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Quantum Mechanics I :- (Prof. A. Sen)

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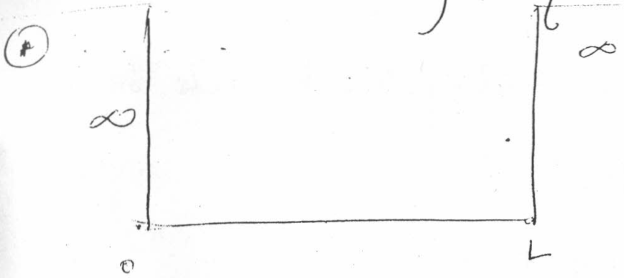
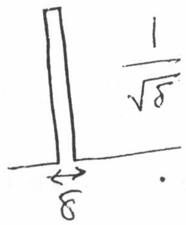
Landau & Lifshitz → Quantum Mechanics



$$\sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \longrightarrow \text{Ground state}$$



$\frac{1}{\sqrt{\delta}}$ {Regularisation technique}

(1) First measure the position

(2) Second measure energy

Problem: Calculate the probability that first expt. gives a result between $L/4$ & L & second expt gives the result equal to the ground state energy

Initially it's in the ground state

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1 dim. classical mechanics

state at any given time is specified by (q, p) — q: coordinate, p: momentum

At a later time, the values $(q(t), p(t))$ is given by eq^ns of motion

Quantum Mechanics

State of the system at any given time is specified by a wavefunction $\underline{\Psi(q)}$ → complex f^n of q

There is some equation that determines $\psi(q,t)$ if we know $\psi(q)$ at some time

Interpretation of $\psi(q)$:

$$\int_{q_1}^{q_2} |\psi(q)|^2 dq = \text{probability of finding the particle between } q_1 \text{ and } q_2$$

Suppose $f(q,p)$ is some $f^{\underline{n}}$ of q & p.

What is the probability that measurement of f gives the result f_n? (f assumes discrete values → $ass^{\underline{n}}$ to simplify)

Postulate (1)

This is given by

$$\int_{q_{min}}^{q_{max}} dq \int_{q_{min}}^{q_{max}} dq' \; \underbrace{\phi^{(f,f_n)}(q,q')}_{\text{Some function of } q \text{ \& } q' \text{ which depend on } f \text{ and } f_n} \psi(q)^* \psi(q')$$

Normalisation

$$\int_{q_{min}}^{q_{max}} |\psi(q)|^2 dq = 1.$$

Postulate (2)

Principle of superposition: If $\psi(q)$ & $\chi(q)$ are two possible wavefunctions, then so is

normalization const. $\mathcal{N}(a\,\psi(q) + b\,\chi(q))$ for any complex nos. a and b.

$a_l = i\Lambda a_k$

$$P^{(n)} = B^{(n)}_{kk} \; |a_k|^2 \left\{ B^{(n)}_{kk} + \Lambda^2 B^{(n)}_{ll} + i\Lambda\left(B^{(n)}_{kl} - B^{(n)}_{lk}\right) \right\}$$

Again, using similar arguments,

$$B^{(n)}_{kl} - B^{(n)}_{lk} = 0 .$$

$$B^{(n)}_{kl} = 0 \quad \text{for } k \neq l, \; n \neq k, l$$

$$\boxed{B^{(n)}_{kk} = 0 \quad \text{for } n \neq k} \longrightarrow \text{not reqd.}$$

$[x, p^2]$

$= x, p$

$2[x, p]p$

$= 2 i\hbar p \neq 0.$

$$B^{(n)}_{kk} = 1 \quad \text{for } n = k$$

$$P^{(n)} = \sum_r \sum_s B^{(n)}_{rs} \, a_r^* a_s$$

$$= |a_n|^2$$

$$\sum_n P^{(n)} = 1 \quad \text{implies} \quad \boxed{\sum_n |a_n|^2 = 1.}$$

Definition

$$C_{rs} = \int dq \, u_r^*(q) \, u_s(q)$$

$C_{rr} = 1$ since u_r is normalized.

Let's take $\psi = a_r u_r + a_s u_s$

$$\int dq \, \psi(q)^* \, \psi(q) = 1 .$$

$$= C_{rr} |a_r|^2 + C_{ss} |a_s|^2 +$$

$$C_{rs} a_r^* a_s + C_{sr} a_s^* a_r$$

$$1 = \underbrace{|a_r|^2 + |a_s|^2}_{1} + C_{rs}\, a_r^* a_s + C_{sr}\, a_s^* a_r$$

$$\therefore C_{rs}\, a_r^* a_s + C_{sr}\, a_s^* a_r = 0.$$

Proof of ~~orthogonality~~ & orthonormality

① Take $a_r = a_s$

$$\Rightarrow (C_{rs} + C_{sr})\,|a_r|^2 = 0$$

$$C_{rs} + C_{sr} = 0 \qquad \therefore C_{rs} = C_{sr} = 0. \quad [r \neq s]$$

② Choose $a_r = i a_s$

$$C_{rs} - C_{sr} = 0$$

$$p^{(n)} = \iint dq\, dq'\, \phi^{(f, f_n)}(q, q')\, \psi(q)^* \psi(q')$$

For $\psi = \boxed{\sum_n a_n u_n(q)}$, $\quad p^{(n)} = |a_n|^2 = a_n^* a_n$

$$a_n = \int dq'\, u_n^*(q')\, \psi(q')$$

$$p^{(n)} = \iint dq\, u_n(q)\, \psi(q)^*\, dq'\, u_n^*(q')\, \psi(q')$$

$$\therefore \boxed{\phi^{(f, f_n)} = u_n(q)\, u_n^*(q')}$$

$\bar{f}$ = average value of f

$$= \sum_n |a_n|^2 f_n$$

$$= \sum_n \int dq \int dq'\, f(n)\, u_n(q)\, u_n^*(q')\, \psi(q)^*\, \psi(q')$$

$$= \int dq \int dq' \, K_f(q,q') \, \psi(q)^* \, \psi(q')$$

$$K_f(q,q') = \sum_n f_n \, u_n(q) \, u_n^*(q')$$

Linear operator $\hat{f}$

$$\hat{f} \, \psi(q) = \int dq' \, K_f(q,q') \, \psi(q')$$

$$\bar{f} = \int dq \, \psi(q)^* \, \hat{f} \, \psi(q) \, .$$

$$K_f(q,q') = \frac{d}{dq} \delta(q-q')$$

$$\int K_f(q,q') \, \psi(q') \, dq'$$

$$= \frac{d\psi}{dq} \qquad K_f(q,q')$$

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$$\hat{f} \, \psi(q) = \int dq' \, K_f(q,q') \, \psi(q')$$

