Nonrelativistic Schrödinger eq.:

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi, \qquad H \text{ "Hamiltonian".}$$

How to get H?

- Take Hamiltonian function $H(x,p)$ from classical mechanics:

$$H(x,p) = \frac{p^2}{2m} + V(x) \qquad \text{total energy}$$

and replace p and x with operators on $L^2(\mathbb{R}^d)$:

$$p \longrightarrow -i\hbar\nabla, \qquad x \longrightarrow [f \mapsto x\cdot f] \qquad \text{"Quantisation"}$$

$\rightsquigarrow$ Schrödinger eq:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + V\psi \qquad (*)$$

Relativistic QM:

Problem with $(*)$: 2nd derivative in space, 1st derivative in time

$\rightsquigarrow$ not Lorentz invariant.

Solution: start with relativistic kinetic energy:

$$H_{rel}(x,p) = \sqrt{c^2p^2 + m^2c^4}, \qquad c = \text{speed of light}$$

Quantisation $\rightsquigarrow$ $$i\hbar\frac{\partial\psi}{\partial t} = \sqrt{-c^2\hbar^2\Delta + m^2c^4}\,\psi \qquad (**)$$

Two options: 1) Square $(**)$: $-\hbar^2\frac{\partial^2\psi}{\partial t^2} = (-c^2\hbar^2\Delta + m^2c^4)\psi$

"Klein-Gordon eq."

2) Compute square root of $-c^2\hbar^2\Delta + m^2c^4$.

Dirac did 2:

Ansatz: $H = c \sum_{i=1}^{3} \alpha_i p_i + \beta m c^2$. Then

$$H^2 = (c\alpha\cdot p + \beta m c^2)(c\alpha\cdot p + \beta m c^2)$$

$$= c^2 (\alpha\cdot p)^2 + \alpha\cdot p \beta m c^2 + \beta m c^2 \alpha\cdot p + \beta^2 m^2 c^4$$

$$= c^2 \sum_{i,j} \alpha_i p_i \alpha_j p_j + \sum_i (\alpha_i \beta + \beta \alpha_i) p m c^2 + \beta^2 m^2 c^4$$

$$= \frac{1}{2} c^2 \sum_{i<j} (\alpha_i \alpha_j + \alpha_j \alpha_i) p_i p_j + \sum_i (\alpha_i \beta + \beta\alpha_i) p m c^2 + \beta^2 m^2 c^4$$

$\rightsquigarrow$ Conditions:

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

$$\alpha_i \beta + \beta \alpha_i = 0 \qquad \text{from } H^2 = -c^2 \hbar^2 \Delta + m^2 c^4.$$

$$\beta^2 = 1 .$$

$\Longrightarrow$ α_i, β have to be matrices.

Possible choice:

$$\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{and}$$

$$\beta := \begin{pmatrix} 1_{2\times2} & 0_{2\times2} \\ 0_{2\times2} & -1_{2\times2} \end{pmatrix}, \qquad \alpha_i = \begin{pmatrix} 0_{2\times2} & \sigma_i \\ \sigma_i & 0_{2\times2} \end{pmatrix}$$

Then $H := -i\hbar c\, \alpha\cdot\nabla + \beta m c^2$ is <u>free Dirac operator</u> and

$$i\hbar \frac{\partial \psi}{\partial t} = -i\hbar c\, \alpha\cdot\nabla + \beta m c^2, \qquad \psi(t,x) = \begin{pmatrix} \psi_1(t,x) \\ \vdots \\ \psi_4(t,x) \end{pmatrix} \in \mathbb{C}^4$$

<u>free Dirac equation</u>

Rigorous definition of the operator:

Hilbert space: $\mathcal{H} := L^2(\mathbb{R}^3)^{\oplus 4}$, $\psi = (\psi_1, \dots, \psi_4)$, $\langle \psi, \phi \rangle = \int \sum_{i=1}^{4} \overline{\psi_i(x)}\, \phi_i(x)\, dx$.

