Differential operators

These are operators with derivatives and are treated as formal operators without acting on functions

Examples: momentum operator in QM

$$p \to \frac{\hbar}{i}\frac{d}{dx}$$

position operator in QM

$$x \to \hat{x}$$

Generally operators do not commute

$$(x\partial_x - \partial_x x)\phi = x\phi' - \phi - x\phi'$$
$$= -\phi$$

$$\Rightarrow x\partial_x - \partial_x x = -1$$

Differential equations for operators

Example: $$\frac{dL}{dt} = i[P, L]$$

Solution $$L(t) = e^{iPt} L(0) e^{-iPt}$$

proof $$\frac{dL}{dt} = iP e^{iPt} L(0) e^{-iPt} + e^{iPt} L(0)(-iP)e^{-iPt}$$
$$= iP\, L(t) + L(t)(-iP)$$
$$= i[P, L(t)]$$

then

$$(u, Lv) = \int_a^b w(x)\, v(x) (L^+ u)^* dx$$

$$= (L^+ u, v)$$

which is exactly the adjoint we had before

<u>Example</u> $L = -i \frac{d}{dx}$

then $u^* L v = -i\, u^* \frac{d}{dx} v$

$$= -i \frac{d}{dx}(u^* v) + i v \frac{d}{dx} u^*$$

$$= -i \frac{d}{dx}(u^* v) + v \left(-i \frac{d}{dx} u\right)^*$$

$$\Rightarrow L^+ = -i \frac{d}{dx}$$

$$Q(u, v) = -i u^* v$$

$\Rightarrow L = L^+ \Rightarrow L$ is self adjoint

Boundary conditions

When a differential operator acts on a domain, we impose boundary conditions on the functions in the domain.
The boundary condition will always be chosen linear an homogeneous. So if y_1 and y_2 satisfy the boundary conditions, then also $\alpha y_1 + \beta y_2$ satisfies the boundary conditions.

Adjoint

Differential operator L
Weight function $w(x)$ on (a,b)
Definition of adjoint

$$w\left(u^* L v - v\left(L^+ u\right)^*\right) = \frac{d}{dx} Q(u,v)$$

Q depends linearly on u an v

$$(u,v) = \int_a^b w(x)\, u^*(x)\, v(x)\, dx$$

$$(u L v) = \int_a^b w(x)\, u^*(x)\, L v\, dx$$

$$= \int_a^b + w(x)\, v\left(L^+ u\right)^* dx + \int_a^b dx \frac{d}{dx} Q(u,v)$$

choose u and v with b.c. $\quad Q(u,v)\Big|_a^b = 0$

Sturm–Liouville operator

$$L = \frac{d}{dx}\left(p_0(x)\frac{d}{dx}\right) + p_2$$

$$u^* p_2 v = v p_2 u^*$$

$$u^* L v$$

$$u^* \frac{d}{dx}\left(p_0(x)\frac{d}{dx}\right) v - \left(\frac{d}{dx} p_0 \frac{d}{dx} u^*\right) v$$

$$= u^* \partial_x p_0 \, \partial_x v + u^* p_0 \partial_x^2 v - \partial_x p_0 \partial_x u^* v - p_0 \partial_x^2 u^* v$$

$$= \frac{d}{dx}\left(u^* p_0 \partial_x v\right) - \cancel{\partial_x u^* p_0 \partial_x v} - \frac{d}{dx}\left(p_0 \partial_x u^* v\right) + \cancel{p_0 \partial_x u^* \partial_x v}$$

$$= \frac{d}{dx}\left(u^* p_0 (\partial_x v) - p_0 (\partial_x u^*) v\right)$$

$\Rightarrow$ Sturm–Liouville operator is selfadjoint.

We can make $L = P_0 \partial_x^2 + P_1 \partial_x + P_2$ selfadjoint by introducing the weight function

$$w = \frac{1}{P_0} e^{\int_a^x \frac{P_1}{P_0} dx'}$$

$$\langle u, v \rangle_w = \int_a^b w\, u^* v \, dx$$

Then $L y = \underline{\frac{1}{w} \frac{d}{dx}} w P_0 \frac{d}{dx} y + P_2 y$

and $\langle u, L v \rangle_w - \langle L u, v \rangle_w = w P_0 (u^* \partial_x v - \partial_x u^* v) \Big|_a^b$

same as for the Sturm Liouville operator with $w = 1$

eigenvalues and selfadjoint operators

We wish to understand when an operator is self-adjoint so that it has a complete set of orthonormal eigenfunctions.