$$K_f(q,q') = \sum_n f_n \, u_n(q) \, u_n(q')^*$$

$$\hat{f}\,(a_1 \psi_1 + a_2 \psi_2) = a_1 \hat{f} \psi_1 + a_2 \hat{f} \psi_2$$

$$\hat{f} \, u_m(q) = \int dq' \, K_f(q,q') \, u_m(q')$$

$$= \int dq' \sum_n f_n \, u_n(q) \, u_n(q')^* \, u_m(q')$$

$$= \sum_n f_n \, u_n(q) \, \delta_{mn}$$

$$= f_m \, u_m(q) \, .$$

$u_m(q)$ is an eigenfunction of $\hat{f}$ with eigenvalue f_m.

Definition

$O^\dagger$ is hermitian conjugate to O if

$$\int (\hat{O}^\dagger \psi(q))^* \chi(q)\, dq$$
$$= \int \psi(q)^* (\hat{O}\chi(q))\, dq$$

for any functions $\psi(q)$, $\chi(q)$

$\hat{O}$ is hermitian if $\hat{O} = \hat{O}^\dagger$

$$\int \psi(q)^* \hat{f} \chi(q)$$
$$= \int dq \int dq' \sum_n f_n u_n(q) u_n(q')^* \chi(q') \psi(q)^*$$

$$\int dq \, (\hat{f}\psi(q))^* \chi(q)$$
$$= \int dq\, \chi(q) \int \left\{ \sum_n f_n u_n(q) u_n^*(q') \psi(q') \right\}^* dq'$$

Interchange q & q' $\longrightarrow$ $\hat{O}^\dagger = \hat{O}$.

$f_n = f_n^*$ $\longrightarrow$ [assumption]

Time evolution is local in time. (Ass$\frac{n}{..}$)

$\Rightarrow$ $\frac{d\psi}{dt}$ is determined in terms of $\psi(q,t)$

Equation should be linear in time

If $\psi_1(q)$ evolves to $\psi_1(q,t)$ and $\psi_2(q)$ evolves to $\psi_2(q,t)$, then $a_1\psi_1(q) + a_2\psi_2(q)$ evolves to

$a_1 \psi_1(q,t) + a_2 \psi_2(q,t)$

$$\frac{d\psi(q,t)}{dt} = a\,\psi(q,t)^2$$

NOT ALLOWED

$$\cancel{\frac{d\psi(q,t)}{dt}} = \psi(q,t) + C$$

General form of the equation is

$$\frac{d\psi(q,t)}{dt} = \hat{O}\,\psi(q,t).$$

$$\int (\psi(q))^* \psi(q)\, dq = 1 \qquad \left\{ \text{some linear operator} \right\}$$

$$\frac{d}{dt}\int (\psi(q,t))^* \psi(q,t)\, dq$$

$$= \int (\hat{O}\psi(q,t))^* \psi(q,t)\, dq + \int (\psi(q,t))^* \hat{O}\psi(q,t)\, dq$$

$$= \int \psi^*(q,t)\, \hat{O}^\dagger \psi(q,t)\, dq + \int (\psi(q,t))^* \hat{O}\psi(q,t)\, dq.$$

$\boxed{\hat{O}^\dagger = -\hat{O}}$ for probability conservation

(anti-hermitian)

$$\psi(q) = \sum_n a_n u_n(q)$$

$$a_n = \int u_n^*(q')\psi(q')\, dq'$$

$$\Rightarrow \psi(q) = \sum_n \int dq'\, u_n^*(q')\psi(q')\,\cancel{dq'}\, u_n(q)$$

$$= \int dq' \underbrace{\sum_n u_n(q)\, u_n^*(q')}_{\delta(q-q')} \psi(q')$$

$$\Rightarrow \sum_n u_n(q)\, u_n^*(q') = \delta(q-q')$$

[Completeness relation]

State $\leftrightarrow$ complex wavefunction

$\Downarrow$ elements of a complex vector space V

~~Take~~ Given any two elements $\psi, \chi \in V$ we can define an inner product $\langle \psi, \chi \rangle$ with the following properties:

1. $\langle \psi, \chi \rangle$ is a complex number
2. $\langle \chi, \psi \rangle = \langle \psi, \chi \rangle^*$
3. $\langle \chi, a\psi_1 + b\psi_2 \rangle = a \langle \chi, \psi_1 \rangle + b \langle \chi, \psi_2 \rangle$

$$\Rightarrow \langle a\chi_1 + b\chi_2, \psi \rangle$$
$$= a^* \langle \chi_1, \psi \rangle + b^* \langle \chi_2, \psi \rangle$$

4. $\langle \psi, \psi \rangle \geq 0$ $\rightarrow$ $\psi \rightarrow$ zero vector

Replace

Space of functions $\longleftrightarrow$ elements of V

2. $\int \psi(q)^* \chi(q)\, dq$
$= \langle \psi, \chi \rangle$

3. Observables $\longrightarrow$ Hermitian operators

(4) Time-evolution operator

$\Rightarrow$ ~~an~~ anti-hermitian operator $\hat{O}$

~~मॉरि महाचार्यं~~

Example

2-state system

V is 2-dimensional

$$\hat{O} = \begin{pmatrix} 0 & ic \\ ic & 0 \end{pmatrix}$$ spin Hamiltonian

Stationary states

$\left\{ \hat{O} \text{ is time-independent here.} \right\}$

$$\hat{O}\, v_n(q) = -i e_n v_n(q)$$

$$\psi(q,t) = e^{-ie_n t} v_n(q) \xleftrightarrow{\text{satisfies}} \frac{\partial \psi}{\partial t} = \hat{O}\psi$$

$$\downarrow$$

$$-ie_n e^{-ie_n t} v_n(q) \qquad -ie_n e^{-ie_n t} v_n(q)$$

$$\psi(q) = \sum a_n v_n(q)$$

$$a_n = \int dq\, v_n(q)^* \psi(q)$$

$$\boxed{\sum_n v_n(q)\, v_n(q')^* = \delta(q-q')}$$

$$\psi(q,t) = \sum_n a_n e^{-ie_n t} v_n(q).$$

Continuous Spectrum

P.T.O.

