C(e^{-ik'x} - e^{-2ik'}e^{ik'x})$$

$$\psi_1(0) = \psi_2(0)$$

$$A(1 - e^{2k}) = C(1 - e^{-2ik'})$$

$$\psi_1'(0) + \psi_2'(0)$$

$$-kA(1 + e^{2k}) = -ik'C(1 + e^{-2ik'})$$

Divide the second equation by the first:

$$-k \frac{1 + e^{2k}}{1 - e^{2k}} = -ik' \frac{1 + e^{-2ik'}}{1 - e^{-2ik'}}$$

$\frac{1+e^{-2ik'}}{1-e^{-2ik'}}$ is pure complex and equal to $\coth(ik') = -i \cot(k')$

$$k \coth(k) = k' \cot(k')$$

That actually has some solutions!

2 some weird basis

Particle in infinite well with $L = 1$.

$$\left(-\frac{d^2}{dx^2} - E\right)\psi(x) = \psi(x)$$

Let

$$f_1(x) = x(1 - x)$$

$$f_2(x) = x\left(\frac{1}{2} - x\right)(1 - x)$$

(without normalization). Orthonormal because f_1 is symmetric around 0.5 and f_2 is antisymmetric. Same applies to the derivatives.

$$\langle f_1 | H - E | f_1 \rangle = 10 - E$$

$$\langle f_2 | H - E | f_2 \rangle = 42 - E$$

Therefore, $E = 10$, $a_1 = 1$ and $E = 42$, $a_2 = 1$. These are clearly not solutions.

Reason: incorrect assumption that $\psi(x) = a_1 f_1(x) + a_2 f_2(x)$.

TODO something to do with bound states?

TODO investigate scattering states.

3 Free particle + self-adjoint boundary conditions

Domain: $[0, a]$

Boundary conditions:

$$\psi(0) = 0$$

$$a \frac{\psi'(a)}{\psi(a)} = B$$

1. Negative energy case:

$$k = \sqrt{-E}$$

$$\psi(x) = A(e^{-kx} - e^{kx})$$

$$a \frac{-ke^{-ka} - ke^{ka}}{e^{-ka} - e^{ka}} = B$$

$$-ka \coth(-ka) = ka \coth(ka) = B$$

For $B > 1$, there exists a single solution with $k > 0$.

2. Zero energy:

$$\psi(x) = Ax$$

$$a \frac{1}{a} = 1 = B$$

3. Positive energy:

$$k = \sqrt{E}$$

$$\psi(x) = A(e^{-ikx} - e^{ikx}) = -2IA \sin(kx)$$

$$a \frac{-ike^{-ika} - ike^{ika}}{e^{-ika} - e^{ika}} = B$$

$$-ika \coth(-ika) = -i^2 ka \cot(ka) = ka \cot(ka) = B$$

A lot of solutions for every value of B .

For $B < 1$: extra solution.

Suppose $B = -1.0$, $a = 1.0$.

No solutions for negative and zero energy.

$k \cot(k)$ tends to straight lines in the neighbourhood of zero.

$$k_n \sim \frac{\pi}{2} + \pi n$$

$$u_n(1) \rightarrow 0$$

$$R(E) = \frac{1}{a} \sum_{\lambda=1}^{\infty} \frac{u_{\lambda}^2(a)}{k_{\lambda}^2 - k^2}$$

3.1 Bounds on the sum

Suppose $a = 1$.

Let k_n be the n th positive root of $x \cot(x) = B$.