Let us first look at some examples

1) $T = -\partial_x^2 \quad D(T) = \{ y, T(y) \in L^2(0,1), \ y(0) = y(1) = 0 \}$

inner product $\langle y_1, y_2 \rangle = \int_0^1 y_1^* y_2 \, dx$

then $\langle y_1, T y_2 \rangle = \int_0^1 y_1^* (-\partial_x^2) y_2$

$$= \int_0^1 \partial_x y_1^* \partial_x y_2 - y_1^* \partial_x y_2 \Big|_0^1$$

$$= \int_0^1 (-\partial_x^2) y_1^* \, y_2 + \underbrace{(\partial_x y_1^*) y_2 \Big|_0^1 - y_1^* \partial_x y_2 \Big|_0^1}_{= 0}$$

$$\Rightarrow T^+ = -\partial_x^2 = T$$

$\Rightarrow$ T is selfadjoint

eigenfunction $\quad y_n = \sin n\pi x$

$\qquad \lambda_n = n^2 \pi^2$

- eigenvalues are real
- eigenfunction are orthogonal

$$\int \sin n\pi x \, \sin m\pi x \sim \delta_{nm}$$

- eigenfunctions are complete

$y \in L^2[0,1]$ then $y = \sum_n a_n \sin n\pi x$

<u>example 2</u>

Now we will see that this is not valid for all Hermition operators

$T = -i\partial_x \qquad D(T) = \{y, Ty \in L^2[0,1], y(0) = y(1) = 0\}$

$$(y_1, Ty_2) = \int_0^1 y_1^* (-i\partial_x) y_2 = \int_0^1 i\partial_x y_1^* y_2 - i y_1^* y_2 \Big|_0^1$$

$$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \| \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad 0$$

$T^+ = T$ but T has no eigenfunctions with these b.c. $\quad T\phi = \phi \Rightarrow \phi \sim e^{-i\lambda x}$ which never vanishes

If $\langle u, Tv \rangle = \langle w, v \rangle \quad \forall v$

then $w = T^{+} u$ if there is a u in the Domain of T^{+} for which this is true.

This is always the case for finite matrices but not for operators.

What we want to find are the conditions on u such that $Q[u, v)$ vanishes for all v. These are the adjoint boundary conditions.

Example: $T = -i\partial_x \quad \mathcal{D}(T) = \{y, Ty \in L^2[0,1],\ y(1) = 0\}$

$$\int_0^1 u^*(-i\partial_x) v = \int_0^1 i\partial_x u^* v - iu^* v \Big|_0^1$$

$$= \int_0^1 i\partial_x u^* v \quad - iu^*(1) v(1) + iu^*(0) v(0)$$

in general the Q term does not vanish. It only vanishes for all v if $u(0) = 0$. So the adjoint boundary condition is

$T^{+} = -i\partial_x \quad \mathcal{D}(T^{+}) = \{y, T^{+}y \in L^2[0,1],\ y(0) = 0\}$

when we impose the b.c. $y(0) = y(1) = 0$ then the boundary term vanishes for all u $\Rightarrow$

$$\mathcal{D}(T^+) = \{ y, T^+(y) \in L^2[0,1] \}$$

$\Rightarrow$ $\mathcal{D}(T^+) \neq \mathcal{D}(T)$

and the operator is not selfadjoint

Self-adjoint boundary conditions

we like to find the boundary conditions that make an operator self-adjoint. These are called the self-adjoint boundary conditions

Example: Let us look at the most general boundary conditions such that $T = -i\partial_x$ becomes selfadjoint.

$$\int_0^1 u^*(-i\partial_x v) = \int_0^1 i\partial_x u^* v + (-i) u^* v \Big|_0^1$$

$$\underbrace{(-i) u^* v \Big|_0^1}_{-i\left(u^*(1) v(1) - u^*(0) v(0)\right)}$$

We demand that $u^*(1)\,v(1) - u^*(0)\,v(0) = 0$

$$\Rightarrow \frac{u^*(1)}{u^*(0)} = \frac{v(1)}{v(0)}$$

this should be true $\forall u, v$

$$\Rightarrow \frac{u^*(1)}{u^*(0)} = \frac{v(0)}{v(1)} = \text{const} = \kappa$$

same conditions on u and v

$$\Rightarrow \frac{u(1)}{u(0)} = \kappa^* = \frac{v(1)}{v(0)} = \frac{1}{\kappa}$$

$$\Rightarrow |\kappa|^2 = 1 \Rightarrow \kappa = e^{i\theta}$$

$$D(T) = D(T^+) = \{y, Ty \in L^2[0,1],\ y(1) = e^{i\theta} y(0)\}$$

twisted periodic boundary conditions

<u>eigenfunction</u> - $e^{i(2\pi n + \theta)x}$

- eigenvalues are real
- eigenfunctions are orthogonal and complete

Example; Sturm Liouville operator

$$L = \frac{d}{dx} p(x) \frac{d}{dx} + q(x)$$

$$\langle u, Lv\rangle = \langle Lu, v\rangle + p(u^* \partial_x v - \partial_x u^* v)\Big|_a^b$$

should vanish for all u and v

$$\Rightarrow \quad u^*(b) v'(b) - u^{*\prime}(b) v(b)$$
$$= u^*(a) v'(a) - u^{*\prime}(a) v(a)$$

This is the case if $\alpha_a u(a) + \beta_a u'(a) = 0$

$\alpha_b u(b) + \beta_b u'(b) = 0$

So we impose the boundary conditions at both ends independently.