Suppose an observable f can take continuous values in the range

can still define eigenfunctions

$$\hat{f}\, u_g(q) = g\, u_g(q)$$

$\boxed{\text{NORMALISATION} \rightarrow ?}$

$$\int u_g(q)^* u_{g'}(q)\, dq = \delta(g-g').$$

DELTA NORMALISATION

Multiply by $u_g(q')$ and integrate over g

$$\int dg\, u_g(q') \int u_g(q)^* u_{g'}(q)\, dq$$

$$= \int dg\, \delta(g-g')\, u_g(q')$$

$$= u_{g'}(q')$$

$$\therefore \quad \int dq \left\{ \int dg\, u_g(q')\, u_g(q)^* \right\} u_{g'}(q) = u_{g'}(q')$$

$$\Rightarrow \quad \int dg\, u_g(q')\, u_g(q)^* = \delta(q-q')$$

$$= \int dg\, u_g^*(q')\, u_g(q)$$

Take any wave $f^{\underline{n}}$ $\Psi(q)$ s.t. $\int dq\, \Psi(q)^* \Psi(q) = 1$

$$\Psi(q) = \int dq'\, \delta(q-q')\, \Psi(q')$$

$$= \int dq' \int dg\, u_g^*(q')\, u_g(q)\, \Psi(q')$$

$$= \int dg \underbrace{\left\{ \int dq'\, u_g^*(q')\, \Psi(q') \right\}}_{a_g} u_g(q)$$

$$\Psi(q) = \int dg \; a_g \, u_g(q)$$

(generalizes $\sum_m a_m u_m(q)$)

$|a_g|^2 dg \longrightarrow$ probability that $\hat{f}$ takes value in the range g to $(g + dg)$

Suppose, f takes value in the range (f_1, f_2)

$$\int_{f_1}^{f_2} |a_g|^2 dg \stackrel{?}{=} 1$$

Ex: Check this. (It's checked)

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Quantum Mechanics

States $\longleftrightarrow$ elements of unit norm of a vector space (complex) with a positive, semi-definite norm

For $\Psi, \phi \in V$, then $\langle \Psi | \phi \rangle$ is a complex number

$$\langle \Psi | \phi \rangle = \langle \phi | \Psi \rangle^*$$

$$\langle \Psi, a\phi_1 + b\phi_2 \rangle = a \langle \Psi, \phi_1 \rangle + b \langle \Psi, \phi_2 \rangle$$

$$\langle \Psi | \Psi \rangle \geqslant 0$$

$$\langle \Psi | \Psi \rangle = 0 \text{ iff } \Psi = 0.$$

$\rightsquigarrow$ HILBERT SPACE

$\Longrightarrow$ (finite / infinite-dimensional).

+ Time-evolution

$$\frac{\partial \Psi}{\partial t} = \hat{O} \Psi \qquad \hat{O}^\dagger = -\hat{O}$$

$\hat{O}$: linear operator

(Prob. conservation)

$$\bar f = \langle \psi, \hat f \psi \rangle$$

$$= \int dq\, \psi(q)^* \hat f \psi(q)$$

$$\frac{d\bar f}{dt} = \left\langle \frac{\partial\psi}{\partial t}, \hat f \psi \right\rangle + \left\langle \psi, \hat f \frac{\partial \psi}{\partial t} \right\rangle$$

$$= \langle \hat O \psi, \hat f \psi \rangle + \langle \psi, \hat f \hat O \psi \rangle$$

$$= \langle \psi, \hat O^\dagger \hat f \psi \rangle + \langle \psi, \hat f \hat O \psi \rangle$$

$$= - \langle \psi, \hat O \hat f \psi \rangle + \langle \psi, \hat f \hat O \psi \rangle$$

$$\therefore \frac{d\bar f}{dt} = \langle \psi, \underbrace{\hat f \hat O - \hat O \hat f}_{[\hat f, \hat O]} \psi \rangle$$

or, $$\frac{d\bar f}{dt} = \overline{[\hat f \;\; \hat O]}$$

Quantization of a classical system

* Classical system is described by a set of coordinates $(q_1, q_2, \cdots q_n)$ and momenta $(p_1, p_2, \cdots, p_n)$ and a Hamiltonian $H(\vec q, \vec p)$.

Equations of motion:

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \quad \& \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}$$

Example

$$H = \frac{p^2}{2m} + V(q)$$

$$\frac{dq}{dt} = \frac{\partial H}{\partial p} = \frac{p}{m} \quad \&$$

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q} = -\frac{\partial V}{\partial q}$$

Given two functions $F(\vec{q}, \vec{p})$ and $\vec{G}(\vec{q}, \vec{p})$, we define,

$$\{F, G\} = \sum_{i=1}^{n} \left[\frac{\partial F}{\partial q_i} \frac{\partial G}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial G}{\partial q_i} \right]$$

Poisson bracket

$$\frac{dF}{dt} = \sum_{i=1}^{n} \left[\frac{\partial F}{\partial q_i} \frac{dq_i}{dt} + \frac{\partial F}{\partial p_i} \frac{dp_i}{dt} \right]$$

$$= \sum_{i=1}^{n} \frac{\partial F}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial H}{\partial q_i}$$

$$= \{F, H\}$$

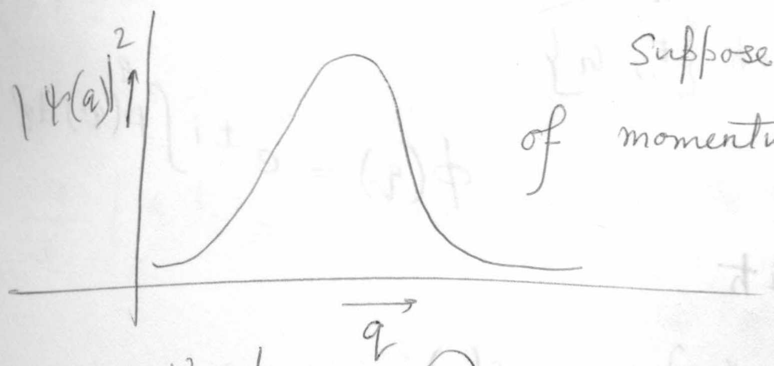
$$\left\{ \begin{aligned} \frac{dq_k}{dt} &= \{q_k, H\} = \frac{\partial H}{\partial p_k} \\ \frac{dp_k}{dt} &= \{p_k, H\} = -\frac{\partial H}{\partial q_k} \end{aligned} \right\}$$ Hamilton's equations

For now, consider the case $\underline{n=1}$.