Domain: $\mathcal{D}(H) = H^1(\mathbb{R}^3)^{\oplus 4}$,

$$H\psi := -i\alpha\cdot\nabla\psi + \beta m \psi, \quad \psi \in \mathcal{D}(H) \qquad (\hbar = c = 1 \text{ from now on})$$

Selfadjointness:

How? Fourier transform! $\mathcal{F}: L^2_x \to L^2_p$

$$\mathcal{F} H \mathcal{F}^{-1} = \begin{pmatrix} m\, 1_{2\times 2} & \sum_{i=1}^{3} p_i \sigma_i \\ \sum_{i=1}^{3} p_i \sigma_i & -m\, 1_{2\times 2} \end{pmatrix} =: h(p).$$

$$\frac{1}{\sqrt{1+v^2}}$$

Eigenvalues of matrix:

$$\lambda_1(p) = \lambda_2(p) = -\lambda_3(p) = -\lambda_4(p) = \sqrt{|p|^2 + m^2}$$
$$=: \lambda(p)$$

Diagonalisation: $u(p) := a_+(p)\, 1_{4\times 4} + a_-(p)\beta \frac{1}{|p|}\sum_{i=1}^{3} p_i \alpha_i$ unitary, where

$$a_\pm(p) := \frac{1}{\sqrt{2}}\sqrt{1 \pm \frac{m}{\lambda(p)}}. \quad = \frac{1}{\sqrt{2}}\sqrt{1 \pm \sqrt{\frac{m^2}{p^2+m^2}}} = \frac{1}{\sqrt{2}}\sqrt{1 \pm \sqrt{1 - \frac{p^2}{p^2+m^2}}}$$

$$\to \frac{1}{\sqrt{2}} \text{ as } p^2 \to \infty$$

Then

$$u(p)\, h(p)\, u(p)^{-1} = \lambda(p)\beta.$$

Hence,

$$(u\mathcal{F}) H (u\mathcal{F})^{-1}(p) = \lambda(p)\beta \quad \text{in } L^2(\mathbb{R}^3_p)^4$$

selfadjoint on $\{ f \in L^2(\mathbb{R}^3)^4 \mid (1+|p|^2)^{\frac{1}{2}} f \in L^2(\mathbb{R}^d)^4 \}$

$\Longrightarrow$ H selfadjoint on $H^1(\mathbb{R}^4)$ and $\sigma(H) = (-\infty, -m] \cup [m, \infty)$

Proof of selfadjointness of h:

$\beta\lambda$ symmetric $\Rightarrow D(\beta\lambda) \subset D((\beta\lambda)^*)$ $\rightsquigarrow$ Only need to show that $D((\beta\lambda)^*) \subset D(\beta\lambda) = \{\phi \in L^2 \mid \lambda\phi \in L^2\}$.

$\phi \in D(H^*) \iff \langle \lambda\psi, \phi\rangle$ continuous in ψ. Assume $\lambda\phi \notin L^2$ for contradiction

Consider $\chi_R\psi$: $\langle \lambda\chi_R\psi, \phi\rangle = \langle \lambda\psi, \chi_R\phi\rangle$

$$= \langle \psi, \lambda\chi_R\phi\rangle \quad , \qquad \chi_R = \chi_{B_R(0)}$$

$\exists\, \psi_R \in L^2$: $\|\psi_R\| = 1$, $\langle \psi_R, \lambda\chi_R\phi\rangle = \|\lambda\chi_R\phi\|_{L^2}$ (by Hahn-Banach thm.)

Since $\lambda\phi \notin L^2$: $\|\lambda\chi_R\phi\|_{L^2} \longrightarrow \infty \quad (R \to \infty)$

$\rightsquigarrow$ sequence (ψ_R) with $\langle \psi_R, \lambda\chi_R\phi\rangle \longrightarrow \infty$

$$\iff \langle \lambda(\chi_R\psi_R), \phi\rangle \longrightarrow \infty, \quad \text{but } \|\chi_R\psi_R\| \leq 1.$$

$$\Rightarrow \langle \lambda\psi, \phi\rangle \text{ not continuous in } \psi \quad \lightning$$

$\square$

Spectral subspaces of H:

Denote $W := u\mathcal{F}$ the diagonalisation: $(WHW^{-1})(p) = \lambda(p)\beta$ in $L^2(\mathbb{R}^3)^{\oplus 4}$.

Define projections

$$P_\pm := W^{-1}\tfrac{1}{2}(1 \pm \beta)W$$

and subspaces

$$\mathcal{H}_\pm := \operatorname{Ran} P_\pm$$

Note that

$$\operatorname{Ran}\tfrac{1}{2}(1+\beta) = \left\{\begin{pmatrix}\psi_1\\ \psi_2\\ 0\\ 0\end{pmatrix}\right\}, \qquad \operatorname{Ran}\tfrac{1}{2}(1-\beta) = \left\{\begin{pmatrix}0\\ 0\\ \psi_3\\ \psi_4\end{pmatrix}\right\}.$$

Hence,

$$L^2(\mathbb{R}^3)^{\oplus 4} = \mathcal{H}_+ \oplus \mathcal{H}_-$$

and $H|_{\mathcal{H}_+}$ positive, $H|_{\mathcal{H}_-}$ negative. In fact,

$$H = U|H|, \quad \text{where} \quad |H| = \sqrt{-\Delta + m^2} \ (\text{positive}) \quad \text{and} \quad U = 1 \oplus (-1) \ \text{w.r.t. } \mathcal{H}_+ \oplus \mathcal{H}_-$$

"Polar decomposition".

