

Lecture 19:

Non-relativistic limit of Dirac eqn:

a) Dirac hamiltonian in $A_0(\vec{r}) = 0, \vec{A} \neq 0$

$$H_D^0 = \vec{\alpha} \cdot \vec{p} + \beta m$$

$$\Rightarrow \text{TISE: } H_D \psi = E \psi$$

Minimal prescription:

$$\begin{aligned} \hat{p} &= -i \vec{\nabla} \rightarrow (\vec{p} - q\vec{A}) \\ &= -i(\vec{\nabla} - i q \vec{A}) \\ &\quad \quad \quad \downarrow \\ &\quad \quad \quad qe \\ &= -i \vec{D} \end{aligned}$$

$$\begin{aligned} \vec{\alpha} &= \gamma^0 \vec{\gamma} \\ &= \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \\ \vec{\beta} &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{aligned}$$

$$\left(\begin{array}{cc} m - E + V & -i \vec{\sigma} \cdot \vec{D} \\ -i \vec{\sigma} \cdot \vec{D} & -m - E + V \end{array} \right) \begin{pmatrix} U \\ L \end{pmatrix} = 0 \quad \left. \vphantom{\begin{pmatrix} m - E + V & -i \vec{\sigma} \cdot \vec{D} \\ -i \vec{\sigma} \cdot \vec{D} & -m - E + V \end{pmatrix}} \right\} \begin{array}{l} H_D \psi = E \psi \\ \psi = \begin{pmatrix} U \\ L \end{pmatrix} \end{array}$$

$$\Rightarrow U = \left(\frac{1}{m - (E - V)} \right) i \vec{\sigma} \cdot \vec{D} L \quad ; \quad L = \left(\frac{-1}{m + (E - V)} \right) i \vec{\sigma} \cdot \vec{D} U$$

Free particle:

$$\begin{pmatrix} \chi \\ \frac{\vec{\sigma} \cdot \vec{p}}{E + m} \chi \end{pmatrix} \xrightarrow[\frac{\vec{p}}{m} \rightarrow 0]{\text{N.R.}} \begin{pmatrix} \chi \\ 0 \end{pmatrix}$$

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix}$$

$$U = \frac{1}{m-E} (\not{\vec{\sigma}} \cdot \vec{D}) \frac{1}{E+m} (\not{\vec{\sigma}} \cdot \vec{D}) U$$

$$= \frac{1}{m^2 - E^2} (\vec{\sigma} \cdot \vec{D})^2 U$$

$$E \approx E_{NR} + m$$

$$(m + E_{NR} + m) (\not{\vec{\sigma}} - (E_{NR} + m))$$

$$\approx -2m E_{NR} + \text{small } (E_{NR} \ll m)$$

$$\bullet \sigma_i \sigma_j D_i D_j = (\delta_{ij} 1 + i \epsilon_{ijk} \sigma_k) D_i D_j$$

$$= \vec{D}^2 + i \vec{\sigma} \cdot \vec{B} (-iqe)$$

$$\text{If we use } E^2 - m^2 = 2m E_{NR};$$

$$E_{NR} U(\vec{r}) = \left(-\frac{1}{2m} \vec{D}^2 - \frac{qe \vec{\sigma} \cdot \vec{B}}{2m} \right) U(\vec{r})$$

$$(\vec{\nabla} - iqe \vec{A}) \quad \downarrow \text{magnetic moment}$$

$$\Rightarrow \mu \sim \vec{S} = \vec{\sigma}/2$$

$$\text{For } \vec{A} \neq 0, A_0 = 0;$$

$$\hookrightarrow H_D^{NR} = \frac{\vec{\pi}^2}{2m} - \vec{\mu} \cdot \vec{B}; \quad \vec{\pi} = \vec{p} - q\vec{A}$$

$$\vec{\mu} = \frac{qe\vec{S}}{m} = \left(\frac{qe}{m} \right) \frac{\vec{\sigma}}{2}; \quad e > 0$$

$$= \left(\frac{geq\hbar}{2mc} \right) \frac{\vec{\sigma}}{2} \Rightarrow \text{Dirac eqn: } g = 2.$$

↓
Landé g-factor

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$i \epsilon_{ijk} \sigma_k D_i D_j$ test function

$$= \epsilon_{ijk} (\partial_i - iqe A_i) (\partial_j - iqe A_j) X$$

$$= \epsilon_{ijk} \left[\cancel{\partial_i \partial_j X}_{\text{sym}} - iqe \partial_i (A_j X) - iqe A_i \partial_j X - \cancel{q^2 e^2 A_i A_j X}_{\text{sym}} \right]$$

$$= \epsilon_{ijk} \left[\cancel{-iqe \partial_i A_j X}_{\text{asym}} - iqe A_j \partial_i X - \cancel{-iqe A_i \partial_j X}_{\text{sym}} \right]$$

$$= \frac{1}{2} \epsilon_{ijk} (-iqe) \underbrace{\partial_i A_j}_{\epsilon_{ijl} B_l} X$$

$$= \delta_{ke} (-iqe) B_e$$

$$b) A_0 \neq 0 \Rightarrow V = qeA_0 ; E \rightarrow E - V$$

$$\text{Dirac equation: } L(\vec{r}) = \frac{1}{E+m-V(\vec{r})} (-i\vec{\sigma} \cdot \vec{\nabla}) U(\vec{r})$$

$$U(\vec{r}) = \frac{1}{E-m-V(\vec{r})} (-i\vec{\sigma} \cdot \vec{\nabla}) L(\vec{r})$$

$$\Rightarrow \frac{1}{E-m-V} \underset{\substack{\uparrow \\ \text{matrix}}}{(-i\vec{\sigma} \cdot \vec{\nabla})} \underset{\substack{\uparrow \\ \text{differential operator}}}{\frac{1}{E+m-V} (-i\vec{\sigma} \cdot \vec{\nabla})} U = U$$

$$\text{Let } \bar{G} = G_- = E - m - V(\vec{r})$$

$$G = G_+ = E + m - V(\vec{r})$$

$$F = -i\vec{\sigma} \cdot \vec{\nabla}$$

$$\Rightarrow FG^{-1} = \underset{\substack{\parallel \\ G^{-1}(FG - GF)G^{-1}}}{G^{-1}F} - G^{-1}[F, G]G^{-1}$$