Let b_n be its asymptotic approximation: $b_n = \frac{\pi}{2} + \pi n$

If $B < 0$, $b_n < k_n$

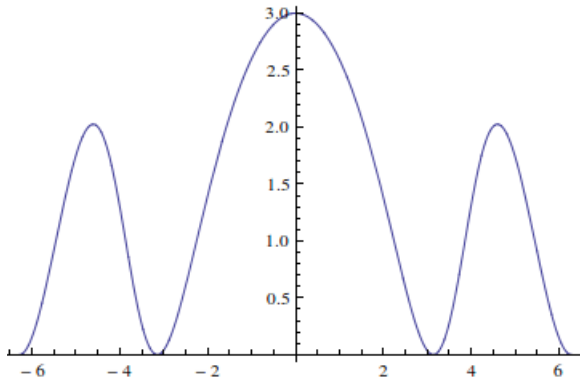
If $B > 0$, $b_n > k_n$

Value of n th eigenfunction square on the boundary is

$$\psi_n^2(a) = \frac{1}{4\left(\frac{a}{2} - \frac{\sin(2k_n a)}{4k_n}\right)} (2 \sin(k_n a))^2 = \frac{\sin^2 k_n}{\frac{1}{2} - \frac{\sin(2k_n)}{4k_n}}$$

As function of k :

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g[k_] := Sin[k]^2 / (0.5 - (Sin[2 * k]) / (4 * k))
Plot[g[k], {k, -2 * Pi, 2 * Pi}]
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That is, for $B < 0$, $\psi^2(b_n) > \psi^2(k_n)$ if k_n is slightly greater than $\frac{\pi}{2}$. So, starting from $i = n$ for which $k_i^2 > k^2$:

$$R_i = \sum_{i=n}^{\infty} \frac{\psi_i^2(1.0)}{k_i^2 - k^2} < \sum \frac{\phi_i^2(1.0)}{b_i^2 - k^2} = \sum \frac{2.0}{b_i^2 - k^2}$$

$$\sum \frac{1}{(\pi/2 + \pi i)^2 - k^2} = \frac{1}{\pi^2} \sum \frac{1}{i^2 + i + 1/4 - \frac{k^2}{\pi^2}}$$

$$D = \sqrt{1 - (1 - 4\frac{k^2}{\pi^2})} = 2\frac{k}{\pi}$$

$$i_{1,2} = -\frac{1}{2} \pm \frac{k}{\pi}$$

$$\frac{1}{i^2 + i + 1/4 - \frac{k^2}{\pi^2}} = \frac{\pi}{2k} \left(\frac{1}{i + 0.5 - \frac{k}{\pi}} - \frac{1}{i + 0.5 + \frac{k}{\pi}} \right)$$

$$R_n \leq -\frac{1}{\pi k} (-PG(0.5 + n + \frac{k}{\pi}) + PG(0.5 + n - \frac{k}{\pi}))$$

Where PG is the polygamma function.

Seems to be working..

3.2 Bounds on the sum: more general case

$$ak \cot(ak) = B$$

$$k_n \sim \frac{1}{a} \left(\frac{\pi}{2} + \pi n \right)$$

$$\psi_n^2(a) = \frac{4 \sin^2(k_n a)}{2a - \frac{\sin(2k_n a)}{k_n}}$$

Asymptotically, $\psi_n^2(a) \leq 2/a$.

$$\left(\frac{1}{a} \left(\frac{\pi}{2} + \pi i \right) \right)^2 - k^2 \leq k_i^2 - k^2$$

$$\frac{1}{a^2} \left(\left(\frac{\pi}{2} + \pi i \right)^2 - a^2 k^2 \right)$$

$$R \leq \frac{1}{a} \sum \frac{2/a}{\frac{1}{a^2} \left(\left(\frac{\pi}{2} + \pi i \right)^2 - a^2 k^2 \right)} = \sum \frac{2}{\left(\frac{\pi}{2} + \pi i \right)^2 - a^2 k^2} = \frac{1}{\pi^2} \frac{\pi}{ak} \sum \frac{1}{i + 0.5 - \frac{ak}{\pi}} - \frac{1}{i + 0.5 + \frac{ak}{\pi}}$$

$$R_{n_0} \leq \frac{1}{\pi^2} \frac{\pi}{ak} (PG(n_0 + 0.5 + \frac{ak}{\pi}) - PG(n_0 + 0.5 - \frac{ak}{\pi}))$$

