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A The Ehrenfest Relations

Ok, we have seen that Schrödinger Eq reduces to Hamilton-Jacobi Eq at the limit $\hbar \Rightarrow 0$, How about $\vec{F} = m\vec{a}$?

① Well HJE ~ F = ma

② Let's work in the Heisenberg picture. ~~and~~ out the EOM

$$\dot{\hat{X}}_H = -\frac{i}{\hbar}[\hat{X}_H, \hat{H}], \quad \dot{\hat{P}}_H = -\frac{i}{\hbar}[\hat{P}_H, \hat{H}]$$

from the HW problem, we know

$$[x_i, f(p)] = i\hbar \frac{\partial f}{\partial p_i} \text{ and } [p_i, g(x)] = -i\hbar \frac{\partial g}{\partial x_i}$$

therefore

$$\dot{X}_H = -\frac{i}{\hbar}\left[\hat{X}_H, \frac{P_H^2}{2m}\right] = \frac{P_H}{m}$$

$$\dot{P}_H = -\frac{i}{\hbar}[P_H, V(\hat{x}_H, t)] = -\nabla_x V(x,t).$$

Now, we check the expectation values of the above

$$\langle \underbrace{\psi_H}_{\text{time-independent}} | \frac{d\hat{X}_H}{dt} | \psi_H \rangle = \frac{d}{dt}\langle \psi_H | \hat{X}_H(t) | \psi_H \rangle = \frac{d}{dt}\langle \psi_s(t) | \hat{X}_s | \psi_s(t) \rangle$$

$$= \langle \psi_H | \frac{\hat{P}_H(t)}{m} | \psi_H \rangle = \frac{1}{m}\langle \psi_s(t) | \hat{P}_s | \psi_s(t) \rangle$$

* this relation is exact !

$$\Rightarrow \frac{d\langle \vec{x} \rangle}{dt} = \frac{1}{m}\langle \vec{P} \rangle \longrightarrow m\frac{d^2}{dt^2}\langle \vec{x} \rangle = -\langle \vec{\nabla} V(x,t) \rangle$$

and

$$\langle \psi_H | \frac{d\vec{P}_H}{dt} | \psi_H \rangle = \cancel{\frac{d}{dt}} \langle \psi_H | -\vec{\nabla}_x V(x,t) | \psi_H \rangle = -\langle \vec{\nabla} V(x,t) \rangle$$

$$= \frac{d}{dt}\langle \psi_H | \vec{P}_H(t) | \psi_H \rangle = \frac{d}{dt}\langle \psi_s(t) | \vec{P}_s | \psi_s(t) \rangle = \frac{d}{dt}\langle P \rangle =$$

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☆ However, these eqs do not say that the expectation value of $\vec{x}$ follows the classical motion!!

It will be, if ~~instead~~

$$m\frac{d^2}{dt^2}\langle \vec{x}\rangle = -\nabla V(\langle x\rangle, t) \quad \text{instead.}$$

☆ On the other hand, if the WF $\psi(x,t)$ is located about $\vec{x}_0 = \langle \vec{x}\rangle$. suppose it is a wave packet. And we consider a function, $f(x,t)$ which is slowly varying on the scale ~ width of ψ.

⇒ (suppress the t dependence ~)

$$\langle f(x)\rangle = \int d^3\vec{x}\, |\psi(x)|^2 f(x)$$

$$\simeq \int d^3\vec{x}\, |\psi(\vec{x})|^2 \Big[f(\vec{x}_0) + \underbrace{(\vec{x}-\vec{x}_0)\cdot \vec{\nabla} f(x_0)}_{\text{vanishes after integration}} + \cdots \Big]$$

$$\simeq f(\vec{x}_0) = f(\langle x\rangle) \qquad \text{a "const" vector}$$

⇒ take $f(x) = -\vec{\nabla} V$

⇒ In this case, the $\langle x\rangle$ of a wave packet moving in a slowly varying potential approximately follows the classical trajectory.

☆ width of the wave packet spread as time goes by — when $\Delta \sim L$ of $V(x)$ ⇒ no longer classical like –

☆ In the special case, $f(x) = ax+b$

⇒ no higher order correction. $\langle f(x)\rangle \overset{\text{exact}}{=} f(\langle x\rangle)$,

identify linear $f(x) = -\nabla V(x)$ ⇒ $V \sim x^2 + x + x^0$ ~~$\sim (x-x_0)^2 + c$~~

⇒ free particle, particle in uniform $\vec{E}$ or gravitational field
SHO, ...