Potentials:

Dirac operator for particle in external field:

$$H := \underbrace{-i\alpha\cdot\nabla + \beta m}_{H_0} + V, \qquad \alpha = (\alpha_1, \alpha_2, \alpha_3)$$

V = multiplication operator by 4×4 matrix.

Types of potentials:

Scalar: $\quad V(x) = \beta\,\phi_{sc}(x), \qquad \phi: \mathbb{R}^3 \longrightarrow \mathbb{R}.$

Electromagnetic: Vector potential: $A = (\phi_{el}, \vec{A})$

$$V(x) = \phi_{el}(x)\, 1_{4\times 4} - \alpha\cdot\vec{A}(x)$$

... and many others ...

Self-adjointness

Thm: $V: \mathbb{R}^3 \longrightarrow \mathbb{C}^4$ hermitian such that for all $i,k = 1,\ldots,4$

$$|V_{ik}(x)| \leq \frac{a}{2|x|} + b \qquad \forall x \in \mathbb{R}^3\setminus\{0\},$$

with $b>0$, $a<1$. Then $H = H_0 + V$ is essentially selfadjoint on $C_0^\infty(\mathbb{R}^3\setminus\{0\})^4$ and selfadjoint on $H^1(\mathbb{R}^3)^4$.

"boundedness $\Longrightarrow$ selfadjointness"

Proof: Assumptions imply that V is rel. bdd. w.r.t. H_0 with relative bound < 1. $\square$

Thm:

V hermitian and for all $i,k = 1,\dots,4$ one has $V \in C^\infty(\mathbb{R}^3)$.

Then $H = H_0 + V$ is essentially self adjoint on $C_0^\infty(\mathbb{R}^3)^4$

"smoothness $\Rightarrow$ selfadjointness"

Proof: Basic criterion plus elliptic regularity. $\square$

Compare this to Schrödinger!

Essential spectrum

$$\sigma_e(H) := \{\lambda \in \sigma(H) \mid \lambda \text{ accumulation point of } \sigma(H) \text{ or } \dim(\ker(\lambda - H)) = \infty\}$$

We have seen last time:

$$\sigma_e(H_0) = (-\infty, m] \cup [m, \infty)$$

Question: How does σ_e change if we add potential?

Abstract criterion:

Thm: Let A, B selfadjoint and

$$(A-z)^{-1} - (B-z)^{-1} \text{ compact for some } z \in \mathbb{C} \setminus \mathbb{R}.$$

Then $\sigma_e(A) = \sigma_e(B)$.

This can be used to prove

Thm: Let $H = H_0 + V$ be selfadjoint and V be H_0-bounded with

$$\lim_{R\to\infty} \| V (H_0 - z)^{-1} \chi_{|x| \geq R} \| = 0. \qquad (*)$$

Then $\sigma_e(H) = (-\infty, m] \cup [m, \infty)$.

Remark:

$(*)$ is implied by $V(x) \to 0$ as $|x| \to \infty$, but allows more general V.

Potentials tending to infinity

Thm:

Let $V = \Phi_{el} \, 1_{4\times4}$ and assume that

(i) $\Phi_{el}(x) = v(|x|)$

(ii) $|v(r)| \longrightarrow \infty$ if $r \to \infty$

(iii) $\left|\frac{v'(r)}{v(r)}\right| \longrightarrow 0$ as $r \to \infty$.

Then $\sigma(H_0 + V) = (-\infty, \infty)$.

Compare to Schrödinger!

Thm:

If $V = \beta \cdot \Phi_{sc}$ and

(i) $|\Phi_{sc}(x)| \longrightarrow \infty$ as $|x| \to \infty$

(ii) $\Phi_{sc}, \nabla\Phi_{sc}$ rel. bdd. w.r.t. $-\Delta + \Phi_{sc}^2$

Then $\sigma(H_0 + V)$ is purely discrete.

Proof:

Supersymmetric methods $\Rightarrow$ $\sigma(D)$ determined by $\sigma(D^*D)$

Schrödinger

$\square$

Remark:

- No explicit knowledge about $D(H_0 + V)$
- No compact resolvent
- H not sectorial $\Rightarrow$ no bilinear form defining H.