4 Trash

$$\psi(x) = e^{-ikx} + Ue^{ikx}$$

$$\frac{\psi'(a)}{\psi(a)} = X$$

$$U = e^{-2ika} \frac{ik + X}{ik - X}$$

5 Delta potential

Suppose we have delta potential at $x = d$: $-a\delta(x - d)$

$$\psi_1(x) = e^{-ikx} - e^{ikx}$$

, we omit the A coefficient and calculate the normalization later.

$$\psi_2(x) = Be^{-ikx} + Ce^{ikx}$$

$$\begin{cases} \psi_1(d) = \psi_2(d) \\ \psi_2'(d) - \psi_1'(d) = -a\psi_1(d) \end{cases}$$

After solving, we get:

$$B = \frac{iae^{2idk} - ia + 2k}{2k}$$

$$C = -\frac{e^{-2idk} (iae^{2idk} - ia + 2ke^{2idk})}{2k}$$

Suppose $d = 1.0$ and $a = 1.0$

$$\psi_2(x) = \frac{(ie^{2ik} - i + 2k)e^{-ikx}}{2k} - \frac{(ie^{2ik} + 2ke^{2ik} - i)e^{-2ik+ikx}}{2k}$$

6 Random definitions

Resonance: pole of resolvent/Green's function continued meromorphically to the lower half-plane.

Real part: energy of the resonance, imaginary part: rate of decay.

6.1 Resolvent of the free particle

$$G(x, s; E) = \int_0^\infty \frac{\psi_\lambda(x)\psi_\lambda^*(s)}{E - \lambda} d\lambda$$

$$\psi_\lambda(x) =$$

7 Question

Green's function is kernel of the resolvent:

$$R_\lambda(f) = \int G(x, s) f(s) ds$$

What is incoming and outgoing Green's function/resolvent?

8 Cylinder delta scattering

$$\Delta \Psi(r, \theta, z) = E \Psi(r, \theta, z)$$

Symmetric w.r.t. to θ , separate variables:

$$\Psi_m(E; r, \theta, z) = \frac{e^{im\theta}}{\sqrt{2\pi}} \psi_m(E; r, z)$$

Each m defines a 2D scattering problem.

$$\left(- \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} - \frac{m^2}{r^2} + \frac{\partial^2}{\partial z^2} \right) + V(r, z) \right) \psi_m(E; r, z) = E \psi_m(E; r, z)$$

Again, separate variables:

$$\psi_m(E; r, z) = \phi(r) \varphi(z)$$

$\phi(r)$: radial equation

$$- \left(\frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \frac{m^2}{r^2} + V_\perp(r) \right) \phi(r) = E_\perp \phi(r)$$

Solutions:

$$\phi_n^m(r) = \frac{\sqrt{2}}{R J_{|m|+1}(x_{mn})} J_m(x_{mn} \frac{r}{R}), n = 1, 2 \dots$$

$$E_{\perp n}^m = \left(\frac{x_{mn}}{R} \right)^2, n = 1, 2 \dots$$

$\varphi(z)$: one-dimensional spatial equation

$$\left(- \frac{d^2}{dz^2} + V_s \right) \varphi(z) = (E - E_\perp) \varphi(z)$$

For fixed n, m two linearly independent solutions.

