Let us consider the Initial Value Problem (IVP)

Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = \Big(\underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)}_{\text{"Hamiltonian" } \hat{\mathcal{H}}} \Big)\psi, \qquad \psi(t=0,x) = \psi_0(x).$$

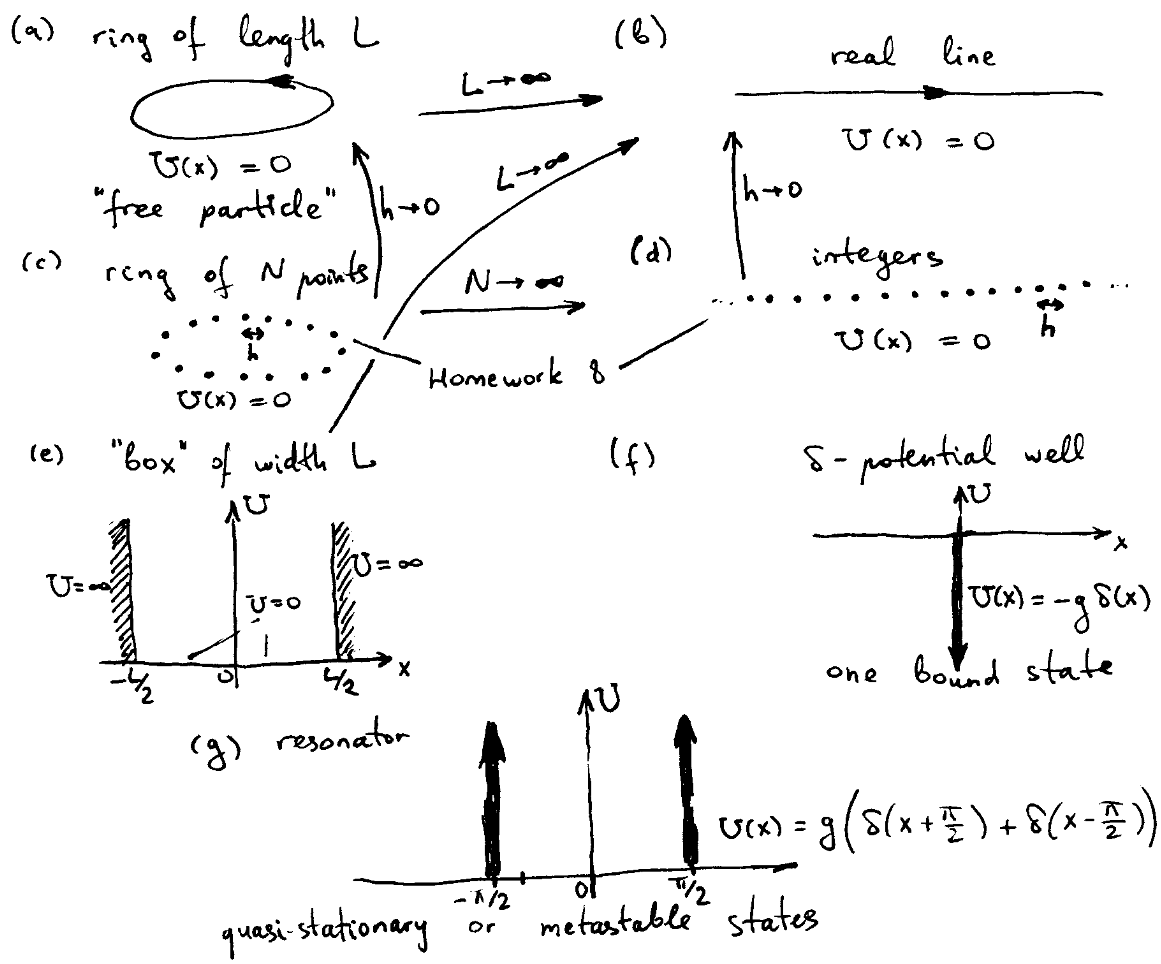
If we rescale space and time: $x = \alpha X$, $t = \beta T$, we get

$$i\frac{\partial \psi}{\partial T} = \Big(-\frac{\hbar}{2m}\frac{\beta}{\alpha^2}\frac{\partial^2}{\partial X^2} + \frac{\beta}{\hbar} U(\alpha X) \Big)\psi.$$

We'll always choose $\beta = m\alpha^2/\hbar$ to set $\hbar = 1$, $m = 1$, so

$$i\frac{\partial \psi}{\partial T} = \Big(-\frac{1}{2}\frac{\partial^2}{\partial X^2} + \alpha^2 \frac{mU}{\hbar^2}(\alpha X) \Big)\psi,$$

the parameter α can be used to stretch (and rescale accordingly) the potential U. We'll consider the following potentials:



Let us proceed with 3 steps: 1) transferring the inhomogeneity from the initial condition to the bulk equation; 2) instead of dealing with arbitrary $\psi_0(x)$, consider δ-functions arbitrarily placed; and 3) do the Fourier transform in time.