☆ In fact, when $\hat{H}(f(x^2), g(p^2))$ ⇒ follow the classical motion

☆ The Ehrenfest relation ~ one way to understand QM → CM

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☆ WKB later

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* Particle in E&M background

Classical

$$\vec{E} = -\vec{\nabla}\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t} \qquad \phi : \text{scalar potential}$$

$$\vec{B} = \nabla \times \vec{A} \qquad \vec{A} : \text{vector potential}$$

& $m\vec{a} = q\left(\vec{E} + \frac{1}{c}\vec{V}\times\vec{B}\right)$

$\vec{V} = \dot{\vec{x}}$, $\vec{a} = \ddot{\vec{x}}$

In classical E&M, the Hamiltonian is

$$H = \frac{1}{2m}\Big(\underbrace{\vec{P}}_{\text{canonical momentum}} - \frac{q}{c}\vec{A}\Big)^2 + q\phi$$

$$\vec{P} = m\vec{V} + \frac{q}{c}\vec{A} \neq \vec{P}_{kinetic} = m\vec{V}$$

Q: How about in QM ?

* $x, p \to \hat{x}, \hat{p}$: quantization of the classical Hamiltonian

$-i\hbar\vec{\nabla}$: generates translation
$\rightsquigarrow$ canonical momentum
(not the kinetic momentum)

* But $\vec{P}\cdot\vec{A} = \vec{A}\cdot\vec{P}$ in CM,
$\neq$ in QM. what do we do ?

* By guessing :

$$\frac{1}{2m}\left[\vec{P} - \frac{q}{c}\vec{A}\right]^2_{cm} \to \frac{1}{2m}\left[\hat{\vec{P}} - \frac{q}{c}\vec{A}(x,t)\right]\cdot\left(\hat{\vec{P}} - \frac{q}{c}\vec{A}(x,t)\right]$$

$$= \frac{1}{2m}\hat{\vec{P}}^2 - \frac{q}{2mc}\left(\hat{P}\cdot\hat{A} + \hat{A}\cdot\hat{P}\right) + \frac{q^2}{2mc^2}\hat{A}^2$$

Such that $\hat{H}$ is Hermitian ($\hat{H} = \hat{H}^+$)

* Stress again : $\frac{1}{2m}\vec{P}^2$ is NOT the kinetic energy !!
The whole expression is.

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* In the configuration representation.

$$\frac{1}{2m}\left[-i\hbar\vec{\nabla}-\frac{q}{c}\vec{A}(x,t)\right]\cdot\left[-i\hbar\vec{\nabla}-\frac{q}{c}\vec{A}(x,t)\right]\psi(x,t)$$
$$+q\phi(x,t)\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)$$

* If $\vec{A}(x,t)=\vec{A}(x)$, $\phi(x,t)=\phi(x)$

we have the time independent Schrödinger eq.

$$\frac{1}{2m}\left[-i\hbar\vec{\nabla}-\frac{q}{c}\vec{A}(x)\right]^2\psi(x)+q\phi(x)\psi(x) = E\psi(x)$$

with ~~eigen~~ energy eigenfunction $\psi(x)$ and eigenvalue E.

* It has a conserved probability current $\vec{J}$

but now $\vec{V}=\frac{1}{m}\left(\vec{P}-\frac{q}{c}\vec{A}(x,t)\right)=\frac{1}{m}\left(-i\hbar\vec{\nabla}-\frac{q}{c}\vec{A}(x,t)\right)$

you shall check that $\rho=|\psi|^2$ and $\vec{J}$ satisfy the continuity eq.

Gauge transformation in QM

* In Classical EDM, ϕ and $\vec{A}$ are not unique.

$\phi'=\phi-\frac{1}{c}\frac{\partial f}{\partial t}$, $\vec{A}'=\vec{A}+\vec{\nabla}f$ $\Rightarrow$ leaves $\vec{E}$ and $\vec{B}$ invariant.

$\Rightarrow$ no physical consequence $\because$ $m\vec{a}=q(\vec{E}+\frac{1}{c}\vec{v}\times\vec{B})$

* What happens in QM?