$$\text{So, we require } [F, G] = [-i\vec{\sigma} \cdot (\vec{\nabla} - iq\vec{A}), (E + m - V(\vec{r}))] \\ = +i\vec{\sigma} \cdot (\vec{\nabla} V)$$

$$U = \bar{G}^{-1} FG^{-1} F U$$

$$= \bar{G}^{-1} (G^{-1} F - G^{-1} (i\vec{\sigma} \cdot \vec{\nabla} V) G^{-1}) F U$$

$$= \bar{G}^{-1} (G^{-1} F^2 - G^{-2} (i\vec{\sigma} \cdot \vec{\nabla} V) F) U$$

$$\text{Approx: } E - V + m = E_{NR} + m + m - V \approx 2m + \text{small}$$

$$\Rightarrow (E - V)^2 - m^2 \approx (E_{NR} - V) 2m$$

$$\mathbf{F} = -i\vec{\sigma} \cdot \vec{D} \Rightarrow F^2 = -(\vec{\sigma} \cdot \vec{D})^2 = -\vec{D}^2 + \text{mag. field}$$

$$\Rightarrow \left(-\frac{1}{2} \frac{D^2}{m} - \frac{qe\vec{\sigma} \cdot \vec{B}}{2m} + V(r) \right) u + \frac{1}{2m} \left(\underbrace{\vec{\nabla} V \cdot \vec{D} u}_{\textcircled{I}} + i\vec{\sigma} \cdot \underbrace{(\vec{\nabla} V \times \vec{D} u)}_{\textcircled{II}} \right) = E_{NR} u$$

NR limit of Dirac eqn.
with $A_0 \neq 0$, $\vec{A} \neq 0$.

1st term: $(\vec{\nabla} V) \cdot (\vec{\sigma} - iqe\vec{A}) u \left(-\frac{1}{4m^2} \right)$
 $\approx (\vec{\nabla} V) \cdot (\vec{\sigma} u)$ $\hookrightarrow O(A^2)$

If V is radial fn: $\Rightarrow \vec{\nabla} V = \hat{r} V'(r) = \hat{r} \frac{\partial V}{\partial r}$

$\Rightarrow \textcircled{I} \approx -\frac{1}{4m^2} V'(r) \frac{\partial u}{\partial r}$ } Darwin term

2nd term: $\frac{-i}{4m^2} \vec{\sigma} \cdot (\underbrace{\vec{\nabla} V}_{\textcircled{a}} \times \underbrace{(\vec{\sigma} - iqe\vec{A}) u}_{\textcircled{b}})$

2-a: $\frac{-i}{4m^2} \vec{\sigma} \cdot (\underbrace{\vec{\nabla} V}_{\hat{r} V'(r)} \times \vec{\nabla} u) = \frac{1}{4m^2} \frac{V'(r)}{r} \vec{\sigma} \cdot (\underbrace{\vec{r} \times (-i\vec{\nabla})}_{\vec{L}}) u$

$= \frac{1}{2m^2} \frac{V'(r)}{r} \underbrace{\left(\frac{\vec{\sigma}}{2} \right)}_{\vec{S}} \cdot \vec{L} u$ } Thomas/Spin orbit term coupling

2-b: $\Delta_{\text{drop}} \sim A_\mu^2$

(also in $\bar{D}^2 u = (\bar{\nabla} - i q e \bar{A})^2 u$)

$$= \bar{\nabla}^2 - \underbrace{q^2 e^2 \bar{A}^2}_{O(A^2)} - i q e (\bar{\nabla} \cdot \bar{A} u) + \bar{A} \cdot \bar{\nabla} u$$

$$= (\bar{\nabla}^2 - 2 i q e \bar{A} \cdot \bar{\nabla}) u + \text{small}$$

$\bar{\nabla} \cdot \bar{A} = 0$
Coulomb gauge

But darwin term is non-hermitian!

$$\rightarrow \langle \psi | \phi \rangle = \int d^3x \psi^*(x) \phi(x)$$

$$(\psi, \hat{O}_D \phi) \neq (\phi, \hat{O}_D \psi)^* \rightarrow \text{non-hermitian.}$$

$$\hat{O}_D = () V'(r) \partial_r$$

$$\left(\int d^3x (\psi^* V'(r) \partial_r \phi) \right)^* \xrightarrow{\substack{\text{integration by parts}}} \int d^3x (-\partial_r (V'(r) \psi(r)) \phi^* \quad \uparrow \text{not hermitian.}$$

Ad-hoc correction:

↳ Retain only hermitian part.

$$\hat{O}_D \rightarrow \frac{\hat{O}_D + \hat{O}_D^\dagger}{2}$$

$$\bullet X = V'(r) \partial_r \quad ; \quad (\psi, X^\dagger \phi) \equiv (X \psi, \phi)$$

$$\begin{aligned} \int \psi^* X^\dagger \phi &= \int d^3r (V' \partial_r \psi)^* \phi \\ &= - \int d^3r \psi^* \frac{1}{r^2} \partial_r (r^2 V'(r) \phi) \end{aligned}$$

$$\Rightarrow \int d\Omega r^2 dr \left(-\psi^* \frac{1}{r^2} \partial_r (r^2 V'(r) \phi) \right)$$

$$\Rightarrow \int \psi^* X^\dagger \phi d^3r = - \int d^3r \psi^* (\nabla^2 V(r) + V' \partial_r \phi)$$

$$\Rightarrow \frac{X + X^\dagger}{2} = -\frac{1}{2} (\nabla^2 V(r))$$

$$\Rightarrow \mathcal{O}_{\text{Darwin}}^{(\text{hermitian})} = \frac{1}{8m^2} (\nabla^2 V)$$

$$V = qeA_0 = -\frac{e^2}{4\pi r} \Rightarrow \nabla^2 \left(\frac{1}{r} \right) = -4\pi \delta(\vec{r})$$