Deficiency indices

$\mathcal{D}_0(L)$ has boundary conditions with
$$y^{(k)}(a) = y^{k}(b) = 0 \quad \forall k < n$$
Then count the number of solutions with eigenvalue $+i$ and $-i$, they are n_+ and n_-.

if $n_+ \neq n_-$ the operator cannot be made selfadjoint. If $n_+ = n_- = n$ then there is an n parameter selfadjoint extention of $\mathcal{D}_0(L)$

Example radial momentum operator.
$$P_r = -i\partial_r \qquad \mathcal{D} = \{ y, P_r y \in L^2(0,\infty) \mid y(0)=0 \}$$

$$P_r^+ = -i\partial_r \qquad \mathcal{D}(P_r^+) = \{ y, P_r^+ y \in L^2(0,\infty) \}$$

$$P_r^+ y = -iy \Rightarrow y \sim e^{-r}$$
$$P_r^+ y = iy \Rightarrow y \sim e^{r} \quad \text{not normalizable}$$
$$\Rightarrow n_+ \neq n_-$$
$\Rightarrow$ this operator cannot be made selfadjoint

Example Schrödinger operator on $[0,\infty)$

$T = -\partial_x^2 \qquad D_0(T) = \{ y,\ Ty \in L^2(0,\infty),\ y(0) = y'(0) = 0 \}$

$T^+ = -\partial_x^2 \qquad D(T^+) = \{ y,\ T(y) \in L^2(0,\infty) \}$

$T^+ y = iy \Rightarrow y = e^{(i-1)x/\sqrt{2}}$

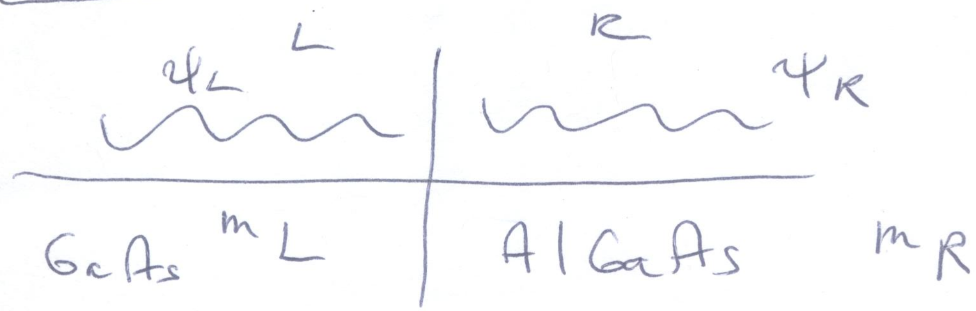
$T^+ y = -iy \Rightarrow y = e^{(-i-1)x/\sqrt{2}}$

Both are normalizable $\Rightarrow n_+ = n_- = 1$

Weyl Neumann: We can relax the condition $y(0) = y'(0) = 0$ so that the operator becomes selfadjoint

this is the domain wit $\frac{y'(0)}{y(0)} = \text{const.}$

Application to semiconductor heterojunction



What is the matching condition between ψ_L and ψ_R

We will use the effective band mass theory

$$H_L = -\frac{1}{2m_L}\partial_x^2 + V_L(x)$$

$$H_R = \frac{1}{-2m_R}\partial_x^2 + V_R(x)$$

The wave function of the effective theory does not have to be continuous

– connection formula between ψ_L and ψ_R should be
- linear
- only involve ψ and ψ'
- make the Hamiltonian selfadjoint

$$\langle\psi_1|H|\psi_2\rangle - \langle H\psi_1|\psi_2\rangle$$

$$=$$

$$-\int \psi_1^* \partial_x^2 \psi_2 = \int \partial_x \psi_1^* \partial_x \psi_2 - \int d(\psi_1^* \partial_x \psi_2)$$

$$= -\int \partial_x^2 \psi_1^* \psi_2 + \int d(\partial_x \psi_1^* \psi_2) - \int d(\psi_1^* \partial_x \psi_2)$$

$$\int = \int_{-\infty}^{\varepsilon_L} + \int_{\varepsilon_R}^{\infty} \qquad \psi(\pm\infty) = 0$$

$$= \langle\psi_1|H|\psi_2\rangle - \langle\psi_2|H|\psi_1\rangle = \frac{1}{2m_L}\left(\psi_{1L}'^{*}\psi_{2L} - \psi_{1L}\psi_{2L}'\right)$$
$$+ \frac{-1}{2m_R}\left(\psi_{1R}'^{*}\psi_{2R} - \psi_{1R}\partial_x\psi_{2R}\right)$$

linear boundary conditi

$$\begin{pmatrix}\psi_{2L}\\ \psi_{2L}'\end{pmatrix} = \begin{pmatrix} a & b \\ c & d\end{pmatrix}\begin{pmatrix}\psi_{2R}\\ \psi_{2R}'\end{pmatrix}$$

