4) Exactly solvable models

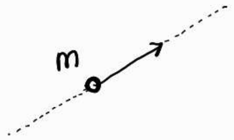
4.1) The free particle

Let us investigate the quantum dynamics of a particle in $\mathbb{R}^d$ $(d=1,2,3)$ assuming that:

- there is no interaction with any external entity;
- $v \ll c \to$ non-relativistic velocities $\rightsquigarrow$ Galilean theory;
- the mass $m>0$ is the unique dimensional parameter (no electric charge, spin, ...)

Classical Mechanics: point particle described by the Hamiltonian $H_{cl}(q,p) = \frac{p^2}{2m}$ $(q,p \in \mathbb{R}^d)$

Admissible motions $\equiv$ solutions of the Cauchy problem



$$\begin{cases} \dot{q} = \frac{\partial H_{cl}}{\partial p} = \frac{p}{m} \\ \dot{p} = -\frac{\partial H_{cl}}{\partial q} = 0 \\ q(0) = q_0, \ p(0) = p_0 \end{cases} \Rightarrow \begin{cases} q(t) = q_0 + \frac{p_0}{m} t \\ p(t) = \text{const.} = p_0 \end{cases} \to \text{Uniform rectilinear motion.}$$

Quantum Mechanics: we consider the canonical quantization of the classical model, referring to the Schrödinger representation in $L^2(\mathbb{R}^d) \equiv L^2$:

$$(Q_j\psi)(x) = x_j\psi(x), \quad D(Q_j) = \{\psi \in L^2 \mid x_j\psi \in L^2\} \text{ self-adjoint in } L^2, \quad \sigma(Q_j) = \sigma_{ac}(Q_j) = \mathbb{R}$$

$$(P_j\psi)(x) = -i\hbar\partial_j\psi(x), \quad D(P_j) = \{\psi \in L^2 \mid \partial_j\psi \in L^2\} \subset H^1 \text{ self-adj. in } L^2, \quad \sigma(P_j) = \sigma_{ac}(P_j) = \mathbb{R} \qquad \underbrace{(j=1,\dots,d)}_{\text{factorization}}$$

$$(H\psi)(x) = \frac{1}{2m}(P^2\psi)(x) = -\frac{\hbar^2}{2m}\Delta_x\psi(x), \quad D(H) = D(P^2) = \{\psi \in L^2 \mid \Delta\psi \in L^2\}$$

Rmk: Dimensionless formulation via the unitary transformation

$$\mathcal{U}: L^2(\mathbb{R}^d, dx) \longrightarrow L^2(\mathbb{R}^d, dy), \quad (\mathcal{U}\psi)(y) := \left(\frac{\hbar}{\sqrt{2m}}\right)^{d/2}\psi\left(\frac{\hbar}{\sqrt{2m}}y\right) \Rightarrow \mathcal{U}H\mathcal{U}^{-1} = -\Delta_y$$

$\hookrightarrow$ this simplifies some formulae, but it makes the comparison with CM less straightforward

Rmk: Consider the unitary Fourier transform

$$\mathcal{F}: L^2(\mathbb{R}^d, dx) \longrightarrow L^2(\mathbb{R}^d, dk), \quad (\mathcal{F}\psi)(k) := \int_{\mathbb{R}^d} dx \, \frac{e^{-ik\cdot x}}{(2\pi)^{d/2}}\psi(x) = \langle \phi_k, \psi \rangle = \hat{\psi}(k)$$

$\to$ plane wave $\phi_k(x) = \frac{e^{ik\cdot x}}{(2\pi)^{d/2}}$

$$\Rightarrow H_{\mathcal{F}} = \mathcal{F}H\mathcal{F}^{-1} = M_{\frac{\hbar^2}{2m}|k|^2} = \text{multiplication operator by } \frac{\hbar^2}{2m}|k|^2$$

Self-adjoint on $D(H_{\mathcal{F}}) = \{\hat{\psi} \in L^2 \mid |k|^2\psi \in L^2\}$, $\quad \sigma(H_{\mathcal{F}}) = \text{essran}\left(\frac{\hbar^2}{2m}|k|^2\right) = [0,\infty)$

$$\langle \hat{\psi}, H_{\mathcal{F}}\hat{\psi} \rangle = \int_{\mathbb{R}^d} dk \, \overline{\hat{\psi}(k)} \frac{\hbar^2}{2m}|k|^2 \hat{\psi}(k) = \int_0^\infty d|k| \, |k|^{d-1} \int_{S^{d-1}} d\omega \, \frac{\hbar^2|k|^2}{2m} |\hat{\psi}(|k|,\omega)|^2$$

$$= \int_0^\infty \lambda \underbrace{\left[\frac{1}{2}\left(\frac{\sqrt{2m}}{\hbar}\right)^d \lambda^{\frac{d-2}{2}} \int_{S^{d-1}} d\omega \left|\hat{\psi}\left(\frac{\sqrt{2m\lambda}}{\hbar}, \omega\right)\right|^2\right] d\lambda}_{d\mu_{H_{\mathcal{F}},\hat{\psi}}(\lambda) = F(\lambda)d\lambda} \quad \text{absolutely continuous w.r.t. Lebesgue}$$

$$\Rightarrow \sigma(H_{\mathcal{F}}) = \sigma_{ac}(H_{\mathcal{F}})$$

Proposition:

- $H = -\frac{\hbar^2}{2m}\Delta_x$ is self-adjoint on $D(H) = \{\psi \in L^2 \mid (1+|k|^2)\mathcal{F}\psi \in L^2\} = H^2(\mathbb{R}^d)$
- $\sigma(H) = \sigma_{ac}(H) = [0,\infty) =$ possible outcomes of kinetic energy measurements.
- $$\langle \psi, E_\lambda\psi \rangle = \begin{cases} \mathbb{1}_{[0,\infty)}(\lambda) \, \frac{1}{2}\left(\frac{2m}{\hbar^2}\right)^{d/2} \int_0^\lambda d\rho \, \rho^{\frac{d-2}{2}} \int_{S^{d-1}} d\omega \left|(\mathcal{F}\psi)\left(\sqrt{\frac{2m\rho}{\hbar^2}}, \omega\right)\right|^2 & \text{if } d \geq 2 \\ \mathbb{1}_{[0,\infty)}(\lambda) \, \frac{1}{2}\sqrt{\frac{2m}{\hbar^2}} \int_0^\lambda d\rho \, \rho^{-1/2} \left[\left|(\mathcal{F}\psi)\left(\sqrt{\frac{2m}{\hbar^2}\rho}\right)\right|^2 + \left|(\mathcal{F}\psi)\left(-\sqrt{\frac{2m}{\hbar^2}\rho}\right)\right|^2\right] & \text{if } d = 1 \end{cases}$$ Spectral measure (PVM)

Proof: $H = \mathcal{F}^{-1}H_{\mathcal{F}}\mathcal{F}$ + $\mathcal{F}$ unitary $\Rightarrow$ H unitarily equivalent to $H_{\mathcal{F}}$

$\langle \psi, H\psi \rangle = \langle \mathcal{U}\psi, \mathcal{U}H\mathcal{U}^{-1}\mathcal{U}\psi \rangle = \langle \hat{\psi}, H_{\mathcal{F}}\hat{\psi} \rangle$ + functional calculus $\blacksquare$

Exercises: • For $d=1$, find a singular Weyl sequence associated to any $\lambda\in[0,\infty)$.
• Check that E_λ is indeed a PVM.

Rmk: $\left\{\phi_k(x)=\frac{e^{ikx}}{(2\pi)^{d/2}}\right\}_{k\in\mathbb{R}^d}$ are distributional solutions of $H\phi_k=\frac{\hbar^2}{2m}|k|^2\phi_k$

However, $\phi_k\notin L^2\Rightarrow$ they are not proper eigenfunct. $\rightsquigarrow$ "generalized/improper eigenvectors

Proposition: the resolvent and time evolution operators act by convolution with integral kernels:

a) $(R_H(z)\psi)(x)=((H-z)^{-1}\psi)(x)=\int_{\mathbb{R}^d}dy\,G_z(x-y)\psi(y)$ $\qquad G_z(x)=\begin{cases} i\sqrt{\frac{m}{2\hbar^2 z}}\,e^{i\sqrt{\frac{2m}{\hbar^2}z}|x|} & \text{for } d=1\\ \frac{m}{2\pi\hbar^2|x|}\,e^{i\sqrt{\frac{2m}{\hbar^2}z}|x|} & \text{for } d=3\end{cases}$

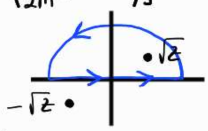
$\forall\psi\in L^2,\ z\in\rho(H)=\mathbb{C}\setminus[0,\infty)$ with $\operatorname{Im}\sqrt{z}>0$

b) $(e^{-i\frac{t}{\hbar}H}\psi)(x)=\int_{\mathbb{R}^d}K_t(x-y)\psi(y)\quad\forall\psi\in L^2,\ t\geq 0\qquad K_t(x)=\left(\frac{m}{2\pi i\hbar t}\right)^{d/2}e^{i\frac{m}{2\hbar t}|x|^2}$ for $d\geq1$

Proof: a) $R_H(z)\psi=(H-z)^{-1}\psi=\mathcal{F}^{-1}\mathcal{F}(H-z)^{-1}\mathcal{F}^{-1}\mathcal{F}\psi=\mathcal{F}^{-1}\left(\frac{\hbar^2}{2m}|k|^2-z\right)^{-1}\mathcal{F}\psi$

$$(R_H(z)\psi)(x)=\int_{\mathbb{R}^d}dk\,\frac{e^{ikx}}{(2\pi)^{d/2}}\left(\frac{\hbar^2}{2m}|k|^2-z\right)^{-1}\int_{\mathbb{R}^d}dy\,\frac{e^{-iky}}{(2\pi)^{d/2}}\psi(y)=\int_{\mathbb{R}^d}dy\left[\int_{\mathbb{R}^d}dk\,\frac{e^{ik\cdot(x-y)}}{(2\pi)^d\left(\frac{\hbar^2}{2m}|k|^2-z\right)}\right]\psi(y)$$

$d=1$: $$\int_{\mathbb{R}}dk\,\frac{e^{ikx}}{2\pi\left(\frac{\hbar^2}{2m}k^2-z\right)}=\left[k=\operatorname{sgn}(x)\sqrt{\tfrac{2m}{\hbar^2}}\right]=\frac{1}{2\pi}\sqrt{\frac{2m}{\hbar^2}}\int_{\mathbb{R}}d\xi\,\frac{e^{i\sqrt{\frac{2m}{\hbar^2}}|x|\xi}}{(\xi-\sqrt{z})(\xi+\sqrt{z})}=$$



$$=\frac{1}{2\pi}\sqrt{\frac{2m}{\hbar^2}}\cdot 2\pi i\,\operatorname{Res}\Big|_{\xi=\sqrt{z}}(\text{integrand function})=i\sqrt{\frac{m}{2\hbar^2 z}}\,e^{i\sqrt{\frac{2m}{\hbar^2}z}|x|}$$

b) $e^{-i\frac{t}{\hbar}H}\psi=\mathcal{F}^{-1}\mathcal{F}e^{-i\frac{t}{\hbar}H}\mathcal{F}^{-1}\mathcal{F}\psi=\mathcal{F}^{-1}e^{-i\frac{t}{\hbar}\left(\frac{\hbar^2}{2m}|k|^2\right)}\mathcal{F}\psi$

$$(e^{-i\frac{t}{\hbar}}\psi)(x)=\int dk\,\frac{e^{ik\cdot x}}{(2\pi)^{d/2}}e^{-i\frac{t}{\hbar}\left(\frac{\hbar^2}{2m}|k|^2\right)}\int dy\,\frac{e^{-ik\cdot y}}{(2\pi)^{d/2}}\psi(y)=\int_{\mathbb{R}^d}dy\left[\lim_{\varepsilon\to0^+}\int_{\mathbb{R}^d}\frac{dk}{(2\pi)^d}\,e^{-(\varepsilon+\frac{i\hbar t}{2m})|k|^2+ik\cdot(x-y)}\right]\psi(y)$$

$$K_t(x-y)=\lim_{\varepsilon\to0^+}\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}dk\,e^{\sum_j\left[-(\varepsilon+\frac{i\hbar t}{2m})k_j^2+ik_j(x_j-y_j)\right]}=\lim_{\varepsilon\to0^+}\prod_{j=1}^d\frac{1}{2\pi}\int_{\mathbb{R}}dk_j\,e^{-(\varepsilon+\frac{i\hbar t}{2m})k_j^2+ik_j(x_j-y_j)}$$

$$=\lim_{\varepsilon\to0^+}\prod_{j=1}^d\frac{1}{2\pi}\frac{1}{(\varepsilon+\frac{i\hbar t}{2m})^{1/2}}e^{-\frac{x_j^2}{4(\varepsilon+\frac{i\hbar t}{2m})}}\int_{\mathbb{R}}d\xi\,e^{-\xi^2}=\prod_{j=1}^d\left(\frac{m}{2\pi i\hbar t}\right)^{1/2}e^{-\frac{x_j^2}{2i\hbar t/m}}$$ ☒

Rmk: $(H-z)\varphi=\psi\ \Rightarrow\ \varphi=(H-z)^{-1}\psi\ \Rightarrow\ \varphi(x)=\int_{\mathbb{R}^d}dy\,G_z(x-y)\psi(y)$

$\hookrightarrow (H-z)\varphi=\left(-\frac{\hbar^2}{2m}\Delta_x-z\right)\int_{\mathbb{R}^d}dy\,G_z(x-y)\psi(y)=\int_{\mathbb{R}^d}dy\left(-\frac{\hbar^2}{2m}\Delta_x-z\right)G_z(x-y)\psi(y)\overset{!}{=}\psi(x)=\int_{\mathbb{R}^d}dy\,\delta(x-y)\psi(y)$

$\hookrightarrow (H_x-z)G_z(x,y)=\delta(x-y)\ \longrightarrow\ G_z=$ "Green function/fundamental solution"

Rmk: $$G_z(x,y)=G_z(x-y)=\int_{\mathbb{R}^d}dk\,\frac{e^{ikx}}{(2\pi)^{d/2}}\frac{1}{\left(\frac{\hbar^2}{2m}|k|^2-z\right)}\frac{e^{-ikx}}{(2\pi)^{d/2}}=\int_{\mathbb{R}^d}dk\,\frac{\phi_k(x)\overline{\phi_k(y)}}{\frac{\hbar^2}{2m}|k|^2-z}$$ "eigenfunction expansion"

Rmk: Explicit expression for $G_z(x-y)$ $\forall d\geq1$ in terms of Bessel functions K_ν.