Necessity of adding X^\dagger ;

$$\int \psi^\dagger \psi d^3\vec{r} = \int (u^\dagger u + L^\dagger L) d^3r$$

$$= \int u^\dagger \left(1 + \frac{\vec{\sigma} \cdot \vec{p}}{2m} \right)^2 u d^3r$$

$$= \int u^\dagger \left(1 + \frac{p^2}{4m^2} \right) u d^3r$$

$$\Rightarrow \boxed{\int u^\dagger u d^3\vec{r} \neq 1} !!$$

So we need to work with $\hat{u} = \sqrt{u} = \left(1 + \frac{\vec{p}^2}{8m^2}\right) u$

$$\hat{u}^\dagger \hat{u} = u^\dagger \left(1 + \frac{\vec{p}^2}{8m^2}\right)^2 u$$

$$\approx u^\dagger \left(1 + \frac{\vec{p}^2}{4m^2}\right) u + \text{small.} = 1$$

If we implement this, we get:

$$\hat{H}_D \approx \frac{\vec{p}^2}{2m} + V(r) + \underbrace{\frac{\nabla^2 V}{8m^2}}_{\text{Darwin}} + \underbrace{\frac{V'(r)}{2m^2 r} \vec{S} \cdot \vec{L}}_{\text{Spin-orbit}} - \underbrace{\frac{(\vec{p}^2)^2}{8m^3}}_{\text{1st relativistic correction}}$$

————— x ——— x ——— x ———

Lecture 20:

$$\Psi \sim \begin{pmatrix} u \\ L \end{pmatrix} e^{i\vec{p}\cdot\vec{r} - iEt}$$

Dirac eqn

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$$(E - V(\vec{r}) - m) u = (-\vec{\sigma} \cdot \vec{D} (E - V + m)^{-1} \vec{\sigma} \cdot \vec{D}) u \\ = (E_{NR} - V(\vec{r})) u$$

Leading terms in NR limit:

$$\left(\frac{1}{2m} (\vec{\nabla} - iqe\vec{A})^2 - g\mu_B \vec{S} \cdot \vec{B} + V(\vec{r}) \right) u = E_{NR} u$$

Problems with NR limit to next order:

$$\textcircled{1} (E - V + m)^{-1} = (E_{NR} - V + 2m)^{-1} \\ = \frac{1}{2m} \left[1 - \frac{(E_{NR} - V)}{2m} + O(m^{-2}) \right]$$

So, $H_{NR} u = E_{NR} u$ is not an eigenvalue eqn in the next order of expansion!

$$\therefore H_{NR} \equiv H_{NR}(E_{NR})$$

$$\textcircled{2} \int \Psi^\dagger \Psi d^3\vec{r} = 1 = \int (u^\dagger u + L^\dagger L) d^3\vec{r}$$

$$L = \frac{\vec{\sigma} \cdot \vec{p}}{2m} u + O(1/m^2) + \dots$$

$$\text{So, we need } \int d^3\vec{r} u^\dagger \left(1 + \frac{\vec{p}^2}{4m^2} + \text{small} \right) u = 1$$

$$\therefore \int d^3\vec{r} u^\dagger u \neq 1 \Rightarrow u \text{ cannot be } \Psi_{NR}!!$$

③ Naively, we obtained $H_{NR} \sim (\vec{\nabla} V) \cdot \vec{\nabla}$

$$\underbrace{O_D}_{\text{Darwin term}} \sim \underbrace{i \vec{E} \cdot \vec{P}}_{\text{non-hermitian}}$$

Adhoc fix: Take $\frac{O_D + O_D^\dagger}{2} \rightarrow$ hermitian part.

A systematic approach to fix these problems:

$$\int d^3\vec{r} \underbrace{u^\dagger \left(1 + \frac{\vec{P}^2}{4m^2}\right) u}_{\Omega^\dagger \Omega} \simeq 1 \quad ; \quad \Omega = 1 + \frac{\vec{P}^2}{8m^2} + \text{small}$$

could be $\Psi_{NR} \rightarrow \boxed{\hat{u} = \Omega u}$

$$\begin{aligned} \bullet H_{NR} u &= \left[\frac{\vec{P}^2}{2m} + V + \frac{1}{2m} \vec{\sigma} \cdot \vec{P} \left(\frac{V}{2m} \right) \vec{\sigma} \cdot \vec{P} - \frac{E_{NR}}{2m} \frac{\vec{P}^2}{2m} \right] u \\ &= E_{NR} u \end{aligned}$$

$$\Rightarrow \underbrace{\Omega^{-1} H_{NR} \Omega^{-1}}_{\hat{H}} \hat{u} = E_{NR} \Omega^{-2} \hat{u} \quad ; \quad \Omega^{-1} = 1 - \frac{\vec{P}^2}{8m^2} + \dots$$

$$\Rightarrow \hat{H} = H_{NR} - \left\{ -\frac{\vec{P}^2}{2m}, \frac{\vec{P}^2}{2m} + V \right\} + \text{small.}$$

$$= \frac{\vec{P}^2}{2m} + V - \frac{E_{NR}}{2m} \frac{\vec{P}^2}{2m} + \frac{1}{4m} \vec{\sigma} \cdot \vec{P} V \vec{\sigma} \cdot \vec{P}$$

$$+ \frac{V}{4m^2} \vec{P}^2 - \underbrace{\frac{\vec{P}^4}{8m^3}}_{\text{first relativistic correction}} - \frac{1}{8m^2} \left\{ \vec{P}^2, V \right\}$$

first relativistic
correction

Now we need $\bar{\sigma} \cdot (\bar{p} V) \bar{\sigma} \cdot \bar{p}$

$$= (\bar{p} V) \cdot \bar{p} + i \bar{\sigma} \cdot ((\bar{p} V) \times \bar{p})$$

$$\begin{aligned} \bullet \left\{ \bar{p}^2, V(r) \right\} \Psi &= \bar{p}^2 (V \Psi) + V(\bar{r}) \bar{p}^2 \Psi \\ &= 2(\bar{p} V) \cdot \bar{p} \Psi + 2V \bar{p}^2 \Psi + (\bar{p}^2 V) \Psi \end{aligned}$$

$$\Rightarrow \frac{1}{4m^2} \left\{ \bar{\sigma} \cdot (\bar{p} V) \bar{\sigma} \cdot \bar{p} - \frac{1}{2} \left\{ \bar{p}^2, V \right\} \right\}$$