1) $$i\frac{\partial\psi}{\partial t} = \underbrace{\left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + U(x)\right)}_{\hat{\mathcal{H}}}\psi, \quad \psi(t=0,x) = \psi_0(x)$$

interested only in $t>0$

is equivalent to $$i\frac{\partial\psi}{\partial t} = \hat{\mathcal{H}}\psi + i\delta(t)\,\psi_0(x), \quad \psi(t<0,x) = 0.$$

creates jump in $\psi(t,x)$ which is $\psi_0(x)$

2) Let us introduce the Green function $G(t;x|y)$ that satisfies the equation

$$i\frac{\partial G}{\partial t} = \hat{\mathcal{H}}G + \delta(t)\,\delta(x-y).$$

acts on variable x

Then (because of superposition principle — our problem is linear) we have

$$\psi(t,x) = i\int dy\, G(t;x|y)\,\psi_0(y), \quad \text{as}$$

$$\psi_0(x) = \int dy\, \delta(x-y)\,\psi_0(y).$$

For arbitrary $\psi_0(x)$ the solution $\psi(t,x)$ is the convolution of the Green function $G(t,x|y)$ with ψ_0.

3) We write $$R_E(x|y) = \int_{-\infty}^{\infty} dt\, e^{iEt}\, G(t;x|y),$$

$$G(t;x|y) = \int_{-\infty}^{\infty}\frac{dE}{2\pi}\, e^{-iEt}\, R_E(x|y).$$

Actually $R_E(x|y) = \int_{-\infty}^{\infty} dt \ldots = \int_0^{\infty} dt \ldots$, so the steps 1) and 3) can be viewed as doin Laplace transform, which is well suited for IVPs: $\mathcal{L}\{f'(t)\}(s) = s\,\mathcal{L}\{f(t)\}(s) - f(0)$.

$\frac{\partial}{\partial t} \longleftrightarrow -iE$, so we have $(E-\hat{\mathcal{H}})R_E(x|y) = \delta(x-y)$.

If you treat $R_E(x|y)$ as an integral kernel of some operator $\hat{R}_E$, then we have $(E-\hat{\mathcal{H}})\hat{R}_E = \hat{I}$ or

$\delta(x-y)$ is the kernel of identity operator I

$$\hat{R}_E = (E-\hat{\mathcal{H}})^{-1}.$$

The operator $\hat{R}_E$ is called the resolvent [operator] of $\hat{\mathcal{H}}$. It depends (in analytic way) on the "spectral parameter" E. Whenever E_0 is an eigenvalue of $\hat{\mathcal{H}}$ (i.e., there is a non-zero solution Ψ of the equation $\hat{\mathcal{H}}\Psi = E_0\Psi$), then $E_0-\hat{\mathcal{H}}$ is non-invertible, or R_{E_0} doesn't exist — $\hat{R}_E$ as a function of E has a singularity at $E=E_0$.

In the simplest case of $\hat{\mathcal{H}}$ being an $n\times n$ matrix with diagonalization

$$\hat{\mathcal{H}} = \hat{T} \cdot \hat{\Lambda} \quad \hat{T}^{-1}$$

right eigenvectors $\hat{\mathcal{H}}\vec{T}_{*k} = \lambda_k \vec{T}_{*k}$

$$\left[\begin{array}{c|c|c|c} \vec{T}_{*1} & \vec{T}_{*2} & \cdots & \vec{T}_{*n} \end{array}\right] \begin{bmatrix} \lambda_1 & & 0 \\ & \lambda_2 & \\ 0 & & \ddots \\ & & & \lambda_n \end{bmatrix} \begin{bmatrix} \vec{t}_{1*} \\ \hline \vec{t}_{2*} \\ \hline \vdots \\ \hline \vec{t}_{n*} \end{bmatrix}$$