Rmk: Singular behavior of $G_z(x-y)$ along the diagonal $x=y$ (UV singularity)

$$G_z(x)\ \underset{x\to0}{\sim}\ \begin{cases}1 & d=1\ \rightarrow \text{continuous, yet not differentiable}\\ \log|x| & d=2\\ |x|^{-(d-2)} & d\geq3\end{cases}$$
$d=2,\ d\geq3$ $\rightarrow$ divergent.

Rmk: Limiting absorption principle (LAP), concerning the limit $z\to\lambda\in\sigma(H)=[0,\infty)$

$z=\lambda\pm i0^+,\ \lambda\geq0\ \rightarrow\ \sqrt{z}=\pm\sqrt{\lambda}\ \Rightarrow\ G_{\lambda\pm i0^+}(x)=\begin{cases}\pm i\sqrt{\frac{m}{2\hbar^2\lambda}}\,e^{\pm i\sqrt{\frac{2m}{\hbar^2}\lambda}|x|} & d=1\\ \frac{m}{2\pi\hbar^2|x|}\,e^{\pm i\sqrt{\frac{2m}{\hbar^2}\lambda}|x|} & d=3\end{cases}$

NB: $R_H(\lambda)\notin B(L^2)$ for $\lambda\in[0,\infty)$

$\hookrightarrow$ incoming/outgoing spherical waves

$\Rightarrow$ the behaviour of $R_H(z)$ for z close to the spectrum $\sigma(H)$ determines the scattering properties of the dynamics generated by H.

Rmk: $\|e^{-i\frac{t}{\hbar}H}\psi\|_{L^2} = \|\psi\|_{L^2}$ → conservation of probability.

$$\|e^{-i\frac{t}{\hbar}H}\psi\|_{L^\infty} = \operatorname*{ess\,sup}_{x\in\mathbb{R}^d}\left|\int_{\mathbb{R}^d} dy\, K_t(x-y)\psi(y)\right| \le \operatorname*{ess\,sup}_{x'\in\mathbb{R}^d}|K_t(x')|\int_{\mathbb{R}^d} dy\,|\psi(y)| = \left(\frac{m}{2\pi\hbar t}\right)^{d/2}\|\psi\|_{L^1(\mathbb{R}^d)}$$

↳ Dispersive estimates: $\psi_0 \in L^2(\mathbb{R}^d)\cap L^1(\mathbb{R}^d) \Rightarrow \|\psi_t\|_{L^\infty} \le \frac{C}{t^{d/2}}\|\psi_0\|_{L^1} \xrightarrow{t\to\infty} 0$

They show that the time evolution ψ_t of any sufficiently regular initial datum ψ_0 vanishes almost everywhere as time increases $t\to\infty$.

Dispersive phenomena are typical in the evolution of unbounded quantum systems (a part of the system flows to infinity if no constraints are present).

Free dynamics of wavepackets for d=1

Wavepackets = states with localized positions and momenta

- they can be realized by superposition of plane waves
- they are natural candidates for reproducing the classical dynamics
- they still manifest purely quantum features → dispersion
  → interference

In the following we consider wavepackets in dimension $d=1$ of the form

$$\psi_0(x) \equiv \psi_{q_0,p_0,\varepsilon}(x) := \frac{1}{\sqrt{\varepsilon}} f\left(\frac{x-q_0}{\varepsilon}\right)e^{i\frac{p_0}{\hbar}x}, \qquad q_0,p_0\in\mathbb{R},\ 0<\varepsilon\ll 1,\ f\in S(\mathbb{R}) \text{ real-valued, even, } \|f\|_{L^2}=1$$

and examine their time evolution $\psi_t := e^{-i\frac{t}{\hbar}H}\psi_0$ for $t\ge 0$.

For brevity, we indicate the associated expectation values of any given observable A by

$$\langle A\rangle_0 \equiv \langle\psi_0, A\psi_0\rangle, \qquad \langle A\rangle_t = \langle\psi_t, A\psi_t\rangle$$

Lemma: For any ψ_0 as above there holds

$$\langle Q\rangle_0 = q_0, \quad \langle\Delta Q\rangle_0^2 = \langle Q^2\rangle_0 - \langle Q\rangle_0^2 = \varepsilon^2\|Qf\|_{L^2}^2 = \varepsilon^2\|(\mathcal{F}f)'\|_{L^2}^2$$
$$\langle P\rangle_0 = p_0, \quad \langle\Delta P\rangle_0^2 = \langle P^2\rangle_0 - \langle P\rangle_0^2 = \varepsilon^{-2}\|Pf\|_{L^2}^2 = \frac{\hbar^2}{\varepsilon^2}\|f'\|_{L^2}^2$$

Rmk: $\langle\Delta Q\rangle_0\cdot\langle\Delta P\rangle_0 = \hbar\|\hat f'\|_{L^2}\|f'\|_{L^2} = \mathcal{O}(\hbar)$ → ψ_0 is an "optimal" state, minimizing Heisenberg's uncertainty relation.

Rmk: Fixing $\varepsilon = \mathcal{O}(\sqrt{\hbar}) \Rightarrow \langle\Delta Q\rangle_0, \langle\Delta P\rangle_0 = \mathcal{O}(\sqrt{\hbar})$ → well localized positions and momenta.

Proof:
$$\langle Q\rangle_0 = \langle\psi_0, Q\psi_0\rangle = \int_{\mathbb{R}} dx\, x|\psi_0(x)|^2 = \int_{\mathbb{R}} dx\,\frac{x}{\varepsilon}\left|f\left(\frac{x-q_0}{\varepsilon}\right)\right|^2 = \int_{\mathbb{R}} dy\,(q_0+\underbrace{\cancel{\varepsilon y}}_{\text{odd}})|f(y)|^2 = q_0\|f\|_{L^2}^2 = q_0$$

$$\langle\Delta Q\rangle_0^2 = \langle\psi_0, Q^2\psi_0\rangle - \langle\psi_0, Q\psi_0\rangle^2 = \int_{\mathbb{R}} dx\, x^2|\psi_0(x)|^2 - q_0^2 = \int_{\mathbb{R}} dy\,(q_0+\varepsilon y)^2|f(y)|^2 - q_0^2$$
$$= \int_{\mathbb{R}} dy\,(\cancel{q_0^2} + \overbrace{\cancel{2q_0\varepsilon y}}^{\text{odd}} + \varepsilon^2 y^2)|f(y)|^2 - \cancel{q_0^2} = \varepsilon^2\int dy\,|y f(y)|^2 = \varepsilon^2\|y f(y)\|_{L^2}^2$$

$$\hat\psi_0(k) = \int_{\mathbb{R}} dx\,\frac{e^{-ikx}}{\sqrt{2\pi}}\psi_0(x) = \int_{\mathbb{R}} dy\,\frac{e^{-ik(q_0+\varepsilon y)}}{\sqrt{2\pi}}\sqrt{\varepsilon}\underbrace{f(y)}_{\text{even}}e^{i\frac{p_0}{\hbar}(q_0+\varepsilon y)} = \sqrt{\varepsilon}\,e^{-i\left(k-\frac{p_0}{\hbar}\right)q_0}\overbrace{\hat f}^{\text{even}}\left(\varepsilon\left(k-\frac{p_0}{\hbar}\right)\right)$$

$$\langle P\rangle_0 = \langle\psi_0, P\psi_0\rangle = \langle\hat\psi_0, \hbar k\hat\psi_0\rangle = \int_{\mathbb{R}} dk\,\hbar k\,\varepsilon\left|\hat f\left(\varepsilon\left(k-\frac{p_0}{\hbar}\right)\right)\right|^2 = \hbar\int_{\mathbb{R}} d\rho\left(\cancel{\frac{\rho}{\varepsilon}} + \frac{p_0}{\hbar}\right)|\hat f(\rho)|^2 = p_0\|\hat f\|_{L^2}^2 = p_0$$

$$\langle\Delta P\rangle_0^2 = \langle\hat\psi_0, (\hbar k)^2\hat\psi_0\rangle - \langle\hat\psi_0, \hbar k\hat\psi_0\rangle^2 = \int dk\,(\hbar k)^2\varepsilon\left|\hat f\left(\varepsilon\left(k-\frac{p_0}{\hbar}\right)\right)\right|^2 - p_0^2 = \hbar^2\int_{\mathbb{R}} d\rho\left(\frac{\rho}{\varepsilon}+\frac{p_0}{\hbar}\right)^2|\hat f(\rho)|^2 - p_0^2$$
$$= \hbar^2\int_{\mathbb{R}} d\rho\left(\frac{\rho^2}{\varepsilon^2} + \underbrace{\cancel{2\frac{p_0}{\hbar}\frac{\rho}{\varepsilon}}}_{\text{odd}} + \cancel{\frac{p_0^2}{\hbar^2}}\right)|\hat f(\rho)|^2 - \cancel{p_0^2} = \frac{\hbar^2}{\varepsilon^2}\|\rho\hat f(\rho)\|_{L^2}^2 = \frac{\hbar^2}{\varepsilon^2}\|f'\|_{L^2}^2.$$
∎

Proposition: For any $\psi_t = e^{-i\frac{t}{\hbar}H}\psi_0$, with ψ_0 as above, there holds

$$\langle Q\rangle_t = q_0 + \frac{p_0}{m}t, \qquad \langle\Delta Q\rangle_t^2 = \langle\Delta Q\rangle_0^2 + \frac{t}{m}\left(\langle QP+PQ\rangle_0 - 2\langle Q\rangle_0\langle P\rangle_0\right) + \frac{t^2}{m^2}\langle\Delta P\rangle_0^2$$
$$\langle P\rangle_t = p_0, \qquad \langle\Delta P\rangle_t^2 = \langle\Delta P\rangle_0^2$$

Rmk: $\langle Q\rangle_t, \langle P\rangle_t$ evolve in time exactly as in CM

$\hookrightarrow$ Ehrenfest theorem: $\frac{d}{dt}\langle Q\rangle_t = \frac{p_0}{m}, \quad \frac{d}{dt}\langle P\rangle_t = -\langle \nabla V(Q)\rangle_t = 0.$

Rmk: $\langle \Delta P\rangle_t = \text{const.}\ \forall t>0$ because $[P,H]=0 \to P$ is a constant of motion

$\Rightarrow$ wavepackets with well-localized momentum $\forall t>0$.

$\langle \Delta Q\rangle_t = \Theta\left(\frac{\hbar t}{\varepsilon m}\right) \xrightarrow{t\to\infty} \infty \Rightarrow$ wavepacket position stays centered in q_0, but it spreads out for large times $\rightsquigarrow$ dispersion.