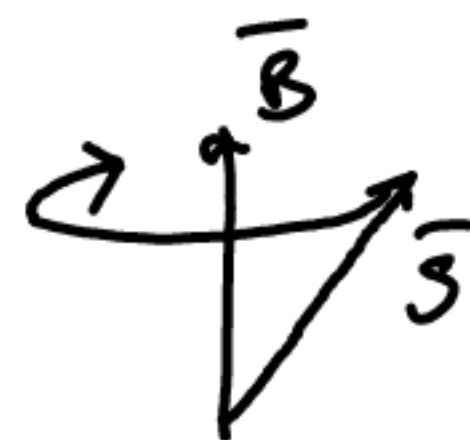
$$= \frac{1}{4m^2} \left\{ i \bar{\sigma} \cdot ((\bar{p} V) \times \bar{p}) - V \bar{p}^2 \Psi - \frac{\bar{p}^2 V}{2} \Psi \right\}$$

$$\Rightarrow \left(\frac{\bar{p}^2}{2m} + V - \underbrace{\frac{\bar{p}^4}{8m^3}}_{\text{first relativistic correction}} - \underbrace{\frac{Q \bar{\sigma} \cdot (\bar{E} \times \bar{p})}{4m^2}}_{\text{thomas spin orbit term}} - \underbrace{Q \frac{\bar{\nabla} \cdot \bar{E}}{8m^2}}_{\text{dewin}} \right) \hat{u} = E_{NR} \hat{u} = \underbrace{\hat{H}_{NR}}_{\text{hamiltonian}} \hat{u}$$

Thomas spin orbit term:

→ Magnetic moment of e^- sees nuclear electric field as a magnetic field. → $-\mu_e \cdot \bar{B}$

→ Moreover, the e^- Spin \bar{S} precesses in \bar{B} .



$$\bar{B} \sim -\bar{v}_e \times \bar{E} \sim -\frac{\bar{p} \times \bar{E}}{m}$$

$$\begin{aligned} (\Delta H) &\approx -\bar{\mu}_e \cdot \left(\frac{\bar{E} \times \bar{p}}{m} \right) ; \mu_e = \frac{Q \hbar}{m} \bar{S} = \frac{Q \hbar}{2m} \bar{\sigma} \\ &= 2 \times \text{Spin orbit / thomas.} \end{aligned}$$

→ Inclusion of spin precession reduces this

Spin orbit term : $V(r) \rightarrow \vec{\nabla} V = V'(r) \hat{r}$

$\hookrightarrow \frac{1}{2m^2} \frac{V'(r)}{r} \vec{S} \cdot \vec{L}$

Darwin term : $-\frac{Qe}{8m^2} \vec{\nabla} \cdot \vec{E}_{\text{nucleus}} = +\frac{Qe}{8m^2} \nabla^2 A_0 = \frac{\nabla^2 V}{8m^2}$

$\vec{\nabla} \cdot \vec{E} = \rho(\vec{r}) = -\nabla^2 A_0$

\hookrightarrow for point nucleus, $\rho(\vec{r}) = q_n \delta^3(\vec{r})$

\hookrightarrow leads to $Z_N |e|^2 \delta^3(\vec{r})$ in H_{NR} .

$\Rightarrow (\Delta E)_{\text{Darwin}} \sim Z_N |e|^2 |\psi(0)|^2$
 $\langle \Psi | \Delta H_{\text{Darwin}} | \Psi \rangle = \int d^3r \Psi^* \Delta H \Psi$ } Only s-wave parts contribute to this.

Physically, darwin term is due to "Jittering motion" with frequency $\sim mc$.

$\Psi(t) \sim e^{iEt}$; $E = m + \text{b.e.} + \text{relativistic}$
($m \gg E_{NR}$)

$\langle V(x + \delta x) \rangle = \langle V(\bar{x}) + \cancel{\delta \bar{x} \cdot \vec{\nabla} V} + \frac{1}{2} \delta x_i \delta x_j \partial_i \partial_j V + \dots \rangle$
high freq. \uparrow
average = 0

$= \langle (\delta \bar{x})^2 \rangle \nabla^2 V \approx \frac{1}{6m^2} \nabla^2 V$

———— x ——— x ——— x ———

Zitterbewegung:

- Heisenberg eqn. of motion for a free particle:
 $[O(t); |\Psi\rangle]$ - independent of t

$$\rightarrow \frac{d}{dt} \Omega_H(t) = -i [\Omega_H(t), H] + \frac{\partial \Omega_H}{\partial t}$$

Constants of motion:

||
0 (Autonomous system)

- $H_0 = \vec{\alpha} \cdot \vec{p} + \beta m$

$$\frac{d}{dt}(\bar{p}_i) = -i [p_{i0}, \vec{\alpha} \cdot \vec{p} + \beta m] = 0$$

$\therefore \vec{p}$ is a const. of motion.

$$\begin{aligned} \frac{d(L_n)_i}{dt} &= -i [\epsilon_{ijk} x^j p^k, \vec{\alpha} \cdot \vec{p} + \beta m] \\ &= (\vec{\alpha} \times \vec{p})_i \end{aligned}$$

$$\frac{d}{dt} \left(\frac{\vec{\Sigma}_H}{2} \right)_i = -(\vec{\alpha} \times \vec{p})_i \Rightarrow \frac{d}{dt} \vec{J} = 0; \quad \vec{J} = \vec{L} + \frac{\vec{\Sigma}}{2}$$

Trajectory of a free Dirac particle of momentum \vec{p} :

$$\dot{\vec{x}}_i = -i [\vec{x}_i, \vec{\alpha} \cdot \vec{p} + \beta m] = +\alpha_i(t) \neq 0 \quad \xrightarrow{\alpha_{\text{Heisenberg}}}$$

$$\vec{\alpha}_s = \gamma^0 \vec{\gamma} \Rightarrow \vec{\alpha}_s^2 = \gamma^0 \gamma^i \gamma^0 \gamma^i = 1_4$$

$$\Rightarrow \vec{\alpha}_H^2 = 1_4$$

\therefore eigenvalues of $\vec{\alpha}$ are ± 1 .

Velocity = $\vec{\alpha}(t)$; and eigenvalues are $\pm 1 (= \pm c)$

So, measurement of velocity of massive Dirac particle should always give c . How??