8.1 Next attempt

Fix channels m and n :

Left region:

$$\psi_n^1(r, z) = \exp(Ik_n z) \phi_n(r) + \sum_{t=1}^{\infty} R_{nt} \exp(-ik_t z) \phi_t(r)$$

Right region:

$$\psi_n^2(r, z) = \sum_{t=1}^{\infty} T_{nt} \exp(ik_t z) \phi_t(r)$$

Boundary conditions at $z = 0$: for any r :

$$\psi_n^1(r, 0) = \psi_n^2(r, 0)$$

$$\partial_z \psi^2(r, 0) - \partial_z \psi_n^1(r, 0) = u \psi_n^1(r, 0)$$

Substituting expressions:

$$\begin{aligned} \phi_n(r) + \sum_{t=1}^{\infty} R_{nt} \phi_t(r) &= \sum_{t=1}^{\infty} T_{nt} \phi_t(r) \\ \sum_{t=1}^{\infty} T_{nt} i k_t \phi_t(r) - (i k_n \phi_n(r) - \sum_{t=1}^{\infty} R_{nt} i k_t \phi_t(r)) &= u \sum_{t=1}^{\infty} T_{nt} \phi_t(r) \end{aligned}$$

For each q , multiply by $\phi_q(r)$ and integrate from 0 to R .

For $q = n$:

$$1 + R_{nn} = T_{nn}$$

$$k_n T_{nn} - (k_n - k_n R_{nn}) = \frac{u}{i} T_{nn}$$

$$\begin{cases} R = \frac{2k_n}{2k_n + iu} \\ T = \frac{-iu}{2k_n + iu} \end{cases}$$

For $q \neq n$:

$$0 + R_{nq} = T_{nq}$$

$$k_q T_{nq} - (0 - k_q R_{nq}) = \frac{u}{i} T_{nq}$$

$$\begin{cases} R = 0 \\ T = 0 \end{cases}$$

9 Cylindric delta well, surrounded by host material

Fix channels m and n :

Left region:

$$\psi_n^1(r, z) = \exp(ik_n z)\phi_n(r) + \sum_{t=1}^{\infty} R_t \exp(-ik_t z)\phi_t(r)$$

Right region:

$$\psi_n^2(r, z) = \sum_{t=1}^{\infty} T_t \exp(ik_t z)\phi_t(r)$$

Boundary conditions at $z = 0$:

$$\forall 0 \leq r \leq RR : \psi_n^1(r, 0) = \psi_n^2(r, 0)$$

$$\forall 0 \leq r \leq R : \partial_z \psi^2(r, 0) = \partial_z \psi_n^1(r, 0) + u\psi_n^1(r, 0)$$

$$\forall R \leq r \leq RR : \partial_z \psi^2(r, 0) = \partial_z \psi_n^1(r, 0)$$

Substituting expressions:

$$\forall 0 \leq r \leq RR : \phi_n(r) + \sum_{t=1}^{\infty} R_t \phi_t(r) = \sum_{t=1}^{\infty} T_t \phi_t(r)$$

$$\forall 0 \leq r \leq R : \sum_{t=1}^{\infty} T_t k_t \phi_t(r) = k_n \phi_n(r) - \sum_{t=1}^{\infty} R_t k_t \phi_t(r) + \frac{u}{i} \sum_{t=1}^{\infty} T_t \phi_t(r)$$

$$\forall R \leq r \leq RR : \sum_{t=1}^{\infty} T_t k_t \phi_t(r) = k_n \phi_n(r) - \sum_{t=1}^{\infty} R_t k_t \phi_t(r)$$

For each q , multiply first equation by $r\phi_q(r)$ and integrate from 0 to RR :

- for $q = n$: $1 + R_n = T_n$

- for $q \neq n$: $R_q = T_q$

For each q , multiply second and third equation by $r\phi_q(r)$, integrate second from 0 to R , third from R to RR , and add them up:

$$\int_0^{RR} \sum_{t=1}^{\infty} T_t k_t r \phi_t(r) \phi_q(r) = \int_0^{RR} k_n r \phi_n(r) \phi_q(r) - \int_0^{RR} \sum_{t=1}^{\infty} R_t k_t r \phi_t(r) \phi_q(r) + \int_0^R \frac{u}{i} \sum_{t=1}^{\infty} T_t r \phi_t(r) \phi_q(r)$$

- for $q = n$: $T_n k_n = k_n - R_n k_n + \frac{u}{i} \sum_{t=1}^{\infty} T_t \int_0^R r \phi_t(r) \phi_n(r)$