left eigenvectors $\vec{t}_{k*}\hat{\mathcal{H}} = \vec{t}_{k*}\lambda_k$

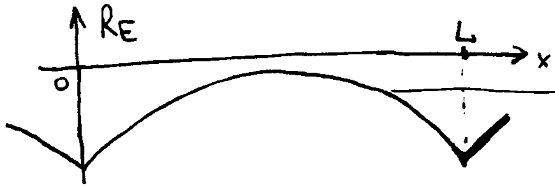
we have $\hat{R}_E = (E-\hat{\mathcal{H}})^{-1} = \hat{T}(E-\hat{\Lambda})^{-1}\hat{T}^{-1} = \sum_{k=1}^{n} \vec{T}_{*k}\frac{1}{E-\lambda_k}\vec{t}_{k*}$

outer product

Resolvent has poles at the eigenvalues, and eigenvectors are extractable from the residues.

In (a), (b), (c), (d) due to translation invariance we are going to have $R_E(x|y) = R_E(x-y|0)$. We would sometimes write $R_E(x|0)$ as $R_E(x)$.

(a) $R_E(x)$ is a periodic function with period L, and $\left(E + \frac{1}{2}\frac{d^2}{dx^2}\right) R_E(x) = \delta(x)$.



$$R_E(x) = A\, e^{i\sqrt{2E}\, x} + B\, e^{i\sqrt{2E}\,(L-x)}$$

some constants yet unknown

Locally integrating the equation near $x=0$ (where it looks like pretty much as $R''_E(x) = 2\delta(x)$), we get

$$\begin{cases} R_E(+0) = \underbrace{R_E(-0)}_{R_E(L-0)} & \text{— continuity at the place of } \delta(x) \\ R'_E(+0) - \underbrace{R'_E(-0)}_{R'_E(L-0)} = 2 & \text{— derivative jump} \end{cases} \quad \Downarrow \; A = B$$

We get $$R_E(x) = \frac{e^{i\sqrt{2E}\,x} + e^{i\sqrt{2E}\,(L-x)}}{i\sqrt{2E}\left(1 - e^{i\sqrt{2E}\,L}\right)}.$$

This expression for $R_E(x)$ contains $\sqrt{2E}$ (which has two different values), but $R_E(x)$ is actually one-valued function of E:

let's exchange

$$R_E(x) = \frac{e^{-i\sqrt{2E}\,L}\left(e^{i\sqrt{2E}x} + e^{i\sqrt{2E}(L-x)}\right)}{i\sqrt{2E}\; e^{-i\sqrt{2E}L}\left(1 - e^{i\sqrt{2E}\,L}\right)} = \frac{e^{i(-\sqrt{2E})x} + e^{i(-\sqrt{2E})(L-x)}}{i(-\sqrt{2E})\left(1 - e^{i(-\sqrt{2E})L}\right)}.$$

The resolvent $R_E(x|y)$ as a function of E has singularities whenever $\sqrt{2E}\,(1-e^{i\sqrt{2E}L})=0$, which happens when $\sqrt{2E}\,L = 2\pi M$ for some integer M. The <u>real</u> (operator $\hat{\mathcal{H}}$ is self-adjoint) numbers $E_M = \frac{2\pi^2}{L^2}M^2$ are the eigenvalues of $\hat{\mathcal{H}} = -\frac{1}{2}\frac{d^2}{dx^2}$ on a ring of length L, with $\frac{e^{i\frac{2\pi M}{L}x}}{\sqrt{L}}$ and $\frac{e^{-i\frac{2\pi M}{L}x}}{\sqrt{L}}$ being the pair of linearly independent normalized eigenfunctions (if $M=0$, then there is just one eigenfunction $\frac{1}{\sqrt{L}}$). An alternative choice would be $\sqrt{\frac{2}{L}}\cos\left(\frac{2\pi M}{L}x\right)$ and $\sqrt{\frac{2}{L}}\sin\left(\frac{2\pi M}{L}x\right)$.