Proof: $\langle P\rangle_t = \langle \psi_t, P\psi_t\rangle = \langle e^{-i\frac{t}{\hbar}H}\psi_0, Pe^{-i\frac{t}{\hbar}H}\psi_0\rangle = \langle \psi_0, e^{i\frac{t}{\hbar}H}Pe^{-i\frac{t}{\hbar}H}\psi_0\rangle = \langle \psi_0, P\psi_0\rangle = \langle P\rangle_0$

$\langle \Delta P\rangle_t^2 = \langle P^2\rangle_t - \langle P\rangle_t^2 = \dots = \langle \Delta P\rangle_0^2$

$\hat{\psi}_t(k) = \mathcal{F}(e^{-i\frac{t}{\hbar}H}\psi_0)(k) = (\mathcal{F}e^{-i\frac{t}{\hbar}H}\mathcal{F}^{-1}\mathcal{F}\psi_0)(k) = e^{-i\frac{t}{\hbar}\left(\frac{\hbar^2k^2}{2m}\right)}\hat{\psi}_0(k) \to$ in momentum representation, time evolution is just a phase shift

$i\partial_k\hat{\psi}_t(k) = \left(\frac{t}{m}\hbar k\hat{\psi}_0 + i\partial_k\hat{\psi}_0\right)e^{-i\frac{t}{\hbar}\left(\frac{\hbar^2k^2}{2m}\right)}$

$\langle Q\rangle_t = \langle \psi_t, Q\psi_t\rangle = \langle \hat{\psi}_t, \mathcal{F}Q\mathcal{F}^{-1}\hat{\psi}_t\rangle = \langle \hat{\psi}_t, i\partial_k\hat{\psi}_t\rangle = \langle \hat{\psi}_0, \left(\frac{t}{m}\hbar k\hat{\psi}_0 + i\partial_k\hat{\psi}_0\right)\rangle$

$= \frac{t}{m}\langle \psi_0, P\psi_0\rangle + \langle \psi_0, Q\psi_0\rangle = p_0\frac{t}{m} + q_0.$

$\langle \Delta Q\rangle_t^2 = \langle Q^2\rangle_t - \langle Q\rangle_t^2 = \langle \psi_t, Q^2\psi_t\rangle - \langle \psi_t, Q\psi_t\rangle^2 = \|Q\psi_t\|_{L^2}^2 - \left(q_0 + \frac{p_0}{m}t\right)^2$

$= \|\mathcal{F}Q\mathcal{F}^{-1}\mathcal{F}\psi_t\|_{L^2}^2 - \left(q_0+\frac{p_0}{m}t\right)^2 = \|i\partial_k\hat{\psi}_t\|_{L^2}^2 - \left(q_0+\frac{p_0}{m}t\right)^2 = \left\|\frac{\hbar t}{m}k\hat{\psi}_0 + i\hat{\psi}_0'\right\|_{L^2}^2 - \left(q_0+\frac{p_0}{m}t\right)^2$

$= \left\|\frac{\hbar t}{m}k\hat{\psi}_0\right\|_{L^2}^2 + 2\mathrm{Re}\langle \frac{\hbar t}{m}k\hat{\psi}_0, i\hat{\psi}_0'\rangle + \|i\hat{\psi}_0'\|_{L^2}^2 - \left(q_0+\frac{p_0}{m}t\right)^2$

$= \frac{t^2}{m^2}\|\hbar k\hat{\psi}_0\|_{L^2}^2 + \frac{t}{m}2\mathrm{Re}\langle \hbar k\hat{\psi}_0, i\partial_k\hat{\psi}_0\rangle + \|i\partial_k\hat{\psi}_0\|_{L^2}^2 - \left(q_0^2 + 2q_0\frac{p_0}{m}t + \frac{p_0^2}{m^2}t^2\right)$

$= \frac{t^2}{m^2}\left(\|P\psi_0\|_{L^2}^2 - p_0^2\right) + \frac{t}{m}\left(2\mathrm{Re}\langle P\psi_0, Q\psi_0\rangle - 2q_0p_0\right) + \left(\|Q\psi_0\|_{L^2}^2 - q_0^2\right)$

$= \frac{t^2}{m^2}\left(\langle \psi_0, P^2\psi_0\rangle - p_0^2\right) + \frac{t}{m}\left(\langle \psi_0, PQ\psi_0\rangle + \langle \psi_0, QP\psi_0\rangle - 2q_0p_0\right) + \left(\langle \psi_0, Q^2\psi_0\rangle - q_0^2\right)$

$= \frac{t^2}{m^2}\langle \Delta P\rangle_0^2 + \frac{t}{m}\left(\langle PQ+QP\rangle_0 - 2\langle Q\rangle_0\langle P\rangle_0\right) + \langle \Delta Q\rangle_0^2.$ ∎

Exercise: Compute explicitly $\psi_t(x), \langle Q\rangle_t, \langle P\rangle_t, \langle \Delta Q\rangle_t, \langle \Delta P\rangle_t$ for the Gaussian state with

$$f(x) = \frac{1}{\pi^{1/4}}e^{-\frac{1}{2}x^2}$$

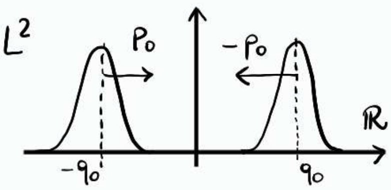
Let us now consider the coherent superposition of two wavepackets

$\psi_0(x) = \psi_0^{(L)}(x) + \psi_0^{(R)}(x) = N_0\left[\psi_{-q_0,p_0,\varepsilon}(x) + \psi_{q_0,-p_0,\varepsilon}(x)\right]$ with $q_0,p_0>0$, $0<\varepsilon\ll 1$, $N_0>0$ s.t. $\|\psi_0\|_{L^2}=1$.

Rmk: Superposition principle: ψ_0 = linear combination of two states $\in L^2$

$\Rightarrow \psi_0$ = admissible state, describing 1! particle (not 2).

$\rightsquigarrow$ single-particle interference phenomena



Rmk: $|\psi_0(x)|^2 = N_0^2\Big[\underbrace{|\psi_{-q_0,p_0,\varepsilon}(x)|^2 + |\psi_{q_0,-p_0,\varepsilon}(x)|^2}_{\text{classical probability densities}} + \underbrace{2\mathrm{Re}\left(\overline{\psi_{-q_0,p_0,\varepsilon}(x)}\,\psi_{q_0,-p_0,\varepsilon}(x)\right)}_{\text{interference Term}}\Big]$

It is possible to fix $q_0,p_0>0$, $f\in\mathcal{C}_c^\infty(\mathbb{R})$ s.t. $\mathrm{supp}(\psi_{-q_0,p_0,\varepsilon}) \cap \mathrm{supp}(\psi_{q_0,-p_0,\varepsilon}) = \emptyset$

$\Rightarrow \overline{\psi_{-q_0,p_0,\varepsilon}(x)}\cdot\psi_{q_0,-p_0,\varepsilon}(x) = 0 \Rightarrow$ NO interference at $t=0$.

Rmk: By linearity, each wavepacket evolves in accordance with the free quantum dynamics

$\left.\begin{array}{l}\langle Q\rangle_{\psi_t^{(L)}} = -q_0 + \frac{p_0}{m}t \\ \langle Q\rangle_{\psi_t^{(R)}} = q_0 - \frac{p_0}{m}t\end{array}\right\} \Rightarrow$ At the classical collision time $t_c = \frac{mq_0}{p_0}$ the centers of the two wavepackets overlap in $x=0$.

Lemma: $\psi_t = e^{-i\frac{t}{\hbar}H}\psi_0 \Rightarrow \psi_{t_c}(x) = 2N_0\cos\left(\frac{p_0}{\hbar}x\right)\left(e^{-i\frac{t_c}{\hbar}H}\psi_{0,0,\varepsilon}\right)(x)\,e^{-i\frac{q_0p_0}{2\hbar}}$

Proof: $\psi_t(x) = N_0\left[\left(e^{-i\frac{t}{\hbar}H}\psi_{-q_0,p_0,\varepsilon}\right)(x) + \left(e^{-i\frac{t}{\hbar}H}\psi_{q_0,-p_0,\varepsilon}\right)(x)\right]$

$$= N_0\,\mathcal{F}^{-1}\left[e^{-i\frac{t}{\hbar}\left(\frac{\hbar^2k^2}{2m}\right)}\left(\hat\psi_{-q_0,p_0,\varepsilon}(k)+\hat\psi_{q_0,-p_0,\varepsilon}(k)\right)\right](x)$$

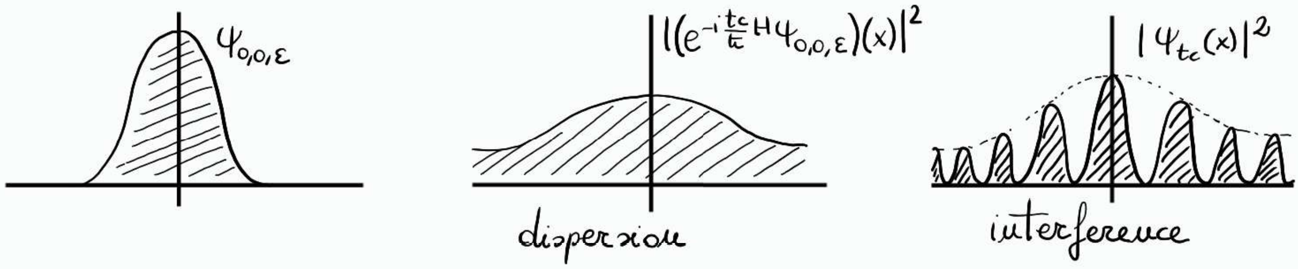
$$= N_0\int dk\,\frac{e^{ikx}}{\sqrt{2\pi}}\,e^{-i\frac{t}{\hbar}\frac{\hbar^2k^2}{2m}}\sqrt{\varepsilon}\left[\hat f\left(\varepsilon\left(k-\frac{p_0}{\hbar}\right)\right)e^{i\left(k-\frac{p_0}{\hbar}\right)q_0} + \hat f\left(\varepsilon\left(k+\frac{p_0}{\hbar}\right)\right)e^{-i\left(k+\frac{p_0}{\hbar}\right)q_0}\right]$$

$$= N_0\sqrt{\frac{\varepsilon}{2\pi}}\,e^{-i\frac{t}{\hbar}\frac{p_0^2}{2m}}\int dk'\left[e^{i\frac{p_0}{\hbar}x-i\frac{t}{\hbar}\frac{\hbar^2k'^2}{2m}+ik'\left(-\frac{p_0t}{m}+q_0+x\right)} + \left(\begin{matrix}q_0\to -q_0\\ p_0\to -p_0\end{matrix}\right)\right]\hat f(\varepsilon k')$$

$$\psi_{t_c}(x) = N_0\sqrt{\frac{\varepsilon}{2\pi}}\,e^{-i\frac{t}{\hbar}\frac{p_0^2}{2m}}\,2\cos\left(\frac{p_0}{\hbar}x\right)\int dk'\,e^{-i\frac{t_c}{\hbar}\frac{\hbar^2k'^2}{2m}+ik'x}\,\hat f(\varepsilon k')$$

$$= 2N_0\cos\left(\frac{p_0}{\hbar}x\right)e^{-i\frac{t_c}{\hbar}\frac{p_0^2}{2m}}\left(e^{-i\frac{t_c}{\hbar}H}\psi_{0,0,\varepsilon}\right)(x). \quad \blacksquare$$

Rmk: $|\psi_{t_c}(x)|^2 = 4N_0^2\left|\left(e^{-i\frac{t_c}{\hbar}H}\psi_{0,0,\varepsilon}\right)(x)\right|^2\cos\left(\frac{p_0}{\hbar}x\right)$



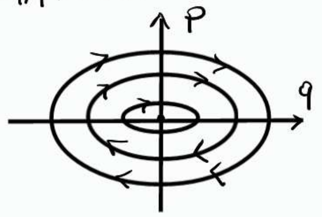
Exercise: Perform the explicit computation for $f(x) = \frac{1}{\pi^{1/4}}e^{-\frac{1}{2}x^2}$.
Examine the limiting regime where $\frac{\varepsilon}{q_0} \ll \frac{\hbar}{\varepsilon p_0} \ll 1$.

4.2) The harmonic oscillator

One of the simplest models with a non-trivial interaction potential, modelling the confinement of a quantum particle.
Let us consider the motion of a quantum particle of mass $m>0$ on a 1D line subject to a conservative force field $F=-\nabla V$ with potential energy $V(x) = \frac{1}{2}m\omega^2x^2$ ($\omega>0$).

Classical Mechanics: Hamiltonian $H_{cl}(q,p) = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2q^2$ with $(q,p)\in\mathbb{R}^2$.

$$\begin{cases}\dot q = \frac{\partial H_{cl}}{\partial p} = \frac{p}{m}\\ \dot p = -\frac{\partial H_{cl}}{\partial q} = -m\omega^2 q\\ q(0)=q_0,\ p(0)=p_0\end{cases} \Rightarrow \begin{cases}\ddot q = -\omega^2 q\\ p = m\dot q\end{cases} \Rightarrow \begin{cases}q(t) = q_0\cos(\omega t)+\frac{p_0}{m\omega}\sin(\omega t)\\ p(t) = -m\omega q_0\sin(\omega t)+p_0\cos(\omega t)\end{cases}$$



Rmk: $\exists$ stationary orbit $\equiv$ stable equilibrium, i.e. $(q_0,p_0)=(0,0)$

Rmk: All orbits in phase space are bounded and closed, whence periodic with period $T=\frac{2\pi}{\omega}$

Quantum Mechanics By canonical quantization we introduce the Hamiltonian operator

$$H = \frac{1}{2m}P^2 + \frac{1}{2}m\omega^2Q^2 = -\frac{\hbar^2}{2m}\Delta_x + \frac{1}{2}m\omega^2x^2$$

Rmk: No ordering problems (such as $QP, PQ, \frac{1}{2}(QP+PQ), \dots$)

Rmk: H symmetric on $D(H) = S(\mathbb{R})\subset L^2(\mathbb{R})$, yet not bounded, not closed, not self-adjoint.
In the sequel it will be argued that H is essentially self-adjoint, proving:

- $\exists\{b_n\}_{n\in\mathbb{N}}$ Hilbert basis of eigenvectors in $L^2(\mathbb{R})$.
- $U: L^2(\mathbb{R})\to \ell^2(\mathbb{N})$ unitary.
- $\sigma(H) = \sigma_{pp}(H)$ pure point spectrum.