Insert into condition for selfadjointness

$$\frac{1}{2m_L}\left(\psi_{1L}^{*}\cdot\left(c\psi_{2R}+d\psi_{2R}'\right)-\psi_{1L}'^{*}\left(a\psi_{2R}+b\psi_{2R}'\right)\right)$$

$$=\frac{1}{2m_R}\left(\psi_{1R}^{*}\psi_{2R}'-\psi_{1R}'^{*}\psi_{2R}\right)$$

This should be true $\forall\ \psi_{2R},\psi_{2R}'$

$$\Rightarrow \begin{pmatrix}\psi_{1R}\\ \psi_{1R}'\end{pmatrix}=\frac{m_R}{m_L}\begin{pmatrix}d^{*} & -b^{*}\\ -c^{*} & a^{*}\end{pmatrix}\begin{pmatrix}\psi_{1L}\\ \psi_{1L}'\end{pmatrix}$$

eg coef of ψ_{2R}

$$\frac{1}{2m_L}\left(c\psi_{1L}^{*}-a\psi_{1L}'\right)=-\frac{1}{2m_R}\psi_{1R}'$$

$$\Rightarrow \psi_{1R}^{*\prime}=-\frac{m_R}{m_L}\left(c\psi_{1L}^{*}-a\psi_{1L}'\right)$$

$$\Rightarrow \psi_{1R}'=\frac{m_R}{m_L}\left(-c^{*}\psi_{1L}+a^{*}\psi_{1L}^{*\prime}\right)$$

$$\Rightarrow \begin{pmatrix}a & b\\ c & d\end{pmatrix}^{-1}=\frac{m_R}{m_L}\begin{pmatrix}d^{*} & -b^{*}\\ -c^{*} & a^{*}\end{pmatrix}$$

so that ψ_1 and ψ_2 have the same boundary conditions

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{ad-bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

$$\Rightarrow \frac{1}{ad-bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix} = \frac{m_R}{m_L}\begin{pmatrix} d^* & -b^* \\ -c^* & a^* \end{pmatrix}$$

$$\Rightarrow \frac{1}{D} d = \frac{m_R}{m_L} d^* \qquad \frac{1}{D} c = \frac{m_R}{m_L} c^*$$

$$\frac{1}{D} b = \frac{m_R}{m_L} b^* \qquad \frac{1}{D} a = \frac{m_R}{m_L} a^*$$

$$\Rightarrow d^* = \frac{m_L}{m_R}\frac{1}{D} d$$

$$\Rightarrow \frac{m_L}{m_R}\frac{1}{D} = e^{i\phi} \qquad \Rightarrow D = |D| e^{-i\phi}$$

$$\Rightarrow d = |d| e^{-i\phi/2} = |d| \sqrt{\frac{m_L}{m_R}}\frac{1}{\sqrt{D}}$$

$$\Rightarrow D = \frac{m_L}{m_R} e^{-i\phi_1}$$

$$d = |d| e^{-i\phi/2} \qquad D = \underbrace{(|a||d| - |b||c|)}_{>0} e^{-i\phi}$$

$$|D| = \frac{m_L}{m_R} \Rightarrow |a||d| - |b||c| = \frac{m_L}{m_R}$$

$$\Rightarrow \qquad |D| = |a||d| - |b||c| = \frac{m_L}{m_R}$$

reduced 8 parameters to 4 parameters

Spectrum of an operator

$$T \phi_n = \lambda_n \phi_n \qquad \sigma(T) = \{\lambda_n\}$$

- discrete spectrum, typical for point spectrum
- continuous spectrum, when eigenfunction are not normalizable on infinite interval

For a discrete spectrum the eigenvalues and eigenfunctions have the same properties as for a finite matrix

$$\int \phi_n^* \phi_n = \delta_{nn} \qquad \text{(orthogonality)}$$

$$\sum_n \phi_n(x) \phi_n(y) = \delta(x-y) \qquad \text{(completeness}$$

$$f(x) = \int f(y)\, \delta(x-y) = \int f(y) \sum_n \phi_n(x) \phi_n(y)$$

$$= \sum_n \phi_n(x) \underbrace{\int f(y) \phi_n(y)}_{a_n}$$

So all functions can be expressed as linear combinations of the basis set $\{\phi_n(x)\}$

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Expansion of y; $y = \sum_{n=0}^{\infty} a_n y_n$

$a_n = \langle y_n, y \rangle$

then the sum converges to y

we will show that next.