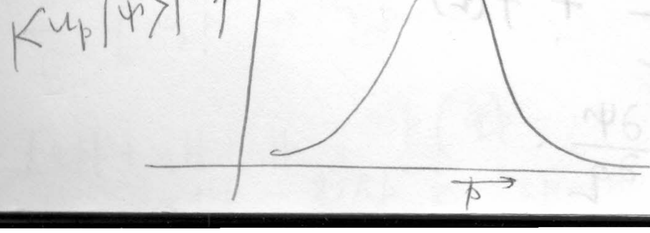
State of a system at a given time is described by (q, p). Classically

In QM, state at " " " is described by a wavefunction $\psi(q)$.

Q. Mech $\Rightarrow$ prob. distr$\underline{^n}$



Suppose, $u_p(q)$ are eigenstates of momentum with eigenvalue p



$\hbar \to$ classical requires wavefunctions with sharply peaked prob. distr$^{\underline{n}}$

We need $\dfrac{d}{dt}\overline{\hat{F}} \simeq \overline{\widehat{\{F, H\}}}$?

connect

$\rightsquigarrow$ required so that averages follow classical equations of motion approximately

$$\frac{d\overline{\hat{F}}}{dt} = \overline{[\hat{F}, \hat{O}]} \quad \text{(actual)}$$

Suppose, we could devise a rule such that

$$\hat{O} \simeq c\hat{H} \qquad [c = \text{constant}]$$

$$[\hat{F}, \hat{G}] \simeq \frac{1}{c}\widehat{\{F, G\}} \quad \text{for all } F, G$$

$$\frac{d\overline{F}}{dt} \simeq \overline{[\hat{F}, c\hat{H}]} = c\,\overline{[\hat{F}, \hat{H}]}$$

$$= \cancel{c}\cdot\frac{1}{\cancel{c}}\overline{\widehat{\{F, H\}}}$$

$$c = \frac{1}{i\hbar}$$

$(\hbar = \text{const.})$

$$\bar{q} = \int \psi^*(q)\, q\, \psi(q)\, dq$$

$$\hat{O} \simeq \frac{1}{i\hbar}\hat{H} \qquad \hat{q}\,\psi(q) = q\,\psi(q)$$

$$[F, G] \simeq i\hbar\widehat{\{F, G\}}$$

$$\{q, p\} = 1 \qquad \phi(q) = e^{\pm i\int^{q} f(q')\,dq'}\,\psi(q)$$

$$[\hat{q}, \hat{p}] \simeq i\hbar$$

Take $\hat{p} = -i\hbar\dfrac{\partial}{\partial q} + f(q)$

$$\hat{p}\,\psi(q) = -i\hbar\frac{\partial\psi}{\partial q}.$$

$$(\hat{q}\hat{p} - \hat{p}\hat{q})\,\psi(q) = i\hbar\,\psi(q)$$

Given any ~~ofe~~ function $F(q,p)$, we define

$$\hat{F} = \left(F(\hat{q},\hat{p})\right)_S \Rightarrow \text{symmetrization}$$

$$F(q,p) = \sum_{m,n} \underbrace{a_{mn}}_{\text{constants}} q^m p^n .$$

Define $\hat{F} = \sum_{m,n} a_{mn} \left(\hat{q}^m \hat{p}^n\right)_S$

$$\left(\hat{A}_1 \quad \hat{A}_n\right)_S \qquad = \sum_{m,n} a_{mn}\, \hat{q}^m \hat{p}^n + O(\hbar)$$

$$= \frac{1}{n!} \left(\hat{A}_1, \ldots \hat{A}_n\right)$$

permutations

$$[\hat{F}, \hat{G}] \cong i\hbar \{F, G\}$$

$$\hat{F}(q,p) = \sum_{m,n} a_{mn} \left(\hat{q}^m \hat{p}^n\right)_S$$

$$= \sum_{m,n} a_{mn}\, \hat{q}^m \hat{p}^n + O(\hbar)$$

$$\boxed{[p, q] \Rightarrow -i\hbar}$$

$$qp - pq = i\hbar$$

$$\frac{1}{(m+n)!}\left[P\left(p^m q^n\right)\right]$$

Let's take $\left(qp^2\right)_S$

$$\frac{1}{6}\left[q p_1 p_2 + q p_2 p_1 + p_1 q p_2 + p_2 q p_1 + p_1 p_2 q + p_2 p_1 q\right]$$

$$= \frac{1}{6}\left[qp^2 + qp^2 + (qp - i\hbar)p + (qp - i\hbar)p + p(qp - i\hbar) + p(qp - i\hbar)\right] = qp^2 - i\hbar p$$

$$= \frac{1}{6}\left[qpp + qpp + qpp + qpp - 2i\hbar p + (qp - i\hbar)p - 2i\hbar p + (qp - i\hbar)p\right]$$

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Classical system $\longleftrightarrow$ What's the corresponding quantum system?

$H(q, p)$ [NO UNIQUE ANSWER]

- We want to have at least one quantum system which goes over to classical limit appropriately.