- for $q \neq n$: $T_q k_q = -R_q k_q + \frac{u}{i} \sum_{t=1}^{\infty} T_t \int_0^R r \phi_t(r) \phi_q(r)$

Substitute $T_n = R_n + 1, T_q = R_q$:

- for $q = n$: $(R_n + 1)k_n = k_n - R_n k_n + \frac{u}{i} \left(\sum_{t=1}^{\infty} R_t \int_0^R r \phi_t(r) \phi_n(r) + \int_0^R r \phi_n(r) \phi_n(r) \right)$

- for $q \neq n$: $R_q k_q = -R_q k_q + \frac{u}{i} \left(\sum_{t=1}^{\infty} R_t \int_0^R r \phi_t(r) \phi_q(r) + \int_0^R r \phi_n(r) \phi_q(r) \right)$

Simplify,

- for $q = n$: $2R_n k_n - \frac{u}{i} \sum_{t=1}^{\infty} R_t \int_0^R r \phi_t(r) \phi_n(r) = \frac{u}{i} \int_0^R r \phi_n(r) \phi_n(r)$
- for $q \neq n$: $2R_q k_q - \frac{u}{i} \sum_{t=1}^{\infty} R_t \int_0^R r \phi_t(r) \phi_q(r) = \frac{u}{i} \int_0^R r \phi_n(r) \phi_q(r)$

DO NOT FORGET TO SET $u = \frac{2\mu}{\hbar^2} u$ IN REAL WORLD CALCULATIONS.

10 Zero width slit, 2D geometry

Domain of the adjoint operator:

$$u(r) = \begin{cases} \beta_1 G_1^E(r, r_{12}, k_0) + u_1(r), & r \in \Omega_1 \\ \beta_{12} G^I(r, r_{12}, k_0) + \beta_{23} G^I(r, r_{23}, k_0) + u_2(r), & r \in \Omega_2 \\ \beta_3 G_3^E(r, r_{23}, k_0) + u_3(r), & r \in \Omega_3 \end{cases}$$

k_0 is some regular (TODO: what's that) value of the spectral parameter.

$u_i \in W_2^2(\Omega_i)$ (TODO what's W_2^2 ?)

Boundary conditions: conservation of flux:

$$\begin{cases} \beta_1 = -\beta_{12} \\ \beta_3 = -\beta_{23} \\ u_1(r_{12}) = u_2(r_{12}) \\ u_3(r_{23}) = u_2(r_{23}) \end{cases}$$

Search solution of scattering problem in form:

$$u(r, k) = \begin{cases} \alpha_1 G_1^E(r, r_{12}, k) + \tilde{u}(x, k), & x \in \Omega_1 \\ \alpha_{12} G^I(r, r_{12}, k) + \alpha_{23} G^I(r, r_{23}, k), & x \in \Omega_2 \\ \alpha_3 G_3^E(r, r_{23}, k), & x \in \Omega_3 \end{cases}$$

10.1 Particle in a 2D box: von Neumann boundary conditions

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \psi(x, y) = E \psi(x, y)$$

$$\begin{cases} \psi(x, y) = X(x)Y(y) \\ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} X(x) = E_x X(x) \\ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} Y(y) = E_y Y(y) \\ E = E_x + E_y \end{cases}$$

$$\begin{cases} X(x) = A_x \sin(k_x x) + B_x \cos(k_x x) \\ Y(y) = A_y \sin(k_y y) + B_y \cos(k_y y) \\ k_x = \sqrt{\frac{2mE_x}{\hbar^2}} \\ k_y = \sqrt{\frac{2mE_y}{\hbar^2}} \end{cases}$$

Boundary conditions:

$$\begin{cases} X'(0) = 0, A_x = 0 \\ X'(L_x) = 0, k_x L_x = \pi n_x \\ Y'(0) = 0, A_y = 0 \\ Y'(L_y) = 0, k_y L_y = \pi n_y \end{cases}$$

$$\begin{cases} \psi(x, y) = \frac{2}{\sqrt{L_x L_y}} \cos(k_x x) \cos(k_y y) \\ k_x = \frac{\pi n_x}{L_x} \\ k_y = \frac{\pi n_y}{L_y} \\ E = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} \right) \end{cases}$$

Let $n = n_x, m = n_y$.