So we have to show that

$$h_n = y - \sum_{m=0}^{n-1} a_m y_n$$

approaches 0 for $n \to \infty$

$h_n \in V_n^{\perp}$

$$\langle h_n | L | h_n \rangle = \langle y L y \rangle - \sum |a_n|^2 \lambda_n$$

$h_n \perp \phi_{m<n}$

$$\Rightarrow \langle h_n | L | h_n \rangle \le \langle y L y \rangle$$

$$\Rightarrow \frac{\langle y\ L\ y \rangle}{\langle h_n\ h_n \rangle} \geq \frac{\langle h_n L h_n \rangle}{h_n h} \geq \lambda_n$$

$$\Rightarrow \frac{\langle y L y \rangle}{\lambda n} \geq \langle h_n h_n \rangle = \left\| y - \sum_{k=0}^{n-1} a_k y_k \right\|^2$$

$\langle y L y \rangle$ does not depend on n and $\lambda_n \sim n^2$ for large $n \Rightarrow \sum_{k=0}^{n-1} a_k y_k$ converges to y for $n \to \infty$

Completeness of the Schrödinger problem (P7)

$$Ly = -y'' + q(x)\, y = \lambda y \qquad x \in [a, b]$$

For large n $q(x)$ is negligible and the eigenvalues are close to the eigenvalues of the free S-operator,

$$\lambda_n \simeq \frac{\pi^2 n^2}{(a-b)^2}$$

This is also the case for the Sturm - Liouville operator

$$Ly = -\frac{d}{dx}\left(p(x) \frac{d}{dx} y\right) + q\, y = \lambda y$$

eigenvalues are the stationary points of $\langle y\, Ly \rangle$ with constraint $(y, y) = 1$

Lowest eigenvalue $\qquad \lambda_0 = \inf\limits_{y \in \mathcal{D}(L)} \dfrac{(y\, Ly)}{(y\, y)}$

This is called Rayleigh - Ritz

The n'th eigenvalue is obtained as follows.

If we know $y_0, \dots, y_{n-1}$

$V_n = \{ y_0, \dots y_{n-1} \}$

then $\lambda_n = \inf\limits_{y \in V_n^\perp} \dfrac{\langle y, Ly \rangle}{\langle y, y \rangle}$

Operator methods

The ho can be solved by operator methods.

$$H = -\partial_x^2 + x^2 = (-\partial_x + x)(\partial_x + x) + 1$$

$$Q = (\partial_x + x)$$
$$Q^+ = (-\partial_x + x)$$

creation and annihilation operators

$$H = Q^+ Q + 1$$

$$Q Q^+ = H + 1 = Q^+ Q + 2$$

If $Q^+ Q \phi = \lambda \phi$

then $Q(Q^+ Q \phi) = \lambda Q \phi$

$$(Q^+ Q + 2)(Q\phi) = \lambda Q \phi$$

$$\Rightarrow \quad Q^+ Q (Q\phi) = (\lambda - 2) Q \phi$$

$Q\phi$ is only a good eigenfunction if it is nonzero. If $Q\phi = 0$ then

$Q^+ Q \phi = 0 \quad \Rightarrow \lambda = 0$

If $\lambda = 0$ then $\langle \psi \, Q^+ Q \psi \rangle = 0 = \langle Q\psi, Q\psi \rangle$

$\Rightarrow Q\psi = 0$

②

We also see that Q^+Q and QQ^+ have the same spectrum with the exception of zero eigenvalues.

$$\psi_0 = e^{-\frac{1}{2}x^2}$$

$$Q\psi_0 = (\partial_x + x)\psi_0 = 0$$

QQ^+ does not have a zero eigenvalue

$$(-\partial_x + x)\, e^{\frac{1}{2}x^2} = 0$$

bus $e^{\frac{1}{2}x^2}$ is not normalizable

If $\quad H\psi_n = (2n+1)\psi_n$

then $\quad HQ^+\psi_n =$

$$(Q^+Q+1)Q^+\psi_n = Q^+(QQ^+ + 1)\psi_n$$

$$= Q^+(H+2)\psi_n = (2(n+1)+1)\psi_n$$

$$H\psi_0 = (QQ^+ + 1)\psi_0 = \psi_0$$

$\Rightarrow (Q^+)^n\psi_0$ are the eigenfunctions of H

$$Q^+ = -\partial_x + x = -e^{\frac{1}{2}x^2}\partial_x e^{-\frac{1}{2}x^2}$$

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$$\Rightarrow \psi_n = (-1)^n \left(e^{\frac{1}{2}x^2} \partial_x e^{-\frac{1}{2}x^2}\right)^n e^{-\frac{1}{2}x^2}$$