$[\hat{q}, \hat{p}] = i\hbar$

Prescription $\rightarrow$

$$\hat{q}\,\psi(q) = q\,\psi(q)$$

$$\hat{p}\,\psi(q) = -i\hbar \frac{\partial \psi(q)}{\partial q}$$

$$F(q,p) = \sum_{m,n} a_{mn}\, q^m p^n$$

$q, p \longrightarrow$ no problem (Ehrenfest)

$$\updownarrow$$

$$\hat{F} = \sum_{m,n} a_{mn} \left(\hat{q}^m \hat{p}^n\right)_S$$

$$= \sum_{m,n} a_{mn}\, \hat{q}^m \hat{p}^n + O(\hbar)$$

$$\frac{d\overline{\hat{F}}}{dt} = \frac{1}{i\hbar} \overline{[\hat{F}, \hat{H}]}$$

We want, for correct classical reduction, is

$$\frac{d\overline{\hat{F}}}{dt} \cong \overline{\widehat{\{F, H\}}}$$

(we can't expect it to be exact)

$$\frac{dF}{dt} = \{F, H\}$$

Classical

Suppose, we could prove, that

$$[\hat{F}, \hat{G}] = i\hbar\, \widehat{\{F, G\}} + O(\hbar^2)$$

for ~~all~~ any F, G

Then

$$\frac{d\overline{\hat{F}}}{dt} = \frac{1}{i\hbar} \overline{[\hat{F}, \hat{H}]}$$

$$= \frac{1}{i\hbar}\left[i\hbar\, \overline{\widehat{\{F, H\}}} + O(\hbar^2)\right]$$

$$\frac{d\overline{\hat{F}}}{dt} = \frac{1}{i\hbar} \overline{[\hat{F}, \hat{H}]}$$

$$= \widehat{\{F, H\}} + O(\hbar).$$

① $[\hat{F}, \hat{G}] = i\hbar\, \widehat{\{F, G\}} + O(\hbar^2)$ (Has to be proved)

② Small $\hbar$ (needed)

same

$\left\{ O(\hbar) \text{ are not detectable by the apparatus in classical Limit} \right\}$

$\rightsquigarrow$ Distribution of $|\psi(q)|^2$ or $|\langle \psi_p | \psi \rangle|^2$ should be sharp

$$\hat{F} = \sum_{m,n} a_{mn} \left(\hat{q}^m \hat{p}^n\right)_s = \sum_{m,n} a_{mn} \hat{q}^m \hat{p}^n + O(\hbar).$$

$$\hat{G} = \sum_{k,l} b_{kl} \left(q^k p^l\right)_s$$

$$= \sum_{k,l} b_{kl} \left(\hat{q}^k \hat{p}^l\right) + O(\hbar)$$

Choose $F = q^m p^n$, $G = q^k p^l$

$$\text{rhs} = i\hbar\, \widehat{\{F, G\}} + O(\hbar^2)$$

$$= i\hbar\, (ml - nk)\, \hat{q}^{k+m-1} \hat{p}^{n+l-1} + O(\hbar^2)$$

[Symmetrization leftovers become $O(\hbar^2)$].

lhs $[\hat{F}, \hat{G}] = [\hat{q}^m \hat{p}^n, \hat{q}^k \hat{p}^l] + O(\hbar^2)$

Use $[A, BC] = [A, B]\, C + B\, [A, C]$

$$[A, B_1 B_2 \cdots B_n]$$

$$= [A, B_1]\, B_2 \cdots B_n + B_1 [A, B_2] B_3 \cdots B_n$$

$$+ B_1 B_2 [A, B_3] B_4 \cdots B_n + \cdots$$

$$+ B_1 B_2 \cdots B_{n-1} [A, B_n]$$

$$[\hat{q}^m \hat{p}^n, \hat{q}^k \hat{p}^l] = [\hat{q}^m \hat{p}^n, \hat{q}^k]\hat{p}^l + \hat{q}^k [\hat{q}^m \hat{p}^n, \hat{p}^l]$$

$$= \left(\hat{q}^m [\hat{p}^n, \hat{q}^k] + \cancel{[\hat{q}^m, \hat{q}^k]} \hat{p}^n\right)\hat{p}^l$$

$$+ \hat{q}^k \left(\hat{q}^m \cancel{[\hat{p}^n, \hat{p}^l]} + [\hat{q}^m, \hat{p}^l]\hat{p}^n\right)$$

$$= \hat{q}^m \Big(\underbrace{[\hat{p}^n, \hat{q}]\hat{q}^{k-1} + \hat{q}[\hat{p}^n, \hat{q}]\hat{q}^{k-2} + \hat{q}^2[\hat{p}^n, \hat{q}]\hat{q}^{k-3} + \cdots + \hat{q}^{k-1}[\hat{p}^n, \hat{q}]}_{k \text{ terms}}\Big)\hat{p}^l$$

$$+ \hat{q}^k \Big(\underbrace{[\hat{q}, \hat{p}^l]\hat{q}^{m-1} + \hat{q}[\hat{q}, \hat{p}^l]\hat{q}^{m-2} + \cdots + \hat{q}^{m-1}[\hat{q}, \hat{p}^l]}_{m \text{ terms}}\Big)\hat{p}^n$$

$$[\hat{p}^n, \hat{q}] = [\hat{p}, \hat{q}]\hat{p}^{n-1} + \hat{p}[\hat{p}, \hat{q}]\hat{p}^{n-2} + \cdots + \hat{p}^{n-1}[\hat{p}, \hat{q}]$$

$$= -i\hbar n \hat{p}^{n-1}$$

$$\therefore \text{LHS} = \hat{q}^m(-i\hbar n)\hat{q}^{k-1}\hat{p}^{n-1}\, k\, \hat{p}^l + \hat{q}^k \quad + O(\hbar^2)$$

$$+ \hat{q}^k \hat{q}^{m-1}\hat{p}^{l-1}\, m\, \hat{p}^n (i\hbar l) + O(\hbar^2)$$

$$= i\hbar(ml - nk)\hat{q}^{k+m-1}\hat{p}^{l+n-1} + O(\hbar^2)$$

On a classical state $\bar{F} = F(\bar{q}, \bar{p}) \cong \sum_{m,n} a_{mn} \bar{q}^m \bar{p}^n$.

We except

Uncertainty principle

Take a state ψ

$$\bar{q} = \langle \psi, \hat{q}\psi \rangle, \quad \bar{p} = \langle \psi, \hat{p}\psi \rangle$$

Standard deviations

$$\left[\begin{array}{l}(\Delta q)^2 = \langle \psi, (\hat{q}-\bar{q})^2 \psi \rangle , \\ (\Delta p)^2 = \langle \psi, (\hat{p}-\bar{p})^2 \psi \rangle \end{array}\right] \begin{array}{l} = \langle \psi, \hat{\mathcal{Q}}^2 \psi \rangle \\ = \langle \psi, \hat{P}^2 \psi \rangle \end{array}$$

How small can we make Δq and Δp?