10.1.1 Green's function

$$G(x, y, x_s, y_s; E) = \sum_{n, m=1}^{\infty} \frac{\psi_{nm}(x, y) \psi_{nm}^*(x_s, y_s)}{E_{nm} - E}$$

TODO investigate convergence on the boundary

$$G(x, y, x_0, y_0; E) = G(x, y, \frac{L_x}{2}, 0; E) = \sum_{n, m=1}^{\infty} \frac{4}{L_x L_y} \frac{\cos(k_n^x x) \cos(k_m^y y) \cos(\frac{\pi}{2} m)}{E_{nm} - E}$$

$$G(x_0, y_0, x_0, y_0; E) = \frac{4}{L_x L_y} \sum_{n, m=1}^{\infty} \frac{\cos(\frac{\pi}{2} n) \cos(\frac{\pi}{2} n)}{E_{nm} - E} = \frac{4}{L_x L_y} \sum_{n, m=1}^{\infty} \frac{\cos^2(\frac{\pi}{2} n)}{E_{nm} - E}$$

$$G(x_0, y_0, x_0, y_0; E) = \frac{4}{L_x L_y} \sum_{n=1}^{\infty} \cos^2(\frac{\pi}{2} n) \sum_{m=1}^{\infty} \frac{1}{E_{nm} - E} = \frac{4}{L_x L_y} \sum_{n'=1}^{\infty} \sum_{m=1}^{\infty} \frac{1}{E_{(2n')m} - E}$$

10.2 1D free particle

We have two fold-eigenvalue degeneracy: for each E , there is $\psi_+^E(x) = N_E e^{ikx}$ and $\psi_-^E(x) = N_E e^{-ikx}$, where $k = \frac{\sqrt{2mE}}{\hbar}$. ψ_+ and ψ_- are orthonormal: $\int \psi_+(x) \psi_-^*(x) dx = \int |N_E|^2 e^{2i\sqrt{E}x} dx = \int |N_E|^2 \frac{1}{2} e^{i\sqrt{E}x} = \frac{1}{2} |N_E|^2 2\pi \delta(k)$, which is zero for non-zero E .

Eigenstates normalization: $\langle \psi_E | \psi_{E'} \rangle = \int_{x=-\infty}^{\infty} \psi_E(x) \psi_{E'}^*(x) dx = N_E N_{E'}^* \int_{x=-\infty}^{\infty} e^{i(k-k')x} dx =$

$$N_E N_{E'}^* 2\pi \delta(k - k')$$

Next, use $\delta(g(x)) = \frac{\delta(x-x_0)}{g'(x_0)}$ (the function has only one root).

$$\langle \psi_E | \psi_{E'} \rangle = N_E N_{E'}^* 2\pi \delta\left(\frac{\sqrt{2mE}}{\hbar} - \frac{\sqrt{2mE'}}{\hbar}\right) = N_E N_{E'}^* 2\pi \sqrt{\frac{2E}{m}} \hbar \delta(E - E')$$

It has to be equal to $\delta(E - E')$. For $E \neq E'$, the normalization could be arbitrary, for $E = E'$ the coefficient should be equal to 1:

$$|N_E|^2 2\pi \sqrt{\frac{2E}{m}} \hbar = 1, \text{ therefore, } |N_E| = \left(\frac{m}{2E}\right)^{1/4} \frac{1}{\sqrt{2\pi\hbar}}$$