Trajectory:

$$-i [\vec{x}, \frac{\vec{p}^2}{2m}] = \frac{\vec{p}}{m} = \vec{v} \quad \text{in NRQM}$$

$$\bullet \frac{d^2 \vec{x}}{dt^2} = \frac{d}{dt} \vec{\alpha}_H(t) = -i [\vec{\alpha}_H(t), \vec{\alpha} \cdot \vec{p} + \beta m]$$

$$\left[\begin{aligned} [A, B] &= AB + BA - 2BA = \{A, B\} - 2BA \\ &\rightarrow -i (\{ \alpha_j, H_0 \} - 2H_0 \alpha_j) \end{aligned} \right.$$

$$\{ \alpha_i, \alpha_j \} = 2\delta_{ij}$$

$$\{ \alpha_i, \beta \} = 0$$

$$\Rightarrow \{ \alpha_j, H_0 \} = 2p_j$$

$$\Rightarrow \frac{d\vec{\alpha}_j}{dt} = -i 2\vec{p}_j + 2i H_0 \alpha_j$$

Consider:

$$\frac{d}{dt} \left(\underbrace{e^{-2iH_D t}}_{\text{integrating factor}} \bar{\alpha}_j \right) = e^{-2iH_D t} \frac{d\bar{\alpha}_j}{dt} - 2i e^{-2iH_D t} H_D \bar{\alpha}_j = -i2p^j e^{-2iH_D t}$$

Integrate this:

$$\Rightarrow e^{-2iH_D t} \bar{\alpha}_j(t) = H_D^{-1} p^j e^{-2iH_D t} + \bar{a} \quad \hookrightarrow \text{const.}$$

$$\bullet \bar{v}(0) = H_D^{-1} \bar{p} + \bar{a}$$

$$\Rightarrow \bar{v}(t) = \bar{\alpha}(t) = H_D^{-1} \bar{p} + \underbrace{e^{2iH_D t}}_{\text{fast fluctuations}} (\bar{v}(0) - H_D^{-1} \bar{p})$$

(freq $\sim 2m + \text{small}$).

$$\langle \bar{v}(t) \rangle_{\text{avg. over } T \gg \frac{1}{2m}} = \frac{\bar{p}}{H_D} = \frac{\bar{p}}{E}$$

$$E = \gamma m \quad ; \quad \bar{p} = \gamma m \bar{v} \quad \Rightarrow \quad \frac{\bar{p}}{E} = \bar{v} !$$

So, on long time scales, the usual relativistic \bar{v} momentum relation $\bar{v} = \frac{\bar{p}}{E}$ holds true. The fast fluctuation does, however, have observable effects, e.g. in the Darwin term where the \bar{e} is an atom instead of seeing a smooth nuclear potential, actually samples a range of \bar{r} value due to its relativistic jitter at freq. $\nu \sim 2m$.

$$\Rightarrow \langle \delta x_i \delta x_j \partial_i \partial_j V \rangle \approx \underbrace{\frac{1}{3} \langle \delta \vec{x}^2 \rangle}_{\text{non-zero for dirac particle}} \cdot \nabla^2 V$$

There are additional counter-intuitive effects for relativistic particles which further invalidates the single particle interpretation.

→ Klein paradox

→ Interference of the and -ve freq. components

These will motivate the foundations of field theory.

————— x ————— x ————— x —————

Lecture 21:

Zitterbewegung: "Jittering motion"

Heisenberg picture: $\frac{d\vec{x}}{dt} = \vec{\alpha}_H(t)$

$$\vec{\alpha}_S = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \quad ; \quad \vec{\alpha}_H(t) = U^\dagger(t) \vec{\alpha}_S U(t) \quad ; \quad U = e^{-iH_D t}$$

$$\vec{\alpha}_H(t) = \vec{p} H_D^{-1} + e^{i2H_D t} (\vec{\alpha}_H(0) - \vec{p} H_D^{-1})$$

$$\stackrel{u}{-i[\vec{\alpha}_H(t), H_D]}$$

↑
Fast fluctuation at freq. $\nu \sim 2m$
(w/ amplitude \sim Compton $\lambda = \frac{h}{mc}$)

$$1 \text{ eV} \sim 10^{15} \text{ Hz}$$

$$1 \text{ MeV} \sim 10^{21} \text{ Hz}$$

Schrodinger picture:

$$\frac{dO_S}{dt} = 0 \quad ; \quad i \frac{d}{dt} |\psi_S(t)\rangle \neq 0.$$

$$\langle \psi_S(t) | \vec{\alpha}_S | \psi_S(t) \rangle$$

$$\psi(\vec{x}, t) = \int \frac{d^3 \vec{p}}{\sqrt{(2\pi)^3} 2E_p}$$

$$\begin{aligned} & \sum_S \left(f_S(\vec{p}) u_S(\vec{p}) e^{-i\vec{p} \cdot \vec{x}} \xleftarrow{\psi_+(\vec{x})} \right. \\ & \quad \left. + \hat{f}_S(\vec{p})^* v_S(\vec{p}) e^{i\vec{p} \cdot \vec{x}} \right) \xleftarrow{\psi_-(\vec{x})} \\ & \quad \parallel \quad \hat{f}_S(-\vec{p})^* v_S(-\vec{p}) e^{iE_p t + i\vec{p} \cdot \vec{x}} \end{aligned}$$

Annotations for the exponentials:
- For $e^{-i\vec{p} \cdot \vec{x}}$: $-iE_p t + i\vec{p} \cdot \vec{x}$
- For $e^{i\vec{p} \cdot \vec{x}}$: $iE_p t - i\vec{p} \cdot \vec{x}$

$$\Rightarrow \Psi(\vec{x}, t) = \sum_{\substack{\vec{p}, s \\ \text{generalized} \\ \text{sum}}} \left(f_s(\vec{p}) u_{\vec{p}, s} + f_s^\dagger(\vec{p}) v_{\vec{p}, s} \right)$$

$$\frac{1}{\sqrt{(2\pi)^3 2E_p}} u_s(\vec{p}) e^{-i\vec{p} \cdot \vec{x}}$$

$$= \sum c_k |e_k\rangle$$

$$E_p = \sqrt{p^2 + m^2}$$

$$\Rightarrow \bar{\Psi}(\vec{x}, t) = \Psi^\dagger(\vec{x}, t) \gamma^0$$

$$= \sum_{\vec{p}, s} \left(f_s^\dagger(\vec{p}) \bar{u}_s(\vec{p}) e^{i\vec{p} \cdot \vec{x}} + \hat{f}_s(\vec{p}) \bar{v}_s(\vec{p}) e^{-i\vec{p} \cdot \vec{x}} \right)$$