Lemma (dimensionless formulation) $\exists\, U : L^2(\mathbb{R}, dx) \to L^2(\mathbb{R}, dy)$ unitary operator s.t.

$$U H U^{-1} = \hbar\omega \hat{H} \quad \text{with} \quad \hat{H} = \frac{1}{2}\hat{P}^2 + \frac{1}{2}\hat{Q}^2, \quad \hat{P} = -i\partial_y, \ \hat{Q} = y.$$

Proof: consider the generic scaling transformation $(U_{\alpha\beta}\psi)(y) = \alpha\psi(\beta y)$, with $\alpha, \beta > 0$.

- demanding $U_{\alpha\beta} : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ to be a unitary operator yields

$$\| U_{\alpha\beta}\psi \|^2_{L^2} = \int dy\, |\alpha\psi(\beta y)|^2 = \alpha^2 \int \frac{dx}{\beta} |\psi(x)|^2 = \frac{\alpha^2}{\beta}\|\psi\|^2_{L^2} \overset{!}{=} \|\psi\|^2_{L^2} \quad \Rightarrow \quad \beta = \alpha^2$$

- demanding $U_{\alpha\beta} H U^{-1}_{\alpha\beta} = \gamma\left(\frac{1}{2}\hat{P}^2 + \frac{1}{2}\hat{Q}^2\right)$ yields

$$(U_{\alpha\beta} H \tilde{\psi})(y) = \alpha\left(-\frac{\hbar^2}{2m}\tilde{\psi}''(\beta y) + \frac{1}{2}m\omega^2(\beta y)^2\tilde{\psi}(\beta y)\right) = \alpha\left(-\frac{\hbar^2}{2m}\frac{1}{\beta^2}\frac{\partial^2}{\partial y^2} + \frac{1}{2}\beta^2 m\omega^2 y^2\right)\tilde{\psi}(\beta y)$$

$$\parallel$$

$$\gamma\left(\frac{1}{2}\hat{P}^2 + \frac{1}{2}\hat{Q}^2\right) U_{\alpha\beta}\tilde{\psi}(y) = \frac{\gamma}{2}\left(-\partial_{yy} + y^2\right)\alpha\tilde{\psi}(\beta y) \quad \Rightarrow \quad \gamma = \frac{\hbar^2}{m\beta^2} = \beta^2 m\omega^2$$

- Summing up, $\beta = \sqrt{\frac{\hbar}{m\omega}}$, $\alpha = \frac{\hbar}{m\omega}$, $\gamma = \hbar\omega$. ∎

Def: the annihilation and creation operators are

$$a := \frac{1}{\sqrt{2}}(\hat{Q} + i\hat{P}) = \frac{1}{\sqrt{2}}(y + \partial_y), \qquad D(a) = S(\mathbb{R}) \subset \overline{D(\hat{Q}) \cap D(\hat{P})} \subset L^2(\mathbb{R}, dy)$$

$$a^+ := \frac{1}{\sqrt{2}}(\hat{Q} - i\hat{P}) = \frac{1}{\sqrt{2}}(y - \partial_y), \qquad D(a^+) = S(\mathbb{R}) \subset \overline{D(\hat{Q}) \cap D(\hat{P})} \subset L^2(\mathbb{R}, dy)$$

Lemma: 1) $\langle \varphi, a\psi \rangle = \langle a^+\varphi, \psi \rangle$

2) $[a, a^+]\psi = \psi$ $\qquad \forall\, \varphi, \psi \in S(\mathbb{R})$

3) $\hat{H}\psi = \left(a^+a + \frac{1}{2}\right)\psi = \left(aa^+ - \frac{1}{2}\right)\psi$

4) $[H, a]\psi = -a\psi$, $[H, a^+]\psi = a^+\psi$

Proof: 1) $\langle \varphi, a\psi \rangle = \int_{\mathbb{R}} dy\, \overline{\varphi}(y)\frac{1}{\sqrt{2}}(y + \partial_y)\psi(y) = \left[\begin{matrix}\text{integration}\\ \text{by parts}\end{matrix}\right] = \int_{\mathbb{R}} \frac{1}{\sqrt{2}}\overline{(y - \partial_y)\varphi(y)}\,\psi(y) = \langle a^+\varphi, \psi \rangle$

3) $aa^+\psi = \frac{1}{\sqrt{2}}(y + \partial_y)\frac{1}{\sqrt{2}}(y - \partial_y)\psi = \frac{1}{2}\left(y^2 - \cancel{y\partial_y} + 1 + \cancel{y\partial_y} - \partial_y^2\right)\psi = \frac{1}{2}\left(-\partial_y^2 + y^2 + 1\right)\psi = \left(\hat{H} + \frac{1}{2}\right)\psi$

$a^+a\psi = \frac{1}{\sqrt{2}}(y - \partial_y)\frac{1}{\sqrt{2}}(y + \partial_y)\psi = \frac{1}{2}\left(y^2 + \cancel{y\partial_y} - 1 - \cancel{y\partial_y} - \partial_y^2\right)\psi = \frac{1}{2}\left(-\partial_y^2 + y^2 - 1\right)\psi = \left(\hat{H} - \frac{1}{2}\right)\psi$

2) $[a, a^+]\psi = (aa^+ - a^+a)\psi = \left[\cancel{\hat{H}} + \frac{1}{2} - \left(\cancel{\hat{H}} - \frac{1}{2}\right)\right]\psi = \psi$

4) $[H, a]\psi = \left[a^+a + \cancel{\tfrac{1}{2}}, a\right]\psi = [a^+, a]\,a\psi = -a\psi$

$[H, a^+]\psi = \left[a^+a + \cancel{\tfrac{1}{2}}, a^+\right]\psi = a^+[a, a^+]\psi = a^+\psi$. ∎

Proposition: Let $\lambda \in \sigma_p(\hat{H})$, $\psi_\lambda \in S(\mathbb{R})$ s.t. $\hat{H}\psi_\lambda = \lambda\psi_\lambda$, $\|\psi_\lambda\|_{L^2} = 1$. Then:

a) $\lambda \geq 1/2$;

b) $\hat{H}(a^+\psi_\lambda) = (\lambda + 1)\,a^+\psi_\lambda$, $\quad \|a^+\psi_\lambda\|_{L^2} = \sqrt{\lambda + 1/2}$;

c) If $\lambda > 1/2$, $\hat{H}(a\psi_\lambda) = (\lambda - 1)\,a\psi_\lambda$, $\quad \|a\psi_\lambda\|_{L^2} = \sqrt{\lambda - 1/2}$.

Proof: a) $\lambda = \langle \psi_\lambda, \hat{H}\psi_\lambda \rangle = \langle \psi_\lambda, (a^+a + \frac{1}{2})\psi_\lambda \rangle = \langle a\psi_\lambda, a\psi_\lambda \rangle + \frac{1}{2}\langle \psi_\lambda, \psi_\lambda \rangle = \|a\psi_\lambda\|^2_{L^2} + \frac{1}{2}\|\psi_\lambda\|^2_{L^2} \geq \frac{1}{2}\|\psi_\lambda\|^2_{L^2} = \frac{1}{2}$

b) $\hat{H}a^+\psi_\lambda = \left([\hat{H}, a^+] + a^+\hat{H}\right)\psi_\lambda = a^+\psi_\lambda + a^+\lambda\psi_\lambda = (\lambda + 1)\,a^+\psi_\lambda$

$\|a^+\psi_\lambda\|^2_{L^2} = \langle a^+\psi_\lambda, a^+\psi_\lambda \rangle = \langle \psi_\lambda, aa^+\psi_\lambda \rangle = \langle \psi_\lambda, (\hat{H} + 1/2)\psi_\lambda \rangle = (\lambda + 1/2)\|\psi_\lambda\|^2_{L^2} = (\lambda + 1/2)$

c) $\hat{H}a\psi_\lambda = \left([\hat{H}, a] + a\hat{H}\right)\psi_\lambda = -a\psi_\lambda + a\lambda\psi_\lambda = (\lambda - 1)\,a\psi_\lambda$

$\|a\psi_\lambda\|^2_{L^2} = \langle a\psi_\lambda, a\psi_\lambda \rangle = \langle \psi_\lambda, a^+a\psi_\lambda \rangle = \langle \psi_\lambda, (\hat{H} - 1/2)\psi_\lambda \rangle = (\lambda - 1/2)\|\psi_\lambda\|^2_{L^2} = (\lambda - 1/2)$

NB: $\lambda > 1/2$, otherwise $\|a\psi_\lambda\|^2_{L^2} \leq 0 \Leftrightarrow a\psi_\lambda = 0$ which is not an eigenstate. ∎

Proposition: $\sigma(\hat{H}) = \sigma_{pp}(\hat{H}) = \{n + \frac{1}{2} \mid n \in \mathbb{N}\}$

$$\left\{\hat{b}_n := \frac{1}{\sqrt{n!}}(a^+)^n b_0, \quad \hat{b}_0(y) = \frac{1}{\pi^{1/4}}e^{-\frac{1}{2}y^2}\right\} \text{ is a Hilbert basis of } L^2(\mathbb{R})$$

Proof: Let $\lambda = n + 1/2$ with $n \in \mathbb{N} = \{0,1,2,\dots\}$. Then:

$\underline{n=0}$: $\lambda_0 = 1/2$, $\hat{H}\psi_0 = \lambda_0 \psi_0 \overset{(a)}{\Rightarrow} \|a\psi_0\|_{L^2} = 0 \Rightarrow 0 = a\psi_0 = (y + \partial_y)\psi_0(y) \Rightarrow \psi_0(y) = c\, e^{-\frac{1}{2}y^2} \in S(\mathbb{R})$ unique solution

Normalization: $1 = \|\psi_0\|^2_{L^2} = c^2 \int dy\, e^{-y^2} = c^2\sqrt{\pi} \Rightarrow c = \pi^{-1/4}$

$\underline{n=1}$: $\lambda_1 = 3/2$, $\hat{H}_1\psi_1 = \lambda_1\psi_1 \overset{(b)}{\Rightarrow} \psi_1 = a^+\hat{b}_0$ is the unique solution

$\left(\text{By contradiction: } \exists\, \varphi_1 \neq \psi_1 \text{ s.t. } H_1\varphi_1 = \lambda_1\varphi_1 \overset{(c)}{\Rightarrow} H(a\varphi_1) = (\lambda_1 - 1)a\varphi_1 = \lambda_0 a\varphi_1 \Rightarrow a\varphi_1 = \hat{b}_0 \right.$
$\left. \Rightarrow \psi_1 = a^+\hat{b}_0 = a^+a\,\varphi_1 = (H - \tfrac{1}{2})\varphi_1 = (\lambda_1 - \tfrac{1}{2})\varphi_1 = \varphi_1 \ \lightning \right)$

Normalization: $1 = \|\psi_1\|^2_{L^2} = \|a^+\hat{b}_0\|^2_{L^2} = \sqrt{\lambda_0 + 1/2} = 1$.

$\underline{n \geq 2}$: by iteration

$\hookrightarrow \{\hat{b}_n\}_{n\in\mathbb{N}}$ are eigenvectors of H with eigenvalues $\lambda_n = n + 1/2 \Rightarrow \hat{b}_n \perp \hat{b}_m$ if $n \neq m$

$\{\hat{b}_n\}$ is a complete system in $L^2(\mathbb{R})$ if and only if $\langle \hat{b}_n, \psi\rangle = 0\ \forall n \Rightarrow \psi = 0$:

- By direct computation we get $\hat{b}_n = \frac{1}{\sqrt{n!}}(a^+)^n\hat{b}_0 = (\text{polynomial in } y \text{ of degree } n)\cdot e^{-\frac{1}{2}y^2}$
  $\Rightarrow \operatorname{span}(\{\hat{b}_n\}) = \operatorname{span}(\{y_n e^{-\frac{1}{2}y^2}\})$
- Let $\varphi \in L^2(\mathbb{R})$ s.t. $\varphi \perp \operatorname{span}(\{\hat{b}_n\})$. Then:

$$\mathcal{F}(\varphi(y)e^{-\frac{1}{2}y^2})(k) = \int dy\, \frac{e^{-iky}}{\sqrt{2\pi}}\varphi(y)e^{-\frac{1}{2}y^2} = \frac{1}{\sqrt{2\pi}}\int dy \sum_{n=0}^{\infty}\frac{(-iky)^n}{n!}e^{-\frac{1}{2}y^2}\varphi(y) = \left[\begin{array}{c}\text{Dominated}\\ \text{convergence}\end{array}\right]$$
$$= \frac{1}{\sqrt{2\pi}}\sum_{n=0}^{\infty}\frac{(-ik)^n}{n!}\int dy\, y^n e^{-\frac{1}{2}y^2}\varphi(y) = \frac{1}{\sqrt{2\pi}}\sum_{n=0}^{\infty}\frac{(-ik)^n}{n!}\cancel{\langle y^n e^{-\frac{1}{2}y^2}, \varphi\rangle_{L^2}} = 0$$

$\mathcal{F}$ is unitary $\Rightarrow \varphi(y)e^{-\frac{1}{2}y^2} = \mathcal{F}^{-1}0 = 0 \Rightarrow \varphi = 0$

Corollary: $\hat{b}_n(y) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(y)\, e^{-\frac{1}{2}y^2}$, where $H_n(y) := (-1)^n e^{y^2}\frac{d^n}{dy^n}e^{-y^2}$ $(n \in \mathbb{N})$
Hermite polynomials

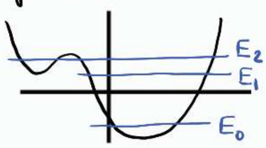
(Proof by induction on $n \in \mathbb{N}$)

Rmk: purely point spectrum with simple eigenvalues $\to$ no degeneracy.