Define $\hat{\mathcal{Q}} = \hat{q} - \bar{q}$, $\hat{P} = \hat{p} - \bar{p}$

$[\hat{\mathcal{Q}}, \hat{P}] = i\hbar$ Define $\phi = (\alpha \hat{\mathcal{Q}} - i\hat{P})\psi$

α = constant (real)

$$\langle \phi, \phi \rangle \geqslant 0$$

$$\Rightarrow \langle (\alpha \hat{\mathcal{Q}} - i\hat{P})\psi , (\alpha\hat{\mathcal{Q}} - i\hat{P})\psi \rangle \geqslant 0 .$$

$$\Rightarrow \langle \psi, (\alpha\hat{\mathcal{Q}} + i\hat{P})(\alpha\hat{\mathcal{Q}} - i\hat{P})\psi \rangle \geqslant 0$$

$$\alpha^2 \hat{\mathcal{Q}}^2 + \hat{P}^2 - i\alpha[\hat{\mathcal{Q}}, \hat{P}]$$

$$= \alpha^2 \hat{\mathcal{Q}}^2 + \hat{P}^2 + \hbar\alpha$$

So, $\langle \psi, (\alpha^2\hat{\mathcal{Q}}^2 + \hat{P}^2 + \hbar\alpha)\psi \rangle \geqslant 0$.

or, $\underbrace{\alpha^2(\Delta q)^2 + (\Delta p)^2 + \hbar\alpha}_{y} \geqslant 0$. (True for all α)

$[\because \langle \psi | \psi \rangle = 1 .]$

Minimize $\quad 2\alpha(\Delta q)^2 + \hbar = 0$

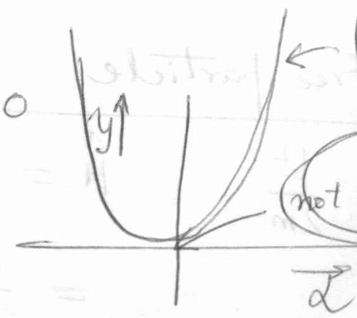
$$\therefore \boxed{\alpha = -\frac{\hbar}{2(\Delta q)^2}}$$

Minimum value

$$\frac{\hbar^2}{4(\Delta q)^4}(\Delta q)^2 + (\Delta p)^2 - \frac{\hbar^2}{2(\Delta q)^2} \geqslant 0$$

$$\Rightarrow (\Delta p)^2 - \frac{\hbar^2}{4(\Delta q)^2} \geqslant 0$$

$$\therefore \Delta p \, \Delta q \geqslant \frac{\hbar}{2}$$



(should not have real roots)

not hitting $y = 0$

Gaussian $\quad \mathcal{N} e^{-\frac{(q-q_0)^2}{2\beta}}$

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$$[\hat{q}', \hat{p}'] = i\hbar + O(\hbar^2)$$

Canonical Transformation

preserve $\{\ \}$ ✓

Heisenberg picture

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$$

Solution $\psi(t) = \exp\left(-\frac{i}{\hbar}\hat{H}t\right)\psi(t=0)$

$$\sum_{n=0}^{\infty} \frac{1}{n!}\left(-\frac{it}{\hbar}\hat{H}\right)^n$$

$$\bar{F}(t) = \langle \psi(t), \hat{F}\psi(t)\rangle$$

$$= \langle e^{-\frac{i}{\hbar}\hat{H}t}\psi(0), \hat{F}e^{-\frac{i}{\hbar}\hat{H}t}\psi(0)\rangle$$

$$= \langle \psi(0), e^{\frac{i}{\hbar}\hat{H}t}\hat{F}e^{-\frac{i}{\hbar}\hat{H}t}\psi(0)\rangle$$

$\hat{F}_H(t)$

$= e^{\frac{i}{\hbar}\hat{H}t}\hat{F}e^{-\frac{i}{\hbar}\hat{H}t}$ $\quad$ [Heisenberg representation of $\hat{F}$]

Define $\psi_H(t) = \psi(0)$. $\qquad \hat{F}(t) = \langle \psi_H | \hat{F}_H(t)\psi_H\rangle$

$$\frac{d\hat{F}_H(t)}{dt} = \frac{i}{\hbar}\hat{H}\hat{F}_H - \frac{i}{\hbar}\hat{F}_H\hat{H}$$

$$= \frac{i}{\hbar}[\hat{H}, \hat{F}_H]$$

Free particle

$$H(q,p) = \frac{p^2}{2m} \qquad \hat{H} = \frac{\hat{p}^2}{2m}$$

$$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2}$$

Eigenstates of $\hat{H}$

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial q^2} = E\psi$$

Solution

$$\psi = u_p(q) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipq}{\hbar}}$$

p = constant

$$\hat{H} u_p(q) = \frac{p^2}{2m} u_p(q).$$

$$\int u_p^*(q) u_{p'}(q)\, dq = \delta(p-p')$$

(Delta normalisation)

$$\hat{p}\, u_p(q) = p\, u_p(q)$$

$$\hat{p} = -i\hbar \frac{\partial}{\partial q}$$

Consider the state $\psi(q) = N \int dp'\, e^{-\frac{\alpha}{2}(p'-p_0)^2 - \frac{iap'}{\hbar}}\, u_{p'}(q)$

$p_0, \alpha, N, a \longrightarrow$ constants

Probability of finding the particles between p and $(p+\delta p)$

$$= \delta p\, N^2 e^{-\alpha(p-p_0)^2}$$

Ex : $\rightarrow$ Calculate $\Delta p = \sqrt{\overline{(p-p_0)^2}}$

Ex : $\rightarrow$ Calculate N

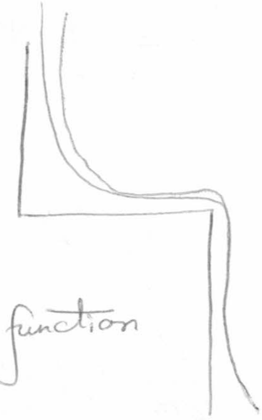
Ex : $\rightarrow$ Show that $\psi(q) = \frac{N}{\sqrt{\alpha\hbar}}\, e^{-\frac{(q-a)^2}{2\alpha\hbar^2} + \frac{i}{\hbar}p_0(q-a)}$