10.2.1 Green's function

$$G(x, s; E) = \frac{1}{2\pi\hbar} \left(\frac{m}{2}\right)^{1/2} \left(\int_0^\infty \frac{1}{\sqrt{\lambda}} \frac{e^{i\frac{\sqrt{2m\lambda}}{\hbar}(x-s)}}{\lambda - E} d\lambda + \int_0^\infty \frac{1}{\sqrt{\lambda}} \frac{e^{-i\frac{\sqrt{2m\lambda}}{\hbar}(x-s)}}{\lambda - E} d\lambda \right)$$

Change the variable of integration:

$$\begin{cases} k = \frac{\sqrt{2m\lambda}}{\hbar} \\ \lambda = \frac{\hbar^2 k^2}{2m} \\ d\lambda = 2 \frac{\hbar^2}{2m} k dk \end{cases}$$

$$\begin{aligned} G(x, s; E) &= C \left(\int + \int \right) \\ &= C \int \frac{1}{\frac{\hbar k}{\sqrt{2m}} \frac{\hbar^2 k^2}{2m} - E} 2 \frac{\hbar^2}{2m} k dk + C \int \\ &= C 2 \frac{\sqrt{2m}}{\hbar} \int_{-\infty}^{\infty} \frac{e^{ikx}}{k^2 - \frac{2mE}{\hbar^2}} dk \\ &= \frac{1}{2\pi\hbar} \sqrt{\frac{m}{2}} 2 \frac{\sqrt{2m}}{\hbar} \int \\ &= \frac{2m}{\hbar^2} \frac{i}{2k_0} e^{ik_0|x-s|} \end{aligned}$$

, where $k_0 = \frac{\sqrt{2mE}}{\hbar}$. That was for positive energy. For negative energy:

$$k_0 = \frac{\sqrt{2m|E|}}{\hbar}.$$

$$\int_{-\infty}^{\infty} \frac{e^{ik|x-s|}}{k^2 - E} dk = 2\pi i \operatorname{Res}_{k=ik_0} f(k) = \frac{e^{iik_0|x-s|}}{2ik_0} = 2\pi \frac{e^{-k_0|x-s|}}{2k_0}$$

$$G(x, s; E) = \frac{2m}{\hbar^2} \frac{1}{2k_0} e^{-k_0|x-s|}$$

That is, we have to choose branch of the square root with positive imaginary part.

10.3 Pipe

Height of the pipe H .

$$\begin{cases} X(x) = N_E e^{ik_x x} \\ Y(y) = \frac{2}{\sqrt{H}} \cos(k_y y) \\ k_x = \frac{\sqrt{2\mu E}}{\hbar} \\ k_y = \frac{\pi m}{H} \end{cases}$$

TODO don't forget the energy normalization and wavefunction normalization

10.3.1 Green's function

Suppose $M(E)$ is the count of open transversal modes for the given energy E .

$$\begin{aligned} G(x, y, x_s, y_s; E) &= \int_0^\infty \frac{\sum_{m=0}^{M(\lambda)} Y_m(y) Y_m^*(y_s) X'(x) X'^*(x_s)}{\lambda - E} d\lambda \\ &= \sum_{m=0}^\infty \int_{E_m^Y}^\infty \frac{Y_m(y) Y_m^*(y_s) X'(x) X'^*(x_s)}{\lambda - E} d\lambda \\ &= \sum_{m=0}^\infty \int_0^\infty \frac{Y_m(y) Y_m^*(y_s) X(x) X^*(x_s)}{\lambda + E_m^y - E} d\lambda \\ &= \sum_{m=0}^\infty Y_m(y) Y_m^*(y_s) \int_0^\infty \frac{X(x) X^*(x_s)}{\lambda - (E - E_m^y)} d\lambda \\ &= \sum_{m=0}^\infty Y_m(y) Y_m^*(y_s) G^x(x, x_s; E - E_m^y) \end{aligned}$$

TODO make clear that negative wavevectors were taken into account.