Rmk: the harmonic oscillator is a case study where the Rellich criterion applies

theorem: Let $V \in L^1_{loc}(\mathbb{R}^d)$, with ess-inf $V \geq V_0$ for some finite $V_0 \in \mathbb{R}$ and $V(x) \xrightarrow{|x|\to\infty} \infty$.
Then, $H = -\Delta + V$ the self-adjoint operator defined by quadratic forms has purely point spectrum, i.e., $\sigma(H) = \sigma_{pp}(H)$.

(the proof relies on quadratic form methods and resolvent compactness, see Reed-Simon Vol. IV, Ch. XIII.14, Thm. XIII.67)



Rmk: $W: L^2(\mathbb{R}) \to \ell^2(\mathbb{N})$, $(W\psi)_n := \langle \hat{b}_n, \psi\rangle$ is a unitary transformation which diagonalizes $\hat{H}$

$(W\hat{H}W^{-1}f)_n = (n + \tfrac{1}{2})f_n \quad \forall f = (f_n)_{n\in\mathbb{N}} \in \ell^2(\mathbb{N}) \quad \longleftrightarrow \quad \hat{H}\psi = s\text{-}\sum_{n=0}^{\infty}(n+\tfrac{1}{2})\langle \hat{b}_n, \psi\rangle \hat{b}_n$

Let us now go back to the original dimensional problem using the unitary inverse operator

$U^{-1}: L^2(\mathbb{R}, dy) \to L^2(\mathbb{R}, dx)$, $\quad (U^{-1}\psi)(x) = \sqrt[4]{\frac{m\omega}{\hbar}}\,\psi\left(\sqrt{\frac{m\omega}{\hbar}}\right)$.

In particular, notice that $\{b_n = U^{-1}\hat{b}_n\}_{n\in\mathbb{N}}$ is an Hilbert basis of $L^2(\mathbb{R})$ consisting of eigenvalues of H with eigenvalues $\{E_n = \hbar\omega(n + \frac{1}{2})\}_{n\in\mathbb{N}}$. From here, it follows that:

Theorem. $\exists!$ self-adjoint extension of the symmetric operator $H = -\frac{\hbar^2}{2m}\Delta_x + \frac{1}{2}m\omega^2$, initially defined on $S(\mathbb{R})$. This extension is given by

$$D(H) = \left\{\psi \in L^2(\mathbb{R}, dx) \,\middle|\, H\psi \in L^2(\mathbb{R}, dx)\right\} = \left\{\psi \in L^2(\mathbb{R}, dx) \,\middle|\, \sum_{n=0}^{\infty}(n + \tfrac{1}{2})|\langle b_n, \psi\rangle|^2 < \infty\right\}$$
$$H\psi = s\text{-}\sum_{n=0}^{\infty}\hbar\omega(n + \tfrac{1}{2})\langle b_n, \psi\rangle b_n$$

- $\sigma(H) = \sigma_{pp}(H) = \{\hbar\omega(n+\frac{1}{2})\}_{n\in\mathbb{N}}$ pure point spectrum.
- $\langle\psi, P_\lambda\psi\rangle = \sum_{\substack{n\in\mathbb{N} \text{ s.t.} \\ \hbar\omega(n+1/2)\leq\lambda}} |\langle b_n,\psi\rangle|^2$ spectral measure.

Rmk: Ground state (fundamental state): $b_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \Rightarrow \langle\Delta Q\rangle_{b_0}\langle\Delta P\rangle_{b_0} = \frac{\hbar}{2}$ (minimal uncertainty)

Excited states: b_n $\forall n\geq 1$

Rmk: $\inf\sigma(H) = \frac{1}{2}\hbar\omega \to$ related to Heisenberg uncertainty principle.

$$\sigma(H)\ni\lambda = \langle\psi, H\psi\rangle = \underbrace{\tfrac{1}{2m}\langle P^2\rangle_\psi}_{a^2} + \underbrace{\tfrac{1}{2}m\omega^2\langle Q^2\rangle_\psi}_{b^2} \geq 2\underbrace{\sqrt{\tfrac{1}{2m}\langle P^2\rangle_\psi}}_{a}\underbrace{\sqrt{\tfrac{1}{2}m\omega^2\langle Q^2\rangle_\psi}}_{b} = \omega\sqrt{\langle P^2\rangle_\psi\langle Q^2\rangle_\psi} \geq \omega\frac{\hbar}{2}$$

Proposition: a) Time evolution described by the strongly continuous one-parameter unitary group

$$\psi_t = e^{-i\frac{t}{\hbar}H}\psi_0 = s\text{-}\sum_{n=0}^{\infty} e^{-i\frac{t}{\hbar}\hbar\omega(n+\frac{1}{2})}\langle b_n,\psi_0\rangle b_n = s\text{-}\sum_{n=0}^{\infty} e^{-it\omega(n+\frac{1}{2})}\langle b_n,\psi_0\rangle b_n$$

b) $\frac{d}{dt}\langle Q\rangle_{\psi_t} = \frac{1}{m}\langle P\rangle_{\psi_t}$, $\frac{d}{dt}\langle P\rangle_{\psi_t} = -m\omega^2\langle Q\rangle_{\psi_t}$ Ehrenfest theorem.

c) $\forall\psi_0\in L^2(\mathbb{R},dx), \forall\varepsilon>0\ \exists R>0$ s.t. $\sup_{t\in\mathbb{R}}\int_{\{|x|>R\}} dx\, |\psi_t(x)|^2 = \sup_t \|\mathbb{1}_{[-R,R]^c}(Q)\psi_t\|_{L^2}^2 < \varepsilon$

Proof: a) Consequence of the spectral theorem.

b)
$$\frac{d}{dt}\langle Q\rangle_{\psi_t} = \frac{d}{dt}\langle e^{-i\frac{t}{\hbar}H}\psi_0, Q e^{-i\frac{t}{\hbar}H}\psi_0\rangle = \langle e^{-i\frac{t}{\hbar}H}\psi_0, \frac{i}{\hbar}[H,Q]e^{-i\frac{t}{\hbar}H}\psi_0\rangle = \langle\psi_t, \frac{i}{\hbar}\left[\frac{1}{2m}P^2,Q\right]\psi_t\rangle$$
$$= \langle\psi_t, \frac{i}{\hbar}\frac{1}{2m}\left(P[P,Q]+[P,Q]P\right)\psi_t\rangle = \langle\psi_t, \frac{i}{\cancel{\hbar}}\frac{1}{\cancel{2}m}\cancel{2}(-i\cancel{\hbar})P\psi_t\rangle = \frac{1}{m}\langle\psi_t, P\psi_t\rangle.$$
$$\frac{d}{dt}\langle P\rangle_{\psi_t} = \frac{d}{dt}\langle e^{-i\frac{t}{\hbar}H}\psi_0, P e^{-i\frac{t}{\hbar}H}\psi_0\rangle = \langle e^{-i\frac{t}{\hbar}H}\psi_0, \frac{i}{\hbar}[H,P]e^{-i\frac{t}{\hbar}H}\psi_0\rangle = \langle\psi_t, \frac{i}{\hbar}\left[\frac{1}{2}m\omega^2Q^2,P\right]\psi_t\rangle$$
$$= \langle\psi_t, \frac{i}{\hbar}\frac{1}{2}m\omega^2\left(Q[Q,P]+[Q,P]Q\right)\psi_t\rangle = \langle\psi_t, \frac{i}{\cancel{\hbar}}\frac{1}{\cancel{2}}m\omega^2\cancel{2}i\cancel{\hbar}Q\psi_t\rangle = -m\omega^2\langle\psi_t, Q\psi_t\rangle$$

Rmk: $\langle Q\rangle_{\psi_t}, \langle P\rangle_{\psi_t}$ make sense if $\psi_t\in D(Q)\cap D(P)$

To differentiate in strong sense one needs $\psi_t\in D(H)$

↳ The above manipulations require $\psi_t\in D(Q)\cap D(P)\cap D(H)\cap D(HQ)\cap D(QH)\cap D(PH)\cap D(HP)$.

Rmk: Exact matching with CM because the potential is quadratic

c)
$$\|\mathbb{1}_{[-R,R]^c}(Q)\psi_t\|_{L^2} = \|\mathbb{1}_{[-R,R]^c}(Q)e^{-i\frac{t}{\hbar}H}\left[\left(\psi_0 - \textstyle\sum_{n=0}^N\langle b_n,\psi_0\rangle b_n\right) + \left(\textstyle\sum_{n=0}^N\langle b_n,\psi_0\rangle b_n\right)\right]\|_{L^2}$$
$$\leq \|\mathbb{1}_{[-R,R]^c}(Q)e^{-i\frac{t}{\hbar}H}\left(\psi_0 - \textstyle\sum_{n=0}^N\langle b_n,\psi_0\rangle b_n\right)\|_{L^2} + \|\mathbb{1}_{[-R,R]^c}(Q)\textstyle\sum_{n=0}^N e^{-it\omega(n+\frac{1}{2})}\langle b_n,\psi_0\rangle b_n\|_{L^2}$$
$$\leq \|\psi_0 - \textstyle\sum_{n=0}^N\langle b_n,\psi_0\rangle b_n\|_{L^2} + \textstyle\sum_{n=0}^N|\langle b_n,\psi_0\rangle|\,\|\mathbb{1}_{[-R,R]^c}(Q)b_n\|_{L^2} < \frac{\sqrt{\varepsilon}}{2}+\frac{\sqrt{\varepsilon}}{2} = \sqrt{\varepsilon}$$

- $\{b_n\}$ Hilbert basis $\Rightarrow \forall\varepsilon>0\ \exists N_\varepsilon>0$ s.t. $\|\psi_0 - \sum_{n=0}^N\langle b_n,\psi_0\rangle b_n\|_{L^2} < \frac{\sqrt{\varepsilon}}{2}$ $\forall N>N_\varepsilon$
- $b_n\in L^2(\mathbb{R}) \Rightarrow \forall\varepsilon>0\ \exists R_\varepsilon>0$ s.t. $\|\mathbb{1}_{[-R,R]^c}(Q)b_n\|_{L^2} \leq \frac{\sqrt{\varepsilon}}{2(N+1)\max_{n\in N}|\langle b_n,\psi\rangle|}$

Exercise: Compute explicitly $\psi_t(x) = (e^{-i\frac{t}{\hbar}H}\psi_0)(x)$ for a Gaussian initial state of the form

$$\psi_0(x) = \frac{1}{\sqrt[4]{\pi\hbar a_0^2}} e^{-\frac{b_0}{2\hbar a_0}(x-q_0)^2 + i\frac{p_0}{\hbar}(x-q_0)} \quad \text{with } a_0,b_0\in\mathbb{C},\ Re\left(\frac{b_0}{a_0}\right) = \frac{1}{|a_0|^2},\ Re\left(\frac{a_0}{b_0}\right) = \frac{1}{|b_0|^2}$$

Compare the result with the CM evolution.

d-dimensional generalization

Let us now examine the case of an anisotropic harmonic oscillator, described by

$$H_d = -\frac{\hbar^2}{2m}\Delta_x + \frac{1}{2}m\sum_{\ell=1}^d \omega_\ell^2 x_\ell^2 \qquad D(H_d) = S(\mathbb{R}^d)\subset L^2(\mathbb{R}^d)$$

Rmk Exploiting the Hilbert space isomorfism $L^2(\mathbb{R}^d)\simeq L^2(\mathbb{R})\otimes\ldots\otimes L^2(\mathbb{R})$ we infer

$$H_d = \sum_{\ell=1}^d\left(-\frac{\hbar^2}{2m}\partial^2_{x_\ell} + \frac{1}{2}m\omega_\ell^2x_\ell^2\right) = H^{(1D)}_{\omega_1}\otimes\mathbb{1}\otimes\ldots\otimes\mathbb{1} + \ldots + \mathbb{1}\otimes\ldots\otimes\mathbb{1}\otimes H^{(1D)}_{\omega_d}$$

Proposition: • $\exists!$ self-adjoint extension of H_d, with $D(H_d)=\{\psi\in L^2(\mathbb{R}^d)\mid H_d\psi\in L^2(\mathbb{R}^d)\}$

• $\sigma(H_d)=\sigma_{pp}(H_d)=\{\hbar(\omega_1 n_1+\dots+\omega_d n_d+\frac{d}{2})\mid n_1,\dots,n_d\in\mathbb{N}\}$

$b_{n_1\dots n_d}(x_1,\dots,x_d)=b_{n_1}(x_1)\dots b_{n_d}(x_d)$ is a Hilbertian base of $L^2(\mathbb{R}^d)$ consisting of eigenvectors of H_d

• explicit expressions for the spectral measure, resolvent, time evolution.

Rmk: If at least two of the frequencies are resonant (i.e., $\exists q\in\mathbb{Q}$ s.t. $\omega_i=q\omega_j$ for some $i\neq j$), then some of the eigenvalues are degenerate.
In particular, if $\omega_1=\dots=\omega_d=\omega$, then all the excited energy levels are degenerate, while the ground state remains unique.

4.3) The hydrogen atom

The hydrogen atom is a system consisting of two interacting particles:

- e^- = electron, mass $m_e\sim 10^{-30}\,kg\sim 0.5\,MeV/c^2$, electric charge $q_e\sim -1.6\cdot 10^{-19}C$;
- p^+ = proton, mass $m_p\sim 2\cdot 10^3 m_e$, electric charge $q_p=-q_e$.