$$\bullet f_r(\vec{q}) = (u_r(\vec{q}), \Psi)$$

$$= \int \frac{d^3 \vec{x}}{\sqrt{2E_q (2\pi)^3}} u_r^\dagger(\vec{q}, \vec{x}) e^{i\vec{q} \cdot \vec{x}} \Psi(\vec{x})$$

$$\bullet \hat{f}_r^\dagger(\vec{q}) = (v_r(\vec{q}), \Psi(\vec{x}))$$

Also, orthonormality $(u_r(\vec{q}), u_s(\vec{p})) = \delta_{rs} \delta^3(\vec{p} - \vec{q})$

$$(v_r(\vec{q}), v_s(\vec{p})) = \delta_{rs} \delta^3(\vec{p} - \vec{q})$$

$$(u_r(\vec{q}), v_s(\vec{p})) = 0.$$

We require $\langle \bar{\alpha}_s \rangle = (\Psi, \bar{\alpha}_s \Psi)$

$$\langle \bar{\alpha}_s \rangle = \sum_{\vec{p}, r} \sum_{\vec{q}, s} \left[f_{\vec{p}, r}^* f_{\vec{q}, s} \int d^3 \vec{x} \mathcal{U}_{\vec{p}, r}^\dagger(\vec{x}) \bar{\alpha} \mathcal{U}_{\vec{q}, s}(\vec{x}) \right. \\
+ \hat{f}_{\vec{p}, r} \hat{f}_{\vec{q}, s}^* \int d^3 \vec{x} \mathcal{V}_{\vec{p}, r}^\dagger(\vec{x}) \bar{\alpha} \mathcal{V}_{\vec{q}, s}(\vec{x}) \\
+ f_{\vec{p}, r}^* f_{\vec{q}, s}^* \int d^3 \vec{x} \mathcal{U}_{\vec{p}, r}^\dagger(\vec{x}) \bar{\alpha} \mathcal{V}_{\vec{q}, s}(\vec{x}) \\
\left. + \text{hermitian conj. } \uparrow \right]$$

$$\bullet \int d^3 \vec{x} e^{i \vec{p} \cdot \vec{x}} e^{-i \vec{q} \cdot \vec{x}} = \int d^3 \vec{x} e^{i(E_p - E_q)t + i(\vec{q} - \vec{p}) \cdot \vec{x}} \\
= (2\pi)^3 \delta^3(\vec{p} - \vec{q}) \underset{E_p = E_q}{e^{i(E_p - E_q)t}} = (2\pi)^3$$

$$\bullet \int d^3 \vec{x} e^{i(E_p t - \vec{p} \cdot \vec{x})} e^{i(E_q t - \vec{q} \cdot \vec{x})} \\
= (2\pi)^3 \delta^3(\vec{p} + \vec{q}) \underset{E_p = E_q}{e^{i(E_p + E_q)t}} = \underbrace{e^{2iE_p t}}_{\text{fast fluctuations!}}$$

$$\Rightarrow \mathcal{U}_{\vec{p}, r}^\dagger \bar{\alpha} \mathcal{V}_{-\vec{p}, s} = (\sqrt{E_p + m})^2 (\chi_r^\dagger, \frac{\vec{\sigma} \cdot \vec{p}}{E_p + m} \chi_r^\dagger) \begin{pmatrix} \bar{\sigma} \chi_r \\ -\frac{\vec{p} (\vec{\sigma} \cdot \vec{p}) \chi_r}{E_p + m} \end{pmatrix} \\
= 2E_p \chi_r^\dagger \bar{\sigma} \chi_r - \frac{2\vec{p}}{E_p + m} \chi_r^\dagger \vec{\sigma} \cdot \vec{p} \chi_r$$

$$\Rightarrow \langle \bar{\alpha} \rangle = \sum_{\vec{p}, r} (|f_{\vec{p}, r}|^2 + |f_{\vec{q}, s}|^2) \frac{\vec{p}}{E_p} \\
+ \sum_{\vec{p}, r} \underbrace{f_{\vec{p}, r}^* \hat{f}_{-\vec{p}, r}^*}_{\text{Zitterbewegung}} e^{-2iE_p t} \chi_r^\dagger \left(\bar{\sigma} - \frac{\vec{p} \vec{\sigma} \cdot \vec{p}}{(E_p + m) E_p} \right) \chi_r + \text{h.c.}$$

\Rightarrow Interference of +ve and -ve frequency oscillations.

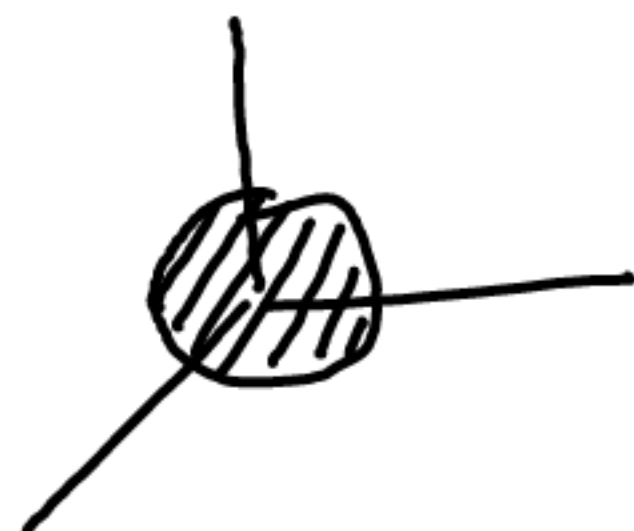
But -ve frequency components are always present to a significant extent for a Dirac particle wave-packet which is localized to a width $\Delta x \lesssim 1/m$.

$$\therefore \left| \frac{\hat{f}_{\bar{p}}}{f_{\bar{p}}} \right| \sim \frac{\bar{p}}{2m} \Rightarrow \text{If } \bar{p} \sim m, \text{ -ve and +ve freq. are comparable.}$$

So, -ve freq. cannot be ignored!

e.g. $\Psi(\bar{x}, 0) = \begin{pmatrix} \phi(\bar{x}) \\ 0 \\ 0 \\ 0 \end{pmatrix}$ $\phi(\bar{x})$ has support $\sim (\Delta \bar{x})$