$$= (-1)^n e^{\frac{1}{2}x^2} \partial_x^n e^{-x^2}$$

$$= -e^{-\frac{1}{2}x^2} H_n(x)$$

see chapter 2

Continuous spectrum

$H = -\partial_x^2$ free Schrödinger operator

We are going to determine its spectrum on the real line by starting with an interval $[-\frac{L}{2}, \frac{L}{2}]$ and then take the limit $L \to \infty$

boundary conditions $\psi(-\frac{L}{2}) = \psi(\frac{L}{2})$

solution $\psi = e^{ikx}$ eigenvalue k^2

$\psi(-\frac{L}{2}) = \psi(\frac{L}{2}) \Rightarrow e^{ikL} = 1$

$\Rightarrow k_n = \frac{2\pi n}{L}$, spectrum $\frac{4\pi^2 n^2}{L^2}$

normalized eigenstate $\psi_n = \frac{1}{\sqrt{L}} e^{ik_n x}$

completeness $\sum_{n=-\infty}^{\infty} \frac{1}{L} e^{ik_n x} e^{-ik_n x'} = \delta(x-x')$

for $L \to \infty$ it becomes a continuous spectrum

$$k^2 = \frac{4\pi^2 n^2}{L^2} \Rightarrow dk = \frac{L}{2\pi} dn$$

$$\sum_n = \int dn = \frac{2\pi}{L} \int dk$$

density of states

$$\frac{dn}{dk} = \frac{2\pi}{L}$$

$$\lambda = \frac{4\pi^2 n^2}{L^2} \Rightarrow \rho(\lambda) = \frac{dn}{d\lambda}$$

$$n = \pm \frac{L}{2\pi} \lambda^{1/2} \Rightarrow \frac{dn}{d\lambda} = 2 \frac{L}{2\pi} \frac{1}{2} \frac{1}{\sqrt{\lambda}}$$

"Radon – Nikodym" derivative

$\pm n$ contribute to the interval

completeness relation

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x-x')} = \delta(x-x')$$

anti-periodic b.c. $\psi(\frac{L}{2}) = -\psi(-\frac{L}{2})$

$$\Rightarrow \quad e^{ikL} = -1 \Rightarrow k = \frac{\pi}{L} + \frac{2\pi n}{L} = \frac{2\pi(n+\frac{1}{2})}{L}$$

eigenvalues $\lambda = \frac{4\pi^2 (n+\frac{1}{2})^2}{L^2}$

$$\rho(\lambda) = 2 \frac{L}{2\pi} \frac{1}{2} \frac{1}{\sqrt{\lambda}}$$ which is

the same.

Spectral density does not depend on boundary conditions.

Phase shifts

Radial Schrödinger equation

$$\left(-\partial_r^2 + V(r)\right)\psi = E\psi \quad \text{on } [0, R]$$

$$\psi(R) = 0$$

$V(r) = 0$ then $\psi \sim \sin kR$

$$\sin k_n R = 0 \Rightarrow k_n = \frac{\pi n}{R}$$

$$\int_0^R \sin k_n r \sin k_m r = \frac{R}{2}\delta_{nm}$$

completeness $\sum_{n=1}^{\infty} \frac{2}{R} \sin k_n r \sin k_n r' = \delta(r-r')$

large R limit $\sum_n \to \int dk$

$$k_n = \frac{n\pi}{R} \Rightarrow dn = \frac{R}{\pi} dk$$

$$\Rightarrow \int_0^\infty dk \frac{R}{\pi} \frac{2}{R} \sin kr \sin kr' = \delta(r-r')$$

Next we look at the case that $V(r) = 0$ for $r > R_0$

For $r > 0$ $\psi(r) = \sin(kr + \eta(k))$

phase shift.

it is some nontrivial function for $r < R_0$

for $r > R_0$: $E = k^2$ because $V(r) = 0$

Example $\quad V(r) = \lambda\,\delta(r-a)$

solution of Schrödinger eq

$$r < a \qquad \psi(r) = A \sin kr$$
$$r > a \qquad \psi(r) = \sin(kr+\eta)$$

$$\int_{a-\varepsilon}^{a+\varepsilon} \left(-\partial_r^2 + V\right)\psi = \int_{a-\varepsilon}^{a+\varepsilon} E\,\psi = O(\varepsilon) \to 0$$

$$\psi'(a-\varepsilon) - \psi'(a+\varepsilon) + \underbrace{\int_{a-\varepsilon}^{a+\varepsilon} \lambda\,\delta(r-a)\,\psi(r)}_{\lambda\,\psi(a)} = 0$$

$$\Rightarrow \quad \psi'(a-\varepsilon) - \psi'(a+\varepsilon) + \lambda\,\psi(a) = 0$$

also $\quad \psi(a-\varepsilon) = \psi(a+\varepsilon)$

if $\psi(r)$ would be discontinuous then already $\partial_r\psi$ would be proportional to a δ-function.