Approximations: • $v_e, v_p\ll c$ (non-relativistic Galilean theory)
• purely electrostatic interaction (negligible magnetic effects)
• scalar particles (negligible spin effects)
} sub-leading order corrections.

Classical Mechanics: Two point particles described by the Lagrangian function

$$L_{cl}(q_e,q_p;\dot q_e,\dot q_p)=\frac{1}{2}m_e|\dot q_e|^2+\frac{1}{2}m_p|\dot q_p|^2+\frac{ke^2}{|q_e-q_p|}\qquad(\bar q_e,\bar q_p,\dot q_e,\dot q_p)\in\mathbb{R}^{3+3}\times\mathbb{R}^{3+3}$$

Passing to center of mass / relative coordinates $\qquad k=\frac{1}{4\pi\varepsilon_0}\simeq 10^{10}\,N\,m^2/C^2$ (ε_0 → vacuum electric permittivity)

$$\left.\begin{aligned}&Q=\frac{m_e q_e+m_p q_p}{m_e+m_p},\quad q=q_e-q_p\\&M=m_e+m_p,\quad \mu=\frac{m_e m_p}{m_e+m_p}\end{aligned}\right\}\Rightarrow L(Q,q;\dot Q,\dot q)=\frac{1}{2}M|\dot Q|^2+\frac{1}{2}\mu|\dot q|^2+\frac{ke^2}{|q|}$$

The associated Hamiltonian funcion is

$$H_{cl}(q_e,q_p;p_e,p_p)=\frac{1}{2m_e}|p_e|^2+\frac{1}{2m_p}|p_p|^2-\frac{ke^2}{|q_e-q_p|}=\frac{1}{2M}|P|^2+\frac{1}{2\mu}|p|^2-\frac{ke^2}{|q|}=H_{CM}(P)+H_r(q,p)$$

$$\Rightarrow\begin{cases}\dot Q=\dfrac{\partial H_{cl}}{\partial P}=\dfrac{P}{M},\quad \dot P=-\dfrac{\partial H_{cl}}{\partial Q}=0\\[2mm]\dot q=\dfrac{\partial H_{cl}}{\partial p}=\dfrac{p}{\mu},\quad \dot p=-\dfrac{\partial H_{cl}}{\partial q}=-\dfrac{ke^2}{|q|^2}\dfrac{q}{|q|}\end{cases}$$

→ the center of mass moves freely (uniform rectilinear motion)

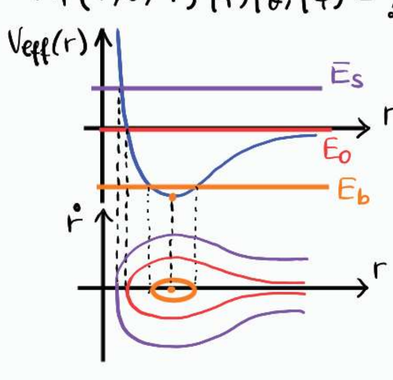
→ the relative coordinate describes a point particle of mass μ subject to a central force field of Coulomb type, with a fixed center.

Regarding the Keplerian model described by $H_r(q,p)$, the following are constants of motion

• $H(q,p)=E$ = total mechanical energy ↔ time translation symmetry
$\bar L=\bar q\wedge\bar p$ = angular momentum ↔ rotational symmetry $SO(3)$ } → completely integrable model

• Passing to polar coordinates $(r,\theta,\varphi)\in\mathbb{R}_+\times[0,\pi)\times[0,2\pi)$, the Hamiltonian becomes

$$H_r(r,\theta,\varphi;p_r,p_\theta,p_\varphi)=\frac{1}{2\mu}p_r^2+\underbrace{\frac{1}{2\mu}\frac{p_\varphi^2}{r^2}-\frac{ke^2}{r}}_{V_{eff}(r)\,=\,\text{effective potential}}\qquad(p_r=m\dot r,\ p_\varphi=mr^2\dot\varphi=|\bar L|=\text{const.})$$

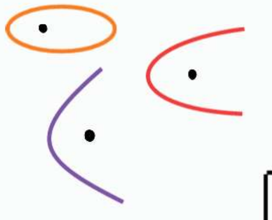


$$\Rightarrow\ \dot r=\pm\sqrt{\frac{2}{m}(E-V_{eff}(r))}\ \longrightarrow\ r=\frac{B}{1+b\cos(\varphi-\varphi_{min})}\qquad B=\frac{|\bar L|^2}{mke^2}\quad b=-1+\frac{B}{r_{min}}$$

$E=E_b<0$ → bounded orbits → elliptic

$E=E_0=0$ → threshold orbits → parabolic

$E=E_s>0$ → scattering orbits (asymptotically free) → hyperbolic



- Accidental/hidden extra symmetry

$A = p\wedge L - mke^2\frac{q}{|q|} = \text{const.} \in \mathbb{R}^3$ Laplace-Runge-Lenz vector $\rightarrow$ full symmetry of the model described by $SO(4)$

$\Rightarrow$ bounded orbits are indeed closed orbits

- Bounded stable orbits are incompatible with classical electrodynamics:

electron = accelerated charge $\Rightarrow$ it loses energy by emitting EM radiation $\Rightarrow$ collapses on the center in finite time !

<u>Quantum mechanics</u>: By canonical quantization we introduce the Hamiltonian operator

$$H = \frac{|P_e|^2}{2m_e} + \frac{|P_p|^2}{2m_p} - ke^2|Q_e - Q_p|^{-1} = -\frac{\hbar^2}{2m_e}\Delta_{x_e} - \frac{\hbar^2}{2m_p}\Delta_{x_p} - \frac{ke^2}{|x_e - x_p|} \quad \text{on } L^2(\mathbb{R}^3, dx_e)\otimes L^2(\mathbb{R}^3, dx_p) \simeq L^2(\mathbb{R}^6)$$

Let us now consider the change of coordinates $X = \frac{m_e x_e + m_p x_p}{m_e + m_p}$, $x = x_e - x_p$ $\left(M = m_e + m_p,\ \mu = \frac{m_e m_p}{m_e + m_p}\right)$, identifying the unitary operator

$$U : L^2(\mathbb{R}^3, dx_e)\otimes L^2(\mathbb{R}^3, dx_p) \longrightarrow L^2(\mathbb{R}^3, dX)\otimes L^2(\mathbb{R}^3, dx)$$
$$\Psi(x_e, x_p) \longmapsto (U\Psi)(X, x) = \Psi\left(X + \frac{m_p}{M}x,\ X - \frac{m_e}{M}x\right)$$

<u>Lemma</u>: $UHU^{-1} = H_{CM}\otimes \mathbb{1} + \mathbb{1}\otimes H_r$ with $H_{CM} = -\frac{\hbar^2}{2M}\Delta_X$, $H_r = -\frac{\hbar^2}{2\mu}\Delta_x - \frac{ke^2}{|x|}$

<u>proof</u>: $\frac{\partial}{\partial x_e^i} = \sum_j\left(\frac{\partial X^j}{\partial x_e^i}\frac{\partial}{\partial X^j} + \frac{\partial x^j}{\partial x_e^i}\frac{\partial}{\partial x^j}\right) = \frac{m_e}{M}\frac{\partial}{\partial X^i} + \frac{\partial}{\partial x^i} \rightarrow \nabla_{x_e} = \frac{m_e}{M}\nabla_X + \nabla_x$

$\frac{\partial}{\partial x_p^i} = \sum_j\left(\frac{\partial X^j}{\partial x_p^i}\frac{\partial}{\partial X^j} + \frac{\partial x^j}{\partial x_e^i}\frac{\partial}{\partial x^j}\right) = \frac{m_p}{M}\frac{\partial}{\partial X^i} - \frac{\partial}{\partial x^i} \rightarrow \nabla_{x_p} = \frac{m_p}{M}\nabla_X - \nabla_x$

$$\begin{aligned} UHU^{-1} &= -\frac{\hbar^2}{2m_e}\left(\frac{m_e}{M}\nabla_X + \nabla_x\right)^2 - \frac{\hbar^2}{2m_p}\left(\frac{m_p}{M}\nabla_X - \nabla_x\right)^2 - \frac{ke^2}{|x|} \\ &= -\frac{\hbar^2}{2m_e}\left(\frac{m_e^2}{M}\Delta_X + \cancel{2\frac{m_e}{M}\nabla_X\cdot\nabla_x} + \Delta_x\right) - \frac{\hbar^2}{2m_p}\left(\frac{m_p^2}{M^2}\Delta_X - \cancel{\frac{2m_p}{M}\nabla_X\cdot\nabla_x} + \Delta_x\right) - \frac{ke^2}{|x|} \\ &= -\frac{\hbar^2}{2M}\Delta_X - \frac{\hbar^2}{2}\left(\frac{1}{m_e} + \frac{1}{m_p}\right)\Delta_x - \frac{ke^2}{|x|} \end{aligned}$$ ∎

<u>Rmk</u>: $H_{CM} \rightarrow$ center of mass moves as a free quantum particle of mass M; $H_r \rightarrow$ particle in $\mathbb{R}^3$ in a central force field. } complete decoupling

<u>Rmk</u>: H_r contains a singular potential $\rightsquigarrow$ non-trivial to establish self-adjointness.

<u>Def</u>: A symmetric operator V is a <u>small perturbation in the sense</u> of Kato (Kato-small perturbation) of a self-adjoint operator H if

$$D(V)\supset D(H) \quad \text{and} \quad \exists\, a\in(0,1),\ C>0 \text{ s.t. } \|V\psi\| \leq a\|H\psi\| + C\|\psi\| \quad \forall\psi\in D(H)$$

<u>Theorem (Kato–Rellich)</u> If V is a Kato-small perturbation of a self-adjoint operator H, then $H+V$ is self-adjoint on $D(H)$

<u>proof</u>: $H+V$ symmetric on $D(H)\cap D(V) = D(H)$. So, it is enough to show that $\exists\,\lambda>0$ s.t. $\operatorname{ran}(H+V\pm i\lambda) = \mathcal{H}$ ($\mathcal{H}$ = Hilbert space, see thm 2.39 in Moscolari's notes)

- H self-adj. $\Rightarrow \exists (H+i\lambda)^{-1}\in B(\mathcal{H}) \Rightarrow (H+V+i\lambda)\psi = \left[\mathbb{1} + V(H+i\lambda)^{-1}\right](H+i\lambda)\psi \quad \forall\psi\in D(H)$

  $\Rightarrow \operatorname{ran}(H+i\lambda) = \operatorname{ran}(H) = \mathcal{H}$
- Since $(H+i\lambda)^{-1}\varphi\in D(H)\ \forall\varphi\in\mathcal{H}$ and V Kato-small wrt H, we obtain

  $\|V(H+i\lambda)^{-1}\varphi\| \leq a\|H(H+i\lambda)^{-1}\varphi\| + C\|(H+i\lambda)^{-1}\varphi\| \leq a\|\varphi\| + \frac{C}{\lambda}\|\varphi\| \leq \tilde{a}\|\varphi\|$ $\forall\varphi\in\mathcal{H}$ and some $\tilde{a}\in(0,1)$ (pick $\lambda > C/(1-a)$)

$\Rightarrow \|V(H+i\lambda)^{-1}\|_{B(\mathcal{H})} < 1 \Rightarrow \exists\ \mathbb{1} + V(H+i\lambda)^{-1}\in B(\mathcal{H})$ with $\ker = \{0\}$, $\operatorname{ran} = \mathcal{H}$

$\Rightarrow \operatorname{ran}(H+V+i\lambda) = \operatorname{ran}\left[(\mathbb{1} + V(H+i\lambda)^{-1})(H+i\lambda)\right] = \mathcal{H} \Rightarrow H+V$ self-adjoint ∎

<u>Theorem</u>: $H_r = -\frac{\hbar^2}{2\mu}\Delta_x - \frac{ke^2}{|x|}$ is:
- essentially self-adjoint on $C_c^\infty(\mathbb{R}^3)$;
- self-adjoint on $D(H_r) = H^2(\mathbb{R}^3)$;
- bounded from below: $\exists\,\lambda_0>0$ s.t. $H_r \geq -\lambda_0\mathbb{1}$.

Proof: We give the proof in separate steps.

Lemma 1 (Sobolev): Let $d\leq 3$. Then $\forall a>0\ \exists b>0$ s.t. $\|\psi\|_{L^\infty}\leq a\|\Delta\psi\|_{L^2}+b\|\psi\|_{L^2}\ \ \forall\psi\in H^2(\mathbb{R}^d)$

In particular: $H^2(\mathbb{R}^d)\hookrightarrow L^\infty(\mathbb{R}^d)$ (continuous embedding)

proof: $|\psi(x)|=\left|\int_{\mathbb{R}^d}dk\,\frac{e^{ik\cdot x}}{(2\pi)^{d/2}}\hat\psi(k)\right|\leq c\int_{\mathbb{R}^d}dk\,|\hat\psi(k)|\frac{|k|^2+\eta^2}{|k|^2+\eta^2}\leq c\left(\int_{\mathbb{R}^d}dk\,\frac{1}{(|k|^2+\eta^2)^2}\right)^{1/2}\left(\int_{\mathbb{R}^d}dk\,(|k|^2+\eta^2)^2|\hat\psi(k)|^2\right)^{1/2}$

$\leq c\left(\int_0^\infty d|k|\,\frac{|k|^{d-1}}{(|k|^2+\eta^2)^2}\right)^{1/2}\|(|k|^2+\eta^2)\hat\psi(k)\|_{L^2}\leq c\,\eta^{\frac{d-4}{2}}\|(-\Delta+\eta^2)\psi\|_{L^2}\leq c\left(\eta^{-\frac{4-d}{2}}\|\Delta\psi\|_{L^2}+\eta^{d/2}\|\psi\|_{L^2}\right)$

↳ the thesis follows by fixing suitably $\eta>0$ (large enough).