$\hookrightarrow \phi(\bar{x}) \neq 0$ in a region of size $|\Delta \bar{x}|$



$$\Psi(\bar{x}, t) = \sum_{\bar{p}, r} f_{\bar{p}, r} \mathcal{U}_{\bar{p}, r}(\bar{x}, t) + \hat{f}_{\bar{p}, s}^* V_{\bar{p}, s}(\bar{x}, t)$$

$$(\mathcal{U}_{\bar{p}, r}(\bar{x}, 0), \Psi(\bar{x}, 0)) \mapsto (V_{\bar{p}, s}(\bar{x}, 0), \Psi(\bar{x}, 0))$$

$$\Rightarrow f_{\bar{p}, r} \approx \tilde{\phi}(\bar{p}) \sqrt{E_{\bar{p}+m}} \left(\mathcal{U}_r^+ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \right)$$

$$\hat{f}_{\bar{p}, r} \approx \tilde{\phi}(\bar{p}) \sqrt{E_{\bar{p}+m}} \mathcal{U}_r^+ \frac{\bar{\sigma} \cdot \bar{p}}{E_{\bar{p}+m}} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$\tilde{\phi}(\bar{p})$

\downarrow
fourier transform
of $\phi(x)$

$$\Rightarrow \frac{\hat{f}_{-\bar{p},1}}{f_{\bar{p},1}} \sim \frac{-p_3}{E_{p+m}} ; \quad \frac{\hat{f}_{-\bar{p},2}}{f_{\bar{p},1}} \sim \frac{-p_+}{E_{p+m}}$$

If $\phi(\bar{p}) \neq 0$ for \bar{p} upto $|\bar{p}| \sim m$

i.e. $\phi(\bar{x})$ is localized to $\Delta x \sim \frac{1}{m}$.

So, if we use only the wave, we cannot localize to scales $< 1/m$.

_____ x _____ x _____ x _____

Klein paradox:

In a region of constant potential $V(x)$, we have from the Dirac eqn.:

$$H_D = \vec{\alpha} \cdot (\vec{p} - \underbrace{q\vec{A}}_0) + \beta m + \underbrace{V(\vec{x})}_{\rightarrow \text{const.}}$$

Solve for u :

$$\underbrace{(\vec{\sigma} \cdot \vec{p})^2}_{\frac{p^2}{p}} u_{\bar{p},r} = (E - V + m)(E - V - m) u_{\bar{p},r}$$

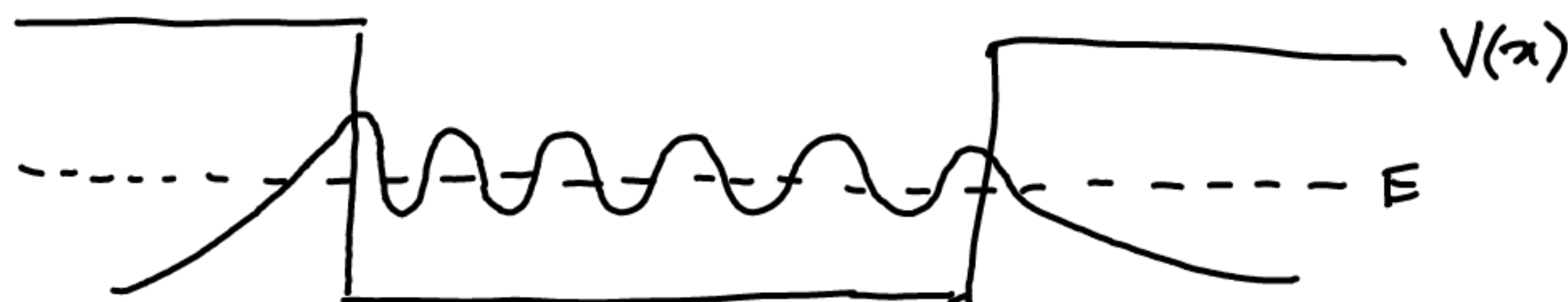
$$\text{So, } \bar{p}^2 = (E - V + m)(E - V - m) = (2m + E_{NR} - V)(E_{NR} - V)$$

$$\boxed{E_{NR} = E - m} \quad \text{Energy rel. to rest mass.}$$

① $V > 0$: Repulsive potential

If $\bar{p}^2 > 0 \Rightarrow$ Wavefn. is oscillatory

$\bar{p}^2 < 0 \Rightarrow$ Wavefn. is damped



• $\bar{p}^2 > 0$ if

i) $E - V + m > 0$, $E - V - m > 0$

is usual ; $2m + E_{NR} > V$ and $E_{NR} > V$

ii) $E - V + m < 0$; $E - V - m < 0$

$\Rightarrow 2m + E_{NR} < V_{\text{repulsive}} > 0$ } again oscillatory??
 $E_{NR} < V_{\text{repulsive}}$