$\bar{q} = a$ Ex. : $\rightarrow$ Calculate Δq and

$(\Delta q)^2 = \;?$ verify $\Delta q\, \Delta p = \frac{\hbar}{2}$

$$\psi(q,t) = N\int dp'\, e^{-\frac{\alpha}{2}(p'-p_0)^2 - \frac{iap'}{\hbar}}\, u_{p'}(q) \times e^{-\frac{ip'^2}{2m}\frac{t}{\hbar}}$$

Ex: Calculate $\bar{p}(t)$, $\bar{q}(t)$, $\Delta p(t)$, $\Delta q(t)$.



$$\bar{p}(t) = p_0$$

$$\bar{q}(t) = a + \frac{p_0}{m} t$$

$$\Delta p(t) = \Delta p(0)$$

$$\Delta q(t) = \; ?$$ (increasing function of t)

Ex:- $m = 1$ gram   Calculate (Δp)

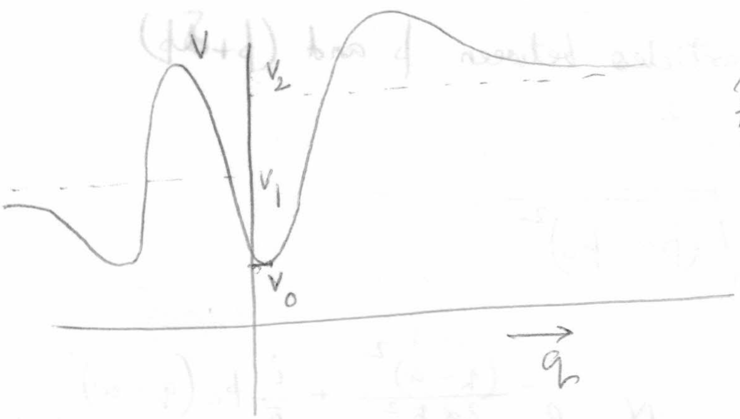
$\Delta q = 0.01$ cm

Calculate Δq after 1 hour

$p_0 = 0, \quad a = 0 \quad (\checkmark)$

One-dimensional particle in a potential

$$H(q, p) = \frac{p^2}{2m} + V(q)$$



$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + V(q)$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial q^2} + V(q)\psi = E\psi$$

$$\frac{\partial^2 \psi}{\partial q^2} = +\frac{2m}{\hbar^2}\left(V(q) - E\right)\psi$$

Asymptotic behaviour

$$\kappa_2 = \sqrt{\frac{2m}{\hbar^2}(V_2 - E)}$$

$$\kappa_1 = \sqrt{\frac{2m}{\hbar^2}(V_1 - E)}$$

$q \longrightarrow \infty$

$$\psi = a\underbrace{e^{\kappa_2 q}}_{f_1} + b\underbrace{e^{-\kappa_2 q}}_{f_2}$$

$$\psi = c e^{\kappa_1 q} + d e^{-\kappa_1 q} \quad \text{for } q \longrightarrow -\infty$$

$f_1(q)$:- The solution that goes to $e^{\kappa_2 q}$ as $q \longrightarrow \infty$. $(a = 1, \; b = 0)$

$f_2(q)$:- The solution for which $a = 0$, $b = 1$.

(goes to $e^{-k_2 q}$ as $q \to \infty$.)

$g_1(q)$:- The solution for which $c = 0$, $d = 1$

$g_2(q)$: " " " " $c = 1$, $d = 0$.

Define coefficients A, B, C, D via :

$$f_2(q) = A(E)\, g_1(q) + B(E)\, g_2(q)$$

$$g_2(q) = C(E)\, f_1(q) + D(E)\, f_2(q)$$

[(f_1, f_2) & (g_1, g_2) are linearly independent]

Define $r(E) = \dfrac{B(E)}{A(E)}$, $t(E) = \dfrac{1}{A(E)}$.

$\downarrow$ reflection $\qquad \downarrow$ transmission

Case- I

$E < V_1, V_2$

κ_1, κ_2 are real and > 0.

$f_2 \to$ ✓ $\quad g_2 \to$ ✓ $\qquad A \longrightarrow 0$.

Need to keep $f_2(q)$ (from $q \to \infty$ study)

" " " $g_2(q)$ (from $q \to -\infty$ ")

$A(E) = 0. \Rightarrow$ discrete set of solutions

$[E_0, E_1, E_2, \dots]$

$r(E)$ and $t(E)$ go to infinity.

$\longrightarrow$ These states are bound states

Case – II

$V_1 < E < V_2$

$$\kappa_1 = \sqrt{2m(V_1 - E)}\,/\hbar = i k_1, \quad k_1 = \sqrt{\frac{2m(E - V_1)}{\hbar^2}}$$

Pick f_2 ($q \to \infty$ side)

$$f_2(q) \longrightarrow e^{-\kappa_2 q} \quad \text{as} \quad q \to \infty$$

$$q \to -\infty$$

$$\begin{aligned} f_2 &= A(E)\, g_1 + B(E)\, g_2 \\ &= A(E)\, e^{-ik_1 q} + B(E)\, e^{+ik_1 q} \qquad q \to -\infty \end{aligned}$$

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Define A, B, C, D through

$$\left\{ \begin{aligned} f_2(q) &= A(E)\, g_1(q) + B(E)\, g_2(q) \\ g_2(q) &= C(E)\, f_1(q) + D(E)\, f_2(q) \end{aligned} \right\} \qquad \boxed{\begin{aligned} r(E) &= \frac{B(E)}{A(E)} \\ t(E) &= \frac{1}{A(E)} \end{aligned}}$$

Case-I

$E < V_1, V_2$ (κ_1 & κ_2 are real and > 0)