Rmk: More generally, there holds $H^s(\mathbb{R}^d)\hookrightarrow \mathcal{C}^{j,\alpha}_b(\mathbb{R}^d)$ for any $j\in\mathbb{N}$, $\alpha\in(0,1)$, $s\geq\frac{d}{2}+j+\alpha$

Notably: $H^2(\mathbb{R})\hookrightarrow\mathcal{C}^{1,\alpha}_b(\mathbb{R})\ \forall\alpha<1/2$; $H^2(\mathbb{R}^2)\hookrightarrow\mathcal{C}^{0,\alpha}_b(\mathbb{R}^2)\ \forall\alpha<1$; $H^2(\mathbb{R}^3)\hookrightarrow\mathcal{C}^{0,\alpha}_b(\mathbb{R}^3)\ \forall\alpha<1/2$

Lemma 2 (Kato): Let $V=V_2+V_\infty$ with $V_2\in L^2(\mathbb{R}^3)$, $V_\infty\in L^\infty(\mathbb{R}^3)$ and $H=-\Delta+V$. Then

a) H is essentially self-adjoint on $\mathcal{C}^\infty_c(\mathbb{R}^3)$, self-adjoint on $D(H)=H^2(\mathbb{R}^3)$

b) $\exists\lambda_0>0$ s.t. $H\geq-\lambda_0\iff\inf\sigma(H)\geq-\lambda_0$.

proof: a) V symmetric on $D(V)\supset\mathcal{C}^\infty_c(\mathbb{R}^3)$.

$\|V\psi\|_{L^2}\leq\|V_2\|_{L^2}\|\psi\|_{L^\infty}+\|V_\infty\|_{L^\infty}\|\psi\|_{L^2}\overset{\text{Lemma 1}}{\leq}\|V_2\|_{L^2}(a\|\Delta\psi\|_{L^2}+b\|\psi\|_{L^2})+\|V_\infty\|_{L^\infty}\|\psi\|_{L^2}\leq a'\|\Delta\psi\|_{L^2}+b'\|\psi\|_{L^2}$

Fixing $a<\|V_2\|_{L^2}^{-1}\Rightarrow a'<1\Rightarrow V$ is a Kato-small perturbation of $H_0=-\Delta$

↳ The thesis follows by Kato-Rellich theorem.

b) Let $\lambda>0$ and put $R_0(-\lambda)=(-\Delta+\lambda)^{-1}$. Then, $R_0(-\lambda)\psi\in D(-\Delta)=H^2(\mathbb{R}^3)\ \forall\psi\in L^2(\mathbb{R}^3)$. Moreover:

$\|VR_0(-\lambda)\psi\|_{L^2}\leq a'\|(-\Delta)R_0(-\lambda)\psi\|_{L^2}+b'\|R_0(-\lambda)\psi\|_{L^2}\leq\left(a'+\frac{b'}{\lambda}\right)\|\psi\|_{L^2}$ with $a'\in(0,1)$, $b'>0$.

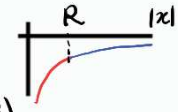
$\Rightarrow\exists\lambda_0>0$ s.t. $\|VR_0(-\lambda)\|_{B(L^2)}<1\ \forall\lambda\geq\lambda_0\Rightarrow\sum_{n=0}^\infty(-1)^n[VR_0(-\lambda)]^n$ unif. convergent in $B(L^2)$

$\Rightarrow(-\Delta+V+\lambda)^{-1}=\left[(\mathbb{1}+V(-\Delta+\lambda)^{-1})(-\Delta+\lambda)\right]^{-1}=R_0(-\lambda)\sum_{n=0}^\infty(-1)^n[VR_0(-\lambda)]^n\in B(\mathcal{H})\ \ \forall\lambda\geq\lambda_0$

$\Rightarrow\lambda\in\rho(-\Delta+V)=\rho(H)$ if $\lambda\geq\lambda_0$.

Lemma 3: $V(x)=-\frac{ke^2}{|x|}\in L^2(\mathbb{R}^3)+L^\infty(\mathbb{R}^3)$

proof: For any $R>0$, let us write $V(x)=\left(-\frac{ke^2}{|x|}\right)\mathbb{1}_{B_R(0)}(x)+\left(-\frac{ke^2}{|x|}\right)\mathbb{1}_{\mathbb{R}^3\setminus B_R(0)}(x)=V_2+V_\infty$



$\|V_2\|_{L^2}^2=\int_{\mathbb{R}^3}dx\left|\left(-\frac{ke^2}{|x|}\right)\mathbb{1}_{B_R(0)}(x)\right|^2=4\pi\int_0^R dr\,\cancel{r^2}\frac{(ke^2)^2}{\cancel{r^2}}=4\pi(ke^2)^2R<\infty\Rightarrow V_2\in L^2(\mathbb{R}^3)$

$\|V_\infty\|_{L^\infty}=\operatorname*{ess\,sup}_{x\in\mathbb{R}^3}\left|\left(-\frac{ke^2}{|x|}\right)\mathbb{1}_{\mathbb{R}^3\setminus B_R(0)}(x)\right|=\sup_{|x|>R}\frac{ke^2}{|x|}=\frac{ke^2}{R}<\infty\ \ \Rightarrow\ \ V_\infty\in L^\infty(\mathbb{R}^3)$

The thesis ultimately follows combining the above lemmas.

Rmk: the arguments in the proof can be easily generalized to prove that the same result holds true for generic power-law potentials of the form

$$V(x)=\frac{\gamma}{|x|^\alpha}\quad\text{with }\gamma\in\mathbb{R},\ \alpha\in(0,3/2)\qquad\boxed{\text{Exercise}}$$

Exercise: Prove that $H_{CM}=-\frac{\hbar^2}{2M}\Delta_X$, $D(H_{CM})=H^2(\mathbb{R}^3)$ (resp., $H_r=-\frac{\hbar^2}{2\mu}\Delta_x-\frac{ke^2}{|x|}$, $D(H_r)=H^2(\mathbb{R}^3)$) is a Kato-small perturb. of $H_p=-\frac{\hbar^2}{2m_p}\Delta_{x_p}$, $D(H_p)=H^2(\mathbb{R}^3)$ (resp. $H_e=-\frac{\hbar^2}{2m_e}\Delta_{x_e}$, $D(H_e)=H^2(\mathbb{R}^3)$)

Corollary: $(e^{-i\frac{t}{\hbar}H_r})_{t\in\mathbb{R}}$ is a strongly continuous, one-parameter unitary group on $L^2(\mathbb{R},dx)$

Proof: direct consequence of the previous theorem and Stone's theorem.

Rmk: $e^{-i\frac{t}{\hbar}(H_{CM}\otimes\mathbb{1}+\mathbb{1}\otimes H_r)}=e^{-i\frac{t}{\hbar}H_{CM}}\otimes e^{-i\frac{t}{\hbar}H_r}$ is a strongly continuous, one parameter unitary group on $L^2(\mathbb{R}^6)\simeq L^2(\mathbb{R}^3,dX)\otimes L^2(\mathbb{R}^3,dx)$

Rmk: The time evolution $e^{-i\frac{t}{\hbar}H}\psi_0$ of a generic initial state $\psi_0 \in L^2(\mathbb{R}^6)$ is well-defined for all times $t\in\mathbb{R}$ (QM dynamics is more regular than CM dynamics).

Proposition (Lower-bound estimate): $H_r \geq -\frac{2m}{\hbar^2}(ke^2)^2 \; (=4E_0)$

Proof: The proof essentially relies on the Hardy inequality (see the proof below)

$$\int_{\mathbb{R}^d} dx\, |\nabla\psi(x)|^2 \geq \left(\frac{d-2}{2}\right)^2 \int_{\mathbb{R}^d} dx\, \frac{|\psi(x)|^2}{|x|^2} \qquad \forall d\geq 3,\ \forall \psi\in H^1(\mathbb{R}^d)$$

For any $\psi\in D(H_r) = H^2(\mathbb{R}^3)\subset H^1(\mathbb{R}^3)$, from here it follows that

$$\langle\psi, H_r\psi\rangle = \int_{\mathbb{R}^3} dx\, \overline{\psi(x)}\left[-\frac{\hbar^2}{2m}\Delta_x\psi(x) - \frac{ke^2}{|x|}\psi(x)\right] = \int_{\mathbb{R}^3} dx \left[\frac{\hbar^2}{2m}|\nabla_x\psi(x)|^2 - \frac{ke^2}{|x|}|\psi(x)|^2\right] \geq \text{(Hardy ineq.)}$$

$$\geq \int_{\mathbb{R}^3} dx \left[\frac{\hbar^2}{2m}\left(\frac{3-2}{2}\right)^2\frac{1}{|x|^2} - \frac{ke^2}{|x|}\right]|\psi(x)|^2 \geq \inf_{r>0}\left(\frac{\hbar^2}{8m}\frac{1}{r^2} - \frac{ke^2}{r}\right)\|\psi\|^2_{L^2} = -\frac{2m}{\hbar^2}(ke^2)^2\|\psi\|^2_{L^2}$$

$$\Rightarrow \inf\sigma(H_r) = \inf_{\psi\in D(H_r)} \frac{\langle\psi, H_r\psi\rangle}{\|\psi\|^2} \geq -\frac{2m}{\hbar^2}(ke^2)^2.$$

Proof of Hardy inequality: For any $\eta>0$, we have the following

$$0 \leq \int_{\mathbb{R}^d} dx \left|\nabla\psi + \eta\frac{x}{|x|^2}\psi\right|^2 = \lim_{\substack{R\to\infty\\ \varepsilon\to 0}} \int_{\{\varepsilon<|x|<R\}} dx \left[|\nabla\psi|^2 + \eta\frac{x}{|x|^2}\cdot\underbrace{(\overline{\psi}\nabla\psi + \overline{\nabla\psi}\psi)}_{=\nabla|\psi|^2} + \eta^2\frac{1}{|x|^2}|\psi|^2\right]$$

$$= \lim_{\substack{R\to\infty\\ \varepsilon\to 0}}\left[\int_{\{\varepsilon<|x|<R\}} dx \left(|\nabla\psi|^2 - \eta\left(\nabla\cdot\frac{x}{|x|^2}\right)|\psi|^2 + \frac{\eta^2}{|x|^2}|\psi|^2\right) + \int_{\partial B_R(0)} d\Sigma_R\, \eta\frac{x}{|x|^2}\cdot\hat{n}_R|\psi|^2 + \int_{\partial B_\varepsilon(0)} d\Sigma_\varepsilon\, \eta\frac{x}{|x|^2}\cdot\hat{n}_\varepsilon|\psi|^2\right]$$

- $\nabla\cdot\frac{x}{|x|^2} = \sum_{i=1}^d \partial_{x_i}\left(\frac{x_i}{|x|^2}\right) = \sum_{i=1}^d\left(\frac{1}{|x|^2} - \frac{2x_i}{|x|^3}\partial_{x_i}|x|\right) = \sum_{i=1}^d\left(\frac{1}{|x|^2} - \frac{2x_i^2}{|x|^4}\right) = \frac{d-2}{|x|^2}$
- $\int_{\partial B_R(0)} d\Sigma_R\, \eta\frac{x}{|x|^2}\cdot\hat{n}_R|\psi|^2 = \frac{\eta}{R^2}\int_{B_R(0)} dx\, \nabla\cdot(x|\psi|^2) = \frac{\eta}{R^2}\int_{B_R(0)} dx\left[(\nabla\cdot x)|\psi|^2 + x\cdot(\overline{\nabla\psi}\psi + \overline{\psi}\nabla\psi)\right]$

  $\leq \frac{\eta}{R^2}\int_{B_R(0)}\left[d|\psi|^2 + 2R|\nabla\psi||\psi|\right] \leq \frac{\eta d}{R^2}\|\psi\|^2_{L^2} + \frac{2\eta}{R}\|\psi\|_{L^2}\|\nabla\psi\|_{L^2} \leq \frac{C}{R}\|\psi\|^2_{H^1} \xrightarrow{R\to\infty} 0$
- $\int_{\partial B_\varepsilon(0)} d\Sigma_\varepsilon\, \eta\frac{x}{|x|^2}\cdot\hat{n}_\varepsilon|\psi|^2 = -\frac{\eta}{\varepsilon}\int_{\partial B_\varepsilon(0)} d\Sigma_\varepsilon|\psi|^2 \leq 0$

$$\leq \int_{\mathbb{R}^d} dx\left(|\nabla\psi|^2 - \eta\frac{d-2}{|x|^2}|\psi|^2 + \frac{\eta^2}{|x|^2}|\psi|^2\right) \leq \int_{\mathbb{R}^d} dx\,|\nabla\psi|^2 - \inf_{\eta>0}\left[\eta^2 - (d-2)\eta\right]\int_{\mathbb{R}^d} dx\,\frac{|\psi|^2}{|x|^2} \Rightarrow \text{thesis.}$$