$\psi \rightarrow e^{\frac{iqf}{\hbar c}}\psi$ need to do a phase rotation to the WF!!

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such that

$$\overbrace{\hat{p}}^{-i\hbar\vec{\nabla}}\!\!-\ldots \qquad (\hat{p} - \frac{q}{c}\hat{A})\psi = \Big(\hat{p} - \frac{q}{c}(\hat{A}' - \vec{\nabla} f)\Big) e^{-\frac{iqf}{\hbar c}}\psi'$$

$$= e^{-\frac{iqf}{\hbar c}}\Big(\hat{p} - \cancel{\frac{q}{c}\vec{\nabla} f} - \frac{q}{c}\hat{A}' + \cancel{\frac{q}{c}\vec{\nabla} f}\Big)\psi'$$

$$= e^{-\frac{iqf}{\hbar c}}\Big[\hat{p} - \frac{q}{c}\hat{A}'\Big]\psi'$$

so

$$\frac{1}{2m}(\hat{p} - \frac{q}{c}\hat{A})^2\psi = e^{-\frac{iqf}{\hbar c}}\Big[\hat{p} - \frac{q}{c}\hat{A}'\Big]^2\psi'$$

Similarly

$$\Big(i\hbar\frac{\partial}{\partial t} - q\phi\Big)\psi = \Big(i\hbar\frac{\partial}{\partial t} - q\big(\phi' + \frac{1}{c}\frac{\partial f}{\partial t}\big)\Big) e^{-\frac{iqf}{\hbar c}}\psi'$$

$$= e^{-\frac{iqf}{\hbar c}}\Big[i\hbar\frac{\partial}{\partial t} + \cancel{\frac{q}{c}\frac{\partial f}{\partial t}} - q\phi' - \cancel{\frac{q}{c}\frac{\partial f}{\partial t}}\Big]\psi'$$

$$= e^{-\frac{iqf}{\hbar c}}\Big[i\hbar\frac{\partial}{\partial t} - q\phi'\Big]\psi'$$

$$\Rightarrow \boxed{\frac{1}{2m}\Big(-i\hbar\vec{\nabla} - \frac{q}{c}\vec{A}'\Big)^2\psi' + q\phi'\psi' = i\hbar\frac{\partial\psi'}{\partial t}}$$

The schrödinger eq is invariant under gauge transformation

Actually, in HEP we do it the reversed way. (symmetry dictate!)
cf. 杨振宁

We require that the Schrödinger eq to be invariant under a local phase transformation.

$$\psi \to e^{\frac{iqf(x,t)}{\hbar c}}\psi$$

$$\frac{1}{2m}(-i\hbar\vec{\nabla})^2\psi = i\hbar\frac{\partial\psi}{\partial t}$$

$$i\hbar\frac{\partial}{\partial t}\Big(e^{\frac{iqf}{\hbar c}}\psi\Big) = e^{\frac{iqf}{\hbar c}}\Big(-\frac{q}{c}\frac{\partial f}{\partial t} + i\hbar\frac{\partial}{\partial t}\psi\Big)$$

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$$(-i\hbar\vec{\nabla})\,\phi\left(e^{\frac{iqf}{\hbar c}}\psi\right)$$
$$= e^{\frac{iqf}{\hbar c}}\left[\frac{q}{c}\vec{\nabla}f - i\hbar\vec{\nabla}\psi\right]$$

Since f arbitrary, the original form has no hope to hold, unless one introduces extra degree of freedom.

$i\hbar\frac{\partial}{\partial t} \longrightarrow i\hbar\frac{\partial}{\partial t} - \frac{q}{c}\phi$, use ϕ to cancell the $-\frac{q}{c}\frac{\partial f}{\partial t}$

$-i\hbar\vec{\nabla} \longrightarrow -i\hbar\vec{\nabla} - \frac{q}{c}\vec{A}$ and use $\vec{A}$ to cancell the $\frac{q}{c}\vec{\nabla}f$

a vector operator

$\Rightarrow$ need the gauge field, the photon!

---

unlike the classical field, we are only able to measure $|\psi|^2$ but it's phase can't be measured unless one choose a certain gauge convention! In a sentence, the absolute phase has **NO physical meaning**. But the phase difference is physical.