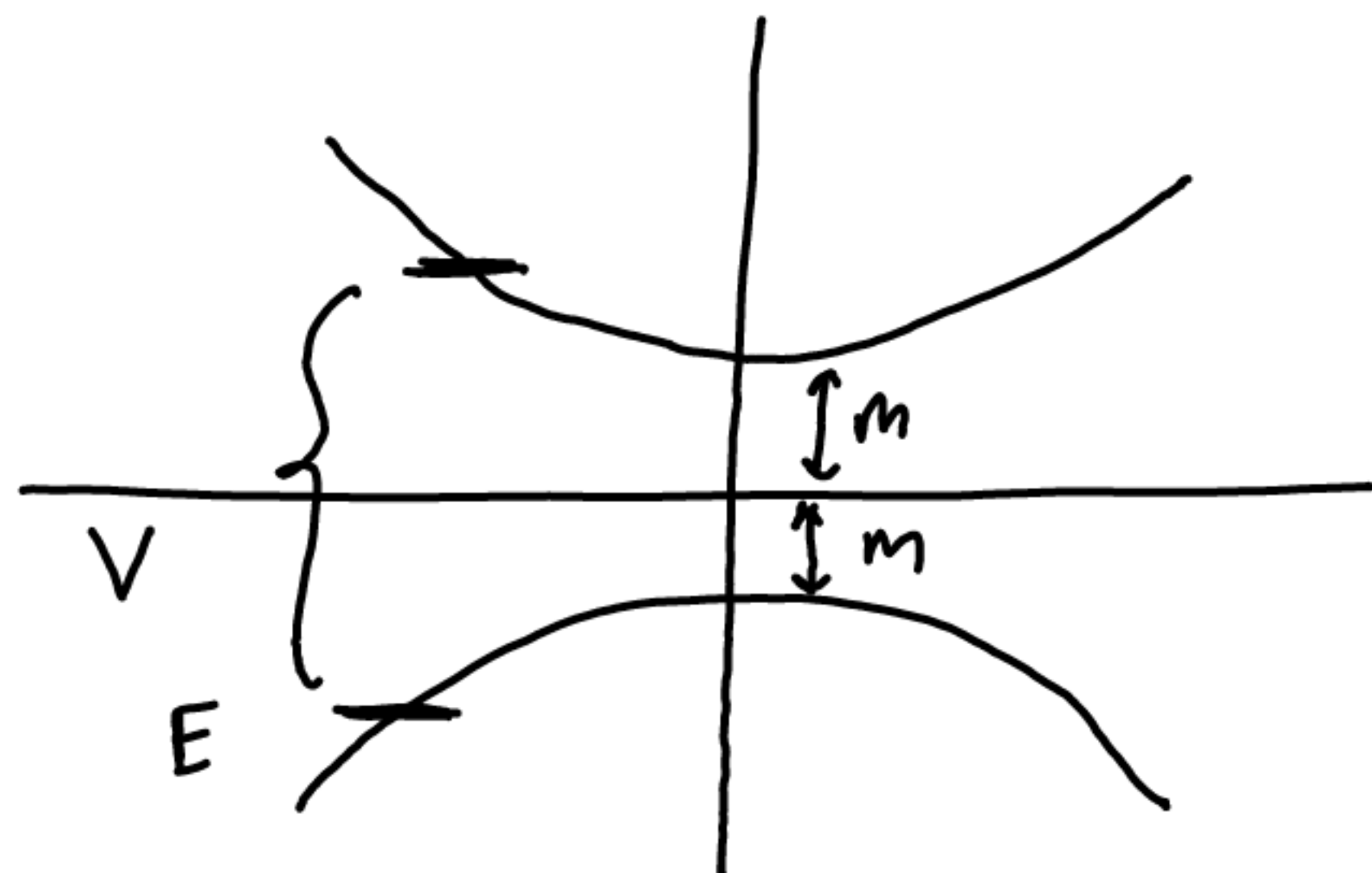
\Rightarrow So, if the potential is so repulsive s.t.

$V > 2m$, then we get oscillatory/undamped particle propagation even in the classically

forbidden region. Since $V > 2m + \dots$

this should be associated with pair creation.

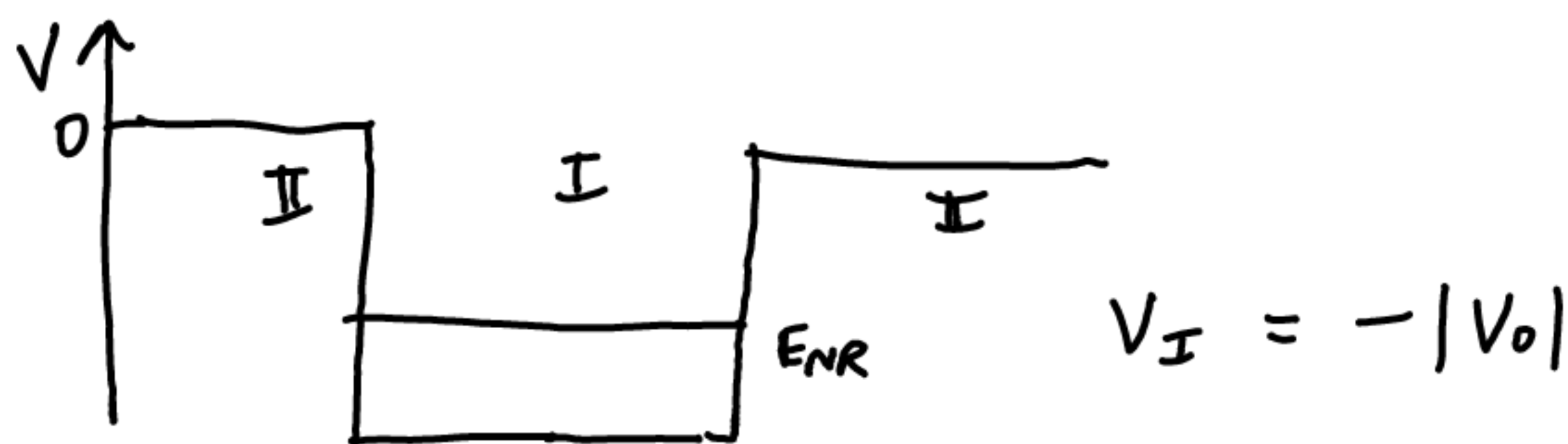
→ These oscillatory solutions are basically -ve energy states raised by $V > 0$ to +ve energy, leaving a hole which itself behaves as a particle of mass m .



$$V + E = V - \sqrt{p^2 + m^2}$$

↳ particle-antiparticle pair which propagates undamped.

② $V < 0$; Attractive potential



N.R case : $p_I = \sqrt{2m(|V_0| + E_{NR})} \sim \text{real}$

$$E_{NR} = \frac{\bar{p}^2}{2m} - |V_0|$$

⇒ In region I → it is oscillatory.

In region II, $p_{II} = \sqrt{2mE_{NR}} \sim \text{img.}$

⇒ Classically forbidden, damped propagation.

In relativistic case,

$$P_I = \sqrt{P^2} = \sqrt{(E_{NR} - V)(2m + E_{NR} - V)} \\ = \sqrt{(|V| - |E_{NR}|)(2m + |V| - |E_{NR}|)}$$

$$P_{II} = \sqrt{|E_{NR}|(|E_{NR}| - 2m)}$$

Suppose the well is very deep:

$$|E_{NR}| > 2m$$

$\Rightarrow P_{II}$ is oscillatory.

\Rightarrow Sufficiently strong attractive potential creates an $e^- - e^+$ pair (out of vacuum!) which propagates without damping.

\rightarrow Thus, the Klein paradox is intelligible as e^+e^- pair creation due to large $|V|$ but again with the Dirac Sea, i.e. ∞ of particles and states playing an essential role.

\rightarrow Thus we require a better theory: QFT!

————— x ————— x ————— x —————