The right and left eigenfunctions for E_M can be chosen as
$$\underset{\text{column}}{\vec{T}_M(x)} = C_M\frac{e^{i\frac{2\pi M}{L}x}}{\sqrt{L}},\qquad \underset{\text{row}}{\vec{t}_M(y)} = \frac{1}{C_M}\frac{e^{-i\frac{2\pi M}{L}x}}{\sqrt{L}},$$
where $C_M \neq 0$ are arbitrary, could depend on M.
We have
$$\int_0^L dx\, \underset{\text{row}\,\cdot\,\text{column}}{\vec{t}_M(x)\vec{T}_N(x)} = \frac{C_N}{C_M}\frac{1}{L}\int_0^L dx\, e^{\frac{2\pi i}{L}(N-M)x} =$$
$$= \frac{C_N}{C_M}\delta_{MN} = \delta_{MN}$$ — analog of $\hat{T}^{-1}\hat{T} = \hat{I}$.

As in our case $\hat{\mathcal{H}}$ is self-adjoint, or $\hat{\mathcal{H}}^* = \hat{\mathcal{H}}$, it is natural to choose $\underset{\text{row}}{\vec{t}_M(x)} = \underbrace{\big(\underset{\text{column}}{\vec{T}_M(x)}\big)^*}_{\text{Hermitian conjugate}}$ —

— analog of $\hat{T}^{-1} = \hat{T}^\dagger$ ($\hat{T}$ is unitary).

In this case we choose $C_M = 1$ for all M.

Let us calculate the residues of $R_E(x|y)$ at $E=E_M$:

$$\operatorname{res}\big(R_E(x|y),\ \underset{E_0}{\overset{\shortparallel}{0}}\big) = \lim_{E\to 0} E R_E(x|y) = \lim_{E\to 0} \frac{E \cdot 2}{i\sqrt{2E}\big(1-\underbrace{e^{i\sqrt{2E}L}}_{\approx\, 1+i\sqrt{2E}L}\big)} =$$

$$= \frac{1}{L} = \frac{1}{\sqrt{L}} \cdot \frac{1}{\sqrt{L}}, \quad \text{and}$$

$$\operatorname{res}\big(R_E(x|y),\ \underset{0}{\overset{\#}{E_M}}\big) = \frac{e^{i\sqrt{2E_M}(x-y)} + e^{i\sqrt{2E_M}(L-x+y)}}{i\sqrt{2E_M}\ \frac{d}{dE}\big(1-e^{i\sqrt{2E}L}\big)\Big|_{E=E_M}} =$$

$$= \frac{2\cos\big(\frac{2\pi M}{L}(x-y)\big)}{i\sqrt{2E_M}\cdot\Big(-i\frac{2}{2\sqrt{2E_M}}L\Big)} = \frac{2\cos\big(\frac{2\pi M}{L}(x-y)\big)}{L} =$$

$$= \frac{e^{-i\frac{2\pi M}{L}y}}{\sqrt{L}} \cdot \frac{e^{i\frac{2\pi M}{L}x}}{\sqrt{L}} + \frac{e^{i\frac{2\pi M}{L}y}}{\sqrt{L}} \cdot \frac{e^{-i\frac{2\pi M}{L}x}}{\sqrt{L}} =$$

$$= \sqrt{\tfrac{2}{L}}\cos\Big(\tfrac{2\pi M}{L}y\Big)\cdot\sqrt{\tfrac{2}{L}}\cos\Big(\tfrac{2\pi M}{L}x\Big) + \sqrt{\tfrac{2}{L}}\sin\Big(\tfrac{2\pi M}{L}y\Big)\cdot\sqrt{\tfrac{2}{L}}\sin\Big(\tfrac{2\pi M}{L}x\Big) -$$

— everything is as it was expected, i.e., residues of the resolvent are related to the eigenfunctions.

We have $1-e^{i\sqrt{2E}L} = -2i\, e^{i\frac{\sqrt{2E}}{2}L}\sin\big(\sqrt{\tfrac{E}{2}}L\big)$, and $\sin z = z\cdot\prod_{M=1}^{\infty}\big(1-\frac{z}{\pi M}\big)\big(1+\frac{z}{\pi M}\big)$. Thinking in "partial fractions" style, an alternative expression for the resolvent is

$$R_E(x|y) = \frac{1}{L}\sum_{M=-\infty}^{\infty} \frac{e^{i\frac{2\pi M}{L}(x-y)}}{E - \frac{2\pi^2}{L^2}M^2},$$

which is an analog of $\hat{R}_E = \sum_k \vec{T}_{xk}\frac{1}{E-\lambda_k}\overleftarrow{T}_{kx}$.