$$\Rightarrow \quad A \sin ka = \sin(ka+\eta)$$
$$A k \cos ka - k\cos(ka+\eta) + \lambda A \sin ka = 0$$

$$\Rightarrow \quad A k \cot ka - \frac{k\cos(ka+\eta)}{\sin ka} + \lambda A = 0$$

$$\Rightarrow \quad k\cot ka - k\cot(ka+\eta) + \lambda = 0$$

$A \sin ka \overset{\wedge}{=} \frac{1}{A}\sin(ka+\eta)$

$$\eta(k) = -ka + \cot^{-1}\left(\frac{\lambda}{k} + \cot ka\right)$$

boundary condition $\sin(kR+\eta)=0$

$\Rightarrow \quad kR + \eta(k) = n\pi$

$\Rightarrow$ for large R $\quad \frac{dn}{dk} = \frac{1}{\pi}\left(R + \frac{d\eta}{dk}\right)$

spectral density $\rho(k) = \frac{1}{\pi}\left(R + \frac{d\eta}{dk}\right)$

$ka = \pi n$ then $\quad \cot ka \to \infty$

to get a finite difference we need that $\quad \cot(ka+\eta) \to 0 \quad \Rightarrow \underset{\pi n}{\eta(\overset{\parallel}{ka})} = 0$

$$\frac{d}{dk}\left(\cot(ka+\eta) - \cos ka\right) = -\frac{\lambda}{k^2}$$

$$-\frac{1}{\sin^2(ka+\eta)}\left(a + \frac{d\eta}{dk}\right) + \frac{a}{\sin^2 ka} = -\frac{\lambda}{k^2}$$

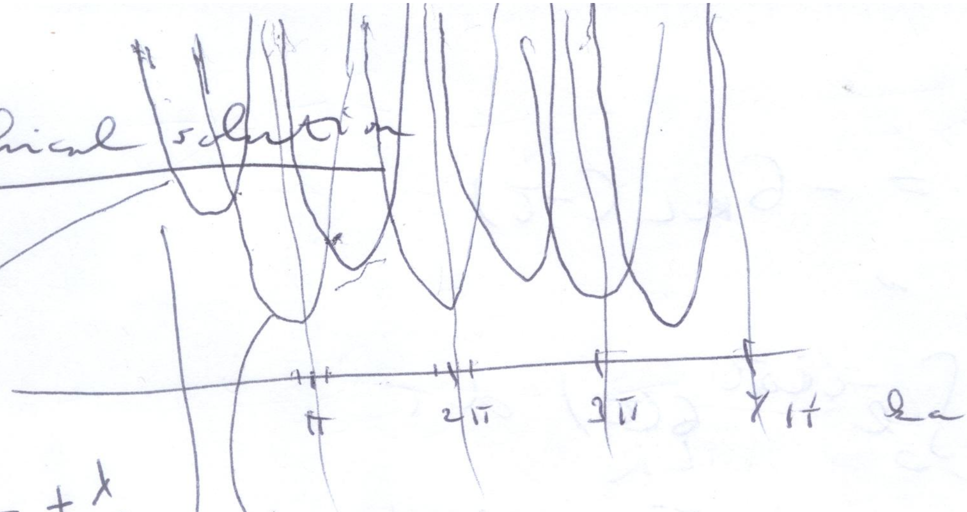
$ka \to \pi n \quad - \quad \eta(ka) \to 0$ and $\left.\frac{d\eta}{dk}\right|_{ka\to\pi n} \to 0$