$\circledast$ Some things about the time-independent Schrödinger Eq for potential motion in 1-D. $\left(\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x)\right)$

(A) Degeneracies in 1-D

say, ψ & ϕ are two solution to S with the same E

$\phi\left(\frac{-\hbar^2}{2m}\psi'' + V\psi = E\psi\right)$
$\psi\left(\frac{-\hbar^2}{2m}\phi'' + V\phi = E\phi\right)$ $\Rightarrow$ $\phi\psi'' - \psi\phi'' = 0 = \frac{d}{dx}W$

$W = \phi\psi' - \psi\phi' = \begin{vmatrix}\phi & \psi \\ \phi' & \psi'\end{vmatrix}$ (Wronskian)

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$\Rightarrow$ $\boxed{W \text{ is independent of } x}$

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Suppose that both ψ and ϕ vanish at some point, (say $\pm\infty$) $\Rightarrow$ $W=0$ Everywhere !!

$$\Rightarrow \quad \frac{\psi'}{\psi} = \frac{\phi'}{\phi} \quad \text{or} \quad \psi = c\phi \qquad c \text{ is a const}$$

$\Rightarrow$ There is no degeneracy. It's true for any bound state

However, if $V(x) \to 0$ when $x \to \pm\infty$,

$E > 0$ eigenfunction $\neq 0$, $\Rightarrow$ degeneracy is possible. (2-fold)

e.g. free particle $e^{\pm ikx}$ $\Rightarrow E = \frac{\hbar^2 k^2}{2m}$

Ⓑ Reality of energy eigenfunction

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x), \qquad \psi^*(x) \text{ is also a solution}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi^*}{dx^2} + V(x)\psi^*(x) = E\psi^*(x)$$

If the energy E is nondegenerate, $\psi = c\psi^*$

and $|\psi|^2 = |c|^2|\psi^*|^2 \Rightarrow c = e^{i\alpha}$

$\Rightarrow \psi = e^{i\alpha}\psi^*$, define $\phi = e^{-\frac{i\alpha}{2}}\psi$

$\Rightarrow \phi = \phi^* \Rightarrow \phi$ is real !!

$\Rightarrow$ Any nondegenerate energy eigenfunction in 1-D can be chosen to be real

* for the denerate ones, linear combinations can be made real.

e.g. $e^{\pm ikx} \Rightarrow \cos kx$ and $\sin kx$

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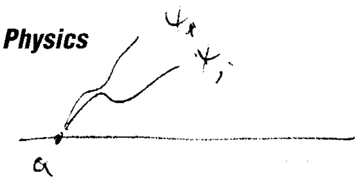


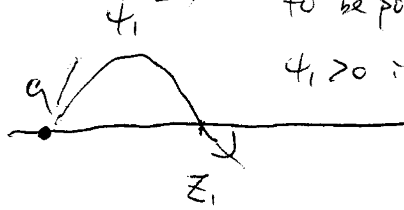
☆ Interleaving of the nodes

$$-\psi_2 \,(-\psi_1'' + \hat{V}\psi_1 = \hat{E}_1 \psi_1)$$
$$+\psi_1 \,(-\psi_2'' + \hat{V}\psi_2 = \hat{E}_2 \psi_2)$$

$\hat{V}$: real ~~bounded from~~

and assume $\hat{E}_2 > \hat{E}_1$

$$\underbrace{(\psi_2\psi_1'' - \psi_1\psi_2'')}_{\displaystyle \frac{d}{dx}(\psi_2\psi_1' - \psi_1\psi_2')} = (\hat{E}_2 - \hat{E}_1)\,\psi_2\psi_1$$



$\psi_1 \to$ can be choosen to be positive

$\psi_1 > 0$ in $[a, z_1]$

z_1: $\uparrow$ first node of ψ_1

$$\int_a^{z_1} dx \;\frac{d}{dx}(\psi_2\psi_1' - \psi_1\psi_2') = (\hat{E}_2 - \hat{E}_1)\int_a^{z_1} \psi_2\psi_1 \, dx$$

$$\Rightarrow (\psi_2\psi_1' - \psi_1\psi_2')\Big|_{z_1} = (\hat{E}_2 - \hat{E}_1)\int_a^{z_1} \psi_2\psi_1 \, dx$$