$q \to \infty \implies$ we must pick $f_2(q)$

$q \to -\infty \implies$ we " " $g_2(q)$

$\implies A(E) = 0$

or, (a) E takes discrete values

(b) $\psi(q)$ goes to zero as $q \to \pm\infty$. (bound state)

(c) $r(E)$ and $t(E)$ go to infinity for the discrete E's

Case-II

$V_1 < E < V_2$

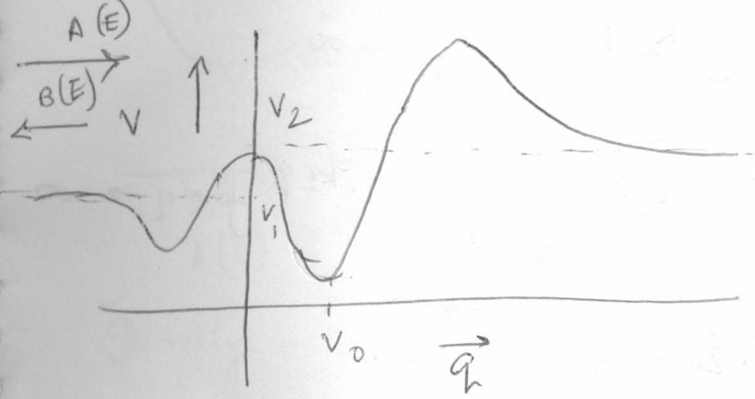
$$\kappa_1 = \sqrt{\frac{2m(V_1 - E)}{\hbar^2}} \quad \text{is imaginary.}$$

Take $\kappa_1 = -ik_1$ $\kappa_2 > 0$

$$k_1 = \sqrt{\frac{2m(E - V_1)}{\hbar^2}}$$

Pick f_2 : $\psi(q) \to 0$ as $q \to \infty$

$\to \quad A(E)\, e^{ik_1 q} + B(E)\, e^{-ik_1 q}$ for $q \to -\infty$.



Reflection coefficient

$$\boxed{r(E) = \frac{B(E)}{A(E)}}$$

($f_2 = g_1$ for no potential)

Case – III

$E > V_1, V_2$

$\kappa_1 = -ik_1$

$\kappa_2 = -ik_2$

$$\boxed{\begin{aligned} k_1 &= \sqrt{\frac{2m(E-V_1)}{\hbar^2}} \\ k_2 &= \sqrt{\frac{2m(E-V_2)}{\hbar^2}} \end{aligned}}$$

$\boxed{\text{Let's pick } f_2 \text{ and } g_2.}$

(We are free to choose among f_1, f_2, g_1, g_2)

(a) $e^{ik_2 q}$ as $q \to \infty$ (Transmitted wave)

$A(E)\, e^{ik_1 q} + B(E)\, e^{-ik_1 q}$ as $q \to -\infty$

incident   reflected

$r(E) = \dfrac{B(E)}{A(E)}$; $t(E) = \dfrac{1}{A(E)}$

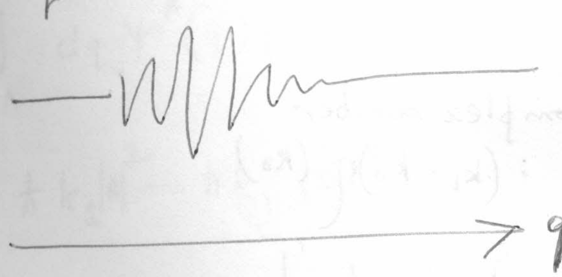
(b) Pick g_2

As $q \to -\infty$, $e^{-ik_1 q}$

As $q \to \infty$ $C(E)\, e^{-ik_2 q} + D(E)\, e^{-ik_2 q}$

← C(E)

→ D(E)



$$\boxed{\begin{aligned} \tilde{r}(E) &= \frac{D(E)}{C(E)} \\ \tilde{t}(E) &= \frac{1}{C(E)} \end{aligned}}$$

Pick the solution

$$\phi(q,E) = \frac{f_2(q,E)}{A(E)} \frac{1}{\sqrt{2\pi\hbar}}$$

$$\begin{cases} = \dfrac{1}{A(E)} \dfrac{1}{\sqrt{2\pi\hbar}} e^{ik_2 q} & \text{as } q \to \infty \\ = \dfrac{1}{\sqrt{2\pi\hbar}} e^{ik_1 q} + \dfrac{B(E)}{A(E)} \dfrac{1}{\sqrt{2\pi\hbar}} e^{-ik_1 q} & \text{for } q \to -\infty \end{cases}$$

as $q \to \infty$.

$$N \int dk_1 \, e^{-\frac{\alpha}{2}(k_1-k_0)^2\hbar^2 - ia(k_1-k_0)} \phi(q,E)$$

$$\phi(q,E) = \frac{1}{\sqrt{2\pi\hbar}} e^{ik_1 q} + \frac{B(E)}{A(E)} \frac{1}{\sqrt{2\pi\hbar}} e^{-ik_1 q}$$

{ Gaussian with peak at a & velocity $\frac{\hbar k_0}{m}$ } [describes a Gaussian with peak at $-a$ & velocity $-\frac{\hbar k_0}{m}$ and amplitude $\frac{B}{A}$]

Take $a = -\Lambda$ (Λ large and $\Lambda > 0$.)

$$k_1 = \sqrt{\frac{2m(E-V_1)}{\hbar^2}} \qquad E = V_1 + \frac{\hbar^2 k_1^2}{2m}.$$

(Assuming B/A is independent of E)

Take $q \to \infty$ sol$^{\underline{n}}$ $\longrightarrow$ not valid again

$$N \int dk_1 \, e^{-\frac{\alpha}{2}(k_1-k_0)^2\hbar^2 - ia(k_1-k_0)} \times \phi(q,E) \times e^{-i\left(\frac{\hbar^2 k_1^2}{2m} + V_1\right) t/\hbar}$$

$$\frac{1}{A(E)} = e^{i\eta(k_1)}$$

$\eta(k_1) \to$ Complex number

$$= e^{i\eta(k_0) + i(k_1-k_0)\eta'(k_0)}$$

effect $\to -i(a - \eta'(k_0))(k_1-k_0)$

$$= -i(a - \mathrm{Re}(\eta'(k_0)) - \mathrm{Im}(\eta'(k_0)))(k_1-k_0)$$