$\eta = -\pi \Rightarrow \sin^2(ka+\eta) = \sin^2 ka$

$$\Rightarrow \quad \frac{1}{\sin^2 ka}\frac{d\eta}{dk} = \frac{\lambda}{k^2}$$

$$\Rightarrow \quad \frac{d\eta}{dk} = \frac{\lambda \sin^2 ka}{k^2}$$

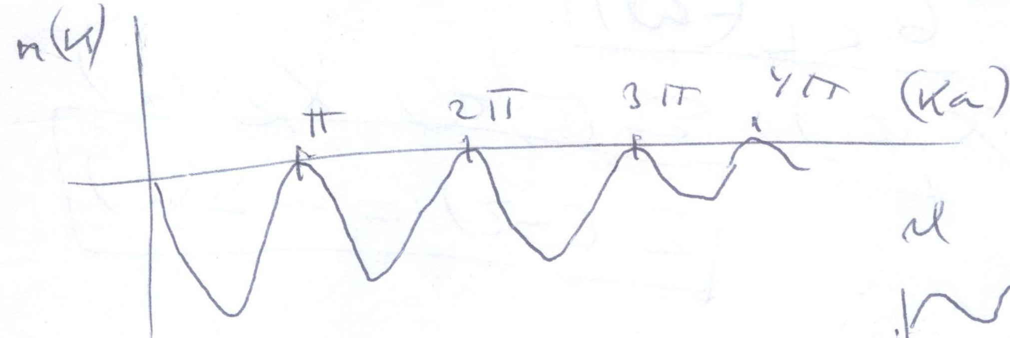
Graphical solution

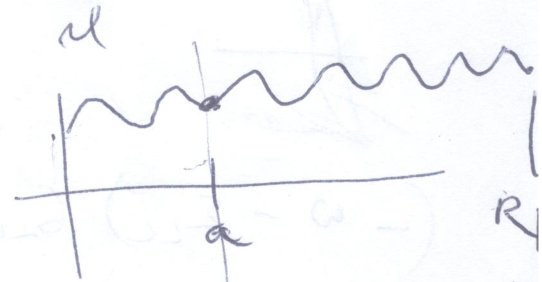


$$\frac{\lambda}{\sin^2 ka} + \frac{\lambda}{k^2}$$

$$\frac{1}{\sin^2(ka+\eta)}$$

also need $\cot(ka+\eta) - \cot ka = \frac{\lambda}{k^2}$



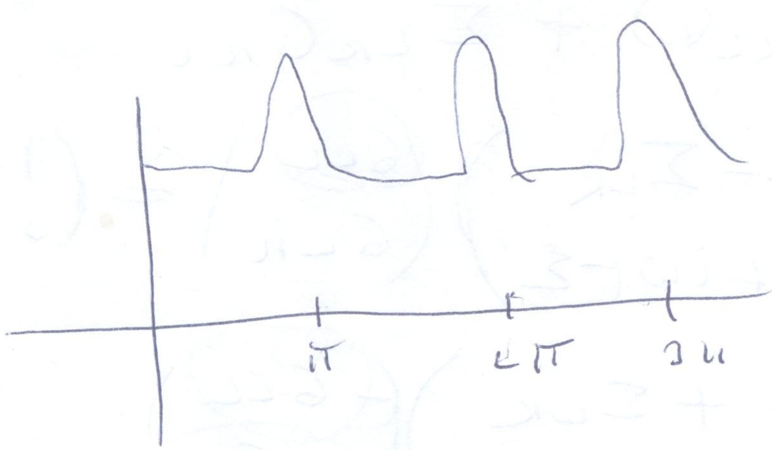


$$\Rightarrow \quad \rho(k) = \frac{1}{\pi}\left(R + \frac{d\eta}{dk}\right)$$

$E = E_k^< + E_k^>$

$\rho^< = \frac{\pi}{a} \quad \rho^> = \frac{R-a}{\pi}$

these states become resonances



Normalization and completeness

we calculate $\int_0^R dr|\psi_k|^2 \equiv \frac{1}{N_k^2}$

$$H\psi = (-\partial_r^2 + V(r))\psi = k^2 \psi$$

then $(k^2 - k'^2)\int \psi_k(r)\psi_{k'}(r)\,dr$

$$= \int_0^R \left((-\partial_r^2 \psi_k)\psi_{k'} - \psi_k(-\partial_r^2)\psi_{k'} \right)$$

$$= \left[\psi_k \partial_r \psi_{k'} - \partial_r \psi_k \psi_{k'} \right]_0^R$$

$\psi_k(0) = 0$

$\psi_k(r > R_0) = \sin(kr + \eta)$

$$= \sin(kR+\eta)\, k' \cos(k'R+\eta) - k\cos(kR+\eta)\sin(k'R+\eta)$$

differentiate wrt k and put $k' = k$

$$2k\int \psi_k \psi_k = k\cos^2(kR+\eta) + k\sin^2(kR+\eta) + k\frac{d\eta}{dk}\cos^2(kR+\eta) + k\frac{d\eta}{dk}\sin^2(kR+\eta) - \frac{1}{2}\sin 2(kR+\eta)$$

$$= -\frac{1}{2}\sin 2(kR+\eta) + k\left(R + \frac{\partial\eta}{\partial k}\right)$$

boundary condition $\sin(kR+\eta) = 0$

$$\Rightarrow \int \psi_k^2 = \frac{1}{2}\left(R + \frac{d\eta}{dk}\right)$$

Completeness relation

$$\sum_{k} \psi_k(r)\, \psi_{k}^{*}(r') = \delta(r-r')$$

$$= \underbrace{\int dk\, \frac{dn}{dk} N_k^2\, \psi_k(r)\, \psi_k(r')}_{\text{continuous part of the spectrum}} + \sum_{n} \psi_n(r)\psi_n(r')$$

↑ bound states

$$\frac{dn}{dk} = \frac{1}{\pi}\left(R + \frac{d\eta}{dk}\right) \qquad N_k^2 = \frac{1}{\frac{1}{2}\left(R + \frac{d\eta}{dk}\right)}$$

$$\Rightarrow \int dk\, \frac{2}{\pi}\, \psi_k(r)\, \psi_k(r') + \sum_{n} \psi_n(r)\, \psi_n(r') = \delta(r-r')$$

↑ bound states