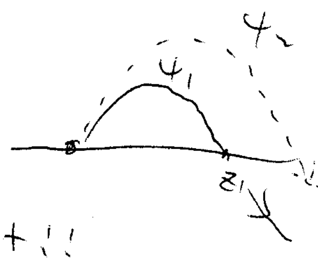
$$\underbrace{\psi_2\psi_1'\Big|_{z_1}}_{<0} = (\hat{E}_2 - \hat{E}_1)\int_a^{z_1} \underbrace{\psi_2\psi_1}_{>0 \text{ in } [a, z_1)} dx$$

If ψ_2 doesn't have a node in $[a\ z_1]$

choose it to be positive (negative)

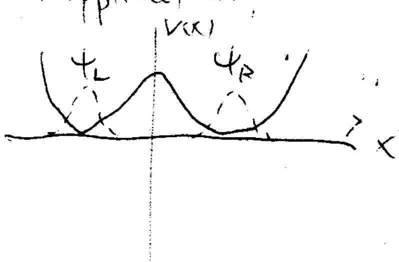
RH > 0, LH < 0.

(RH < 0), (LH > 0) Inconsistent!!

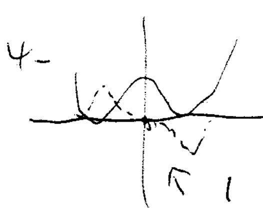


$\Rightarrow$ $\boxed{\psi_2 \text{ must have a node in } [a, z_1]}$

☆ Application.



$\Rightarrow$ eigenfunction $\psi_\pm = \frac{1}{\sqrt{2}}(\psi_L \pm \psi_R)$



No node

$\nwarrow$ 1 node

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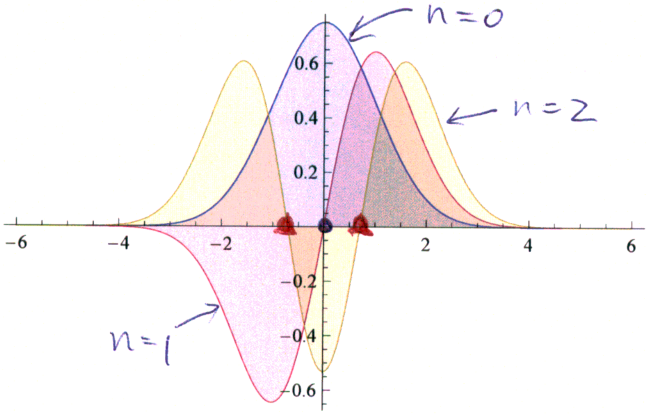
$\Rightarrow$ ψ_- is the excited state / ψ_+ is the ground state!!

In[14]:=
```
SHOWF[{n_, x_}] := Sqrt[1 / (2^n * n!)] * Sqrt[1 / Sqrt[Pi]] * Exp[-x^2 / 2] HermiteH[n, x]
```

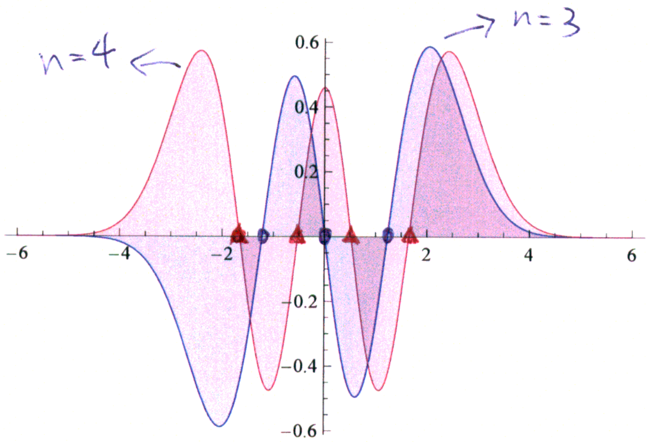
In[17]:=
```
Plot[Evaluate[Table[SHOWF[{n, x}], {n, 0, 2}]], {x, -6, 6}, PlotRange → Full, Filling → Axis]
```

Out[17]=



In[18]:=
```
Plot[Evaluate[Table[SHOWF[{n, x}], {n, 3, 4}]],
  {x, -6, 6}, PlotRange → Full, Filling → Axis]
```

Out[18]=



In[19]:=
```
Plot[Evaluate[Table[SHOWF[{n, x}], {n, 5, 6}]], {x, -6, 6}, PlotRange → Full, Filling → Axis]
```

Out[19]=