Rmk: Hardy inequality is optimal. In fact:

$$H = -\Delta - \frac{\gamma}{|x|^2} \text{ is not bounded from below if } \gamma > \left(\frac{d-2}{2}\right)^2$$

Def: A bounded operator $A\in\mathcal{B}(\mathcal{H})$ is compact if $\psi_n \xrightarrow{w} \psi_\infty \Rightarrow A\psi_n \xrightarrow{s} A\psi_\infty$

Example (finite-range operators) Let $A\in\mathcal{B}(\mathcal{H})$ be such that $\operatorname{ran}(A)\subset\operatorname{span}(b_1,\dots,b_N)$
$\Rightarrow A\psi = \sum_{i=1}^N \lambda_i\langle c_i,\psi\rangle b_i$ with $\{b_i\}_{i=1,\dots,N}, \{c_i\}_{i=1,\dots,N}$ orthonormal systems.
If $\psi_n\xrightarrow{w}0$, then $\|A\psi_n\|^2 = \sum_{i=1}^N|\lambda_i|^2|\langle c_i,\psi_n\rangle|^2 \xrightarrow{n\to\infty} 0$, i.e., $A\psi_n\xrightarrow{s}0 \Rightarrow A$ compact

Theorem
- $A\in\mathcal{B}(\mathcal{H})$ compact $\Rightarrow \exists\{A_N\}_{N\in\mathbb{N}}\subset\mathcal{B}(\mathcal{H})$ finite-range s.t. $A_N\xrightarrow{u}A$
- $\{A_N\}_{N\in\mathbb{N}}\subset\mathcal{B}(\mathcal{H})$ compact $\Rightarrow u\text{-}\lim_{N\to\infty} A_N\in\mathcal{B}(\mathcal{H})$ is compact.
- Riesz-Schrauder: A compact $\Rightarrow \sigma(A) = \sigma_{disc}(A)$
  $\Rightarrow 0$ is the only possible accumulation point
  $\Rightarrow \forall\lambda\in\sigma(A)$ is an eigenvalue with finite multiplicity
- Hilbert-Schmidt: A compact $\Rightarrow \exists\{b_i\}_{i\in\mathbb{N}}, \{c_i\}_{i\in\mathbb{N}}$ orthonormal systems, $\{\lambda_i\geq 0\}$
  s.t. $A\psi = \sum_{i\in\mathbb{N}}\lambda_i\langle c_i,\psi\rangle b_i$ and $\lim_{i\to\infty}\lambda_i = 0$.
- A compact, B bounded $\Rightarrow AB$ and BA is compact.
- $(A\psi)(x) = \int_\Omega dy\, K(x,y)\psi(y)$, $\int_{\Omega\times\Omega} dx\,dy\,|K(x,y)|^2 < \infty \Rightarrow A$ is compact.

Theorem (Weyl): Let A, B be two self-adjoint operators, $\exists z \in \rho(A), \rho(B)$ s.t. $(A-z)^{-1} - (B-z)^{-1}$ is compact $\Big\} \Rightarrow \sigma_{ess}(A) = \sigma_{ess}(A)$

Proof: $\lambda \in \sigma_{ess}(A) \Rightarrow \exists \{\psi_n\}_{n\in\mathbb{N}} \subset D(A)$ singular Weyl sequence: $\|\psi_n\| = 1$, $\psi_n \xrightarrow{w} 0$, $(A-\lambda)\psi_n \xrightarrow{s} 0$

Let us set $\varphi_n := (B-z)^{-1}\psi_n$. Then:

- $\varphi_n \in D(B)$ $\forall n \in \mathbb{N}$ and $\varphi_n \xrightarrow{w} 0$
- $\varphi_n = \underbrace{[(B-z)^{-1} - (A-z)^{-1}]\psi_n}_{\text{compact } + \psi_n \xrightarrow{w} 0,\ \xrightarrow{s} 0} + \underbrace{[(A-z)^{-1} - (\lambda - z)^{-1}]\psi_n}_{= -\frac{1}{z-\lambda}(A-z)^{-1}\underbrace{(A-\lambda)\psi_n}_{\xrightarrow{s} 0}} + (\lambda - z)^{-1}\psi_n \Big\} \Rightarrow \lim_{n\to\infty}\|\varphi_n\| = \lim_{n\to\infty}\frac{\|\psi_n\|}{|\lambda - z|} = \frac{1}{|\lambda - z|} > 0$
- $\|(B-\lambda)\varphi_n\| = \|(B-z+z-\lambda)(B-z)^{-1}\psi_n\| = \|[1+(z-\lambda)(B-z)^{-1}]\psi_n\| = |z-\lambda| \, \|[(B-z)^{-1} + \frac{1}{z-\lambda}]\psi_n\|$
$= |z-\lambda| \, \|[(B-z)^{-1} - (A-z)^{-1} + (A-z)^{-1} - (\lambda - z)^{-1}]\psi_n\| \leq |z-\lambda| \, \underbrace{\|[(B-z)^{-1} - (A-z)^{-1}]\psi_n\|}_{\xrightarrow{s} 0} + \|(A-z)^{-1}\underbrace{(A-\lambda)\psi_n}_{\xrightarrow{s} 0}\| \to 0$

The above arguments show that $\left\{\frac{\varphi_n}{\|\varphi_n\|}\right\}_{n\in\mathbb{N}}$ is a singular Weyl sequence for λ w.r.t. B, so $\lambda \in \sigma_{ess}(B)$. By the arbitrariness of $\lambda \in \sigma_{ess}(A)$, we deduce

$$\sigma_{ess}(A) \subset \sigma_{ess}(B)$$

Exchanging A and B and repeating the same arguments, we infer $\sigma_{ess}(B) \subset \sigma_{ess}(A)$. Together with the previous inclusion, this ultimately proves the thesis. ∎

Proposition: $\sigma_{ess}(H_r) = [0, \infty)$

Proof: Setting $H_0 = -\frac{\hbar^2}{2\mu}\Delta_x$, we have $\sigma(H_0) = \sigma_{ess}(H_0) = [0,\infty)$. Then, the thesis follows from Weyl's theorem as soon as we can show that

$$\exists z \in \rho(H_r) \cap \rho(H_0) \text{ s.t. } (H_r - z)^{-1} - (H_0 - z)^{-1} \text{ is compact}$$

Since we previously proved that $\sigma(H_r) \subset [-\frac{2\mu}{\hbar^2}(ke^2)^2, \infty)$, yielding $(-\infty, -\frac{2\mu}{\hbar^2}(ke^2)^2) \subset \rho(H_r) \cap \rho(H_0)$, it is sufficient to prove that

$$(H_r + \lambda)^{-1} - (H_0 + \lambda)^{-1} \text{ is compact for some } \lambda > \frac{2\mu}{\hbar^2}(ke^2)^2$$

By the second resolvent identity we get $(H_r+\lambda)^{-1} - (H_0+\lambda)^{-1} = -(H_r+\lambda)^{-1}(H_r - H_0)(H_0+\lambda)^{-1}$

$(H_r+\lambda)^{-1}$ is a bounded operator

(bounded operator) $\times$ (compact operator) = compact operator $\Rightarrow$ it suffices to prove that $(H_r - H_0)(H_0+\lambda)^{-1} = V(H_0+\lambda)^{-1}$ is a compact operator.

Let us put $V = V \mathbb{1}_{B_n(0)} + V \mathbb{1}_{\mathbb{R}^3 \setminus B_n(0)} = V_{2,n} + V_{\infty,n} \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$

- $(V_{2,n}(H_0+\lambda)^{-1}\psi)(x) = V_{2,n}(x)\int_{\mathbb{R}^3} dy \, \frac{\mu}{2\pi\hbar^2} \frac{e^{-\sqrt{\frac{2\mu}{\hbar^2}\lambda}|x-y|}}{|x-y|}\psi(y) = \int_{\mathbb{R}^3} dy \, K_n(x,y)\psi(y) \Rightarrow V_{2,n}(H_0+\lambda)^{-1}$ is compact

$\|K_n\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} = c\int_{\mathbb{R}^3\times\mathbb{R}^3} dx\,dy \, |V_{2,n}(x)|^2 \frac{e^{-\gamma|x-y|}}{|x-y|^2} = c\|V_{2,n}\|_{L^2}^2 \int_0^\infty dr \, \cancel{r^2} \frac{e^{-\gamma r}}{\cancel{r^2}} < \infty \Rightarrow K_n \in L^2(\mathbb{R}^3\times\mathbb{R}^3)$

- $\|V(H_0+\lambda)^{-1} - V_{2,n}(H_0+\lambda)^{-1}\|_{B(L^2)} = \|W_n(H_0+\lambda)^{-1}\|_{B(L^2)} \leq \|W_n\|_{L^\infty}\|(H_0+\lambda)^{-1}\|_{B(L^2)} \to 0$

$\Rightarrow V(H_0+\lambda)^{-1}$ is the limit in uniform topology of a sequence of compact operators, so $V(H_0+\lambda)^{-1}$ is compact as well, ultimately proving the thesis. ∎

We report the following result, without discussing its proof.

Proposition: $\sigma_{sc}(H_r) = \emptyset$

Proposition (virial theorem): Let $\lambda \in \sigma_p(H_r)$, $\psi \in D(H_r)$ s.t. $H_r\psi = \lambda\psi$, $\|\psi\| = 1$. Then,

$$\lambda = \langle\psi, H_r\psi\rangle = -\langle\psi, H_0\psi\rangle = \frac{1}{2}\langle\psi, V\psi\rangle < 0$$

Proof: Let us consider the scaling operators $(U_s\psi)(x) = e^{3s/2}\psi(e^s x)$ $(s\in\mathbb{R})$. Then, we have:

- $\{U_s\}_{s\in\mathbb{R}}$ is a strongly continuous unitary group, with generators $A = \frac{3}{2}\mathbb{1} + x\cdot\nabla_x$

- $U_s H_r U_s^* = e^{-2s} H_0 + e^{-s} V$ (the explicit form of $H_r = -\frac{\hbar^2}{2\mu}\Delta_x - \frac{ke^2}{|x|}$ plays a role)
- $0 = \langle U_s\psi, (H_r-\lambda)\psi\rangle = \langle U_s\psi, (H_0+V-\lambda)\psi\rangle$

$0 = \langle (H_r-\lambda)\psi, U_s^*\psi\rangle = \langle \psi, (H_r-\lambda)U_s^*\psi\rangle = \langle U_s\psi, U_s(H_r-\lambda)U_s^*\psi\rangle = \langle U_s\psi, (e^{-2s}H_0 + e^{-s}V-\lambda)\psi\rangle$

$\Rightarrow 0 = \langle U_s\psi, [(1-e^{-2s})H_0 + (1-e^{-s})V]\psi\rangle$

$\Rightarrow 0 = \lim_{s\to 0} \frac{\langle U_s\psi, [(1-e^{-2s})H_0 + (1-e^{-s})V]\psi\rangle}{s} = 2\langle\psi, H_0\psi\rangle + \langle\psi, V\psi\rangle \Rightarrow \langle \psi, V\psi\rangle = -2\langle\psi, H_0\psi\rangle$

$\Rightarrow \lambda = \langle \psi, H_r\psi\rangle = \langle\psi, H_0\psi\rangle + \langle\psi, V\psi\rangle = -\langle\psi, H_0\psi\rangle = \frac{1}{2}\langle\psi, V\psi\rangle$ $\blacksquare$

Proposition: $\sigma_p(H_r) = \{E_n\}_{n\in\mathbb{N}}$ (infinite sequence) s.t.

$E_n < 0 \ \forall n\in\mathbb{N}$; $E_n < E_{n+1}$; $E_1 = \inf\sigma(H_r)$; $\lim_{n\to\infty} E_n = 0$; finite multiplicity $\forall n\in\mathbb{N}$

Proof:
- $\psi\in D(H_r) = H^2(\mathbb{R}^3) \Rightarrow U_s^*\psi = U_{-s}\psi = e^{-3s/2}\psi(e^{-s}x) \in D(H_r)$

$\Rightarrow H_0\psi = -\frac{\hbar^2}{2\mu}\Delta_x\psi \in L^2(\mathbb{R}^3) \Rightarrow 0 \le \langle\psi, H_0\psi\rangle < \infty$

$\Rightarrow V\psi \in L^2(\mathbb{R}^3)$ by Hardy inequality $\Rightarrow -\infty < \langle\psi, V\psi\rangle \le 0$

$\Rightarrow \langle U_s^*\psi, H_r U_s^*\psi\rangle = \langle\psi, U_s H_r U_s^*\psi\rangle = e^{-2s}\langle\psi, H_0\psi\rangle + e^{-s}\langle\psi, V\psi\rangle < 0$ by fixing $s \gg 1$

$\Rightarrow \exists$ negative eigenvalue $E\in\sigma_{disc}(H_r)$, $E<0$, since $\sigma_{ess}(H_r) = [0,\infty)$.

- Let $\varphi\in C_c^\infty(\mathbb{R}^3)$ s.t. $\|\varphi\|_{L^2} = 1$, $\operatorname{supp}\varphi \subset B_2(0)\setminus B_1(0)$ and let $\varphi_n(x) = (U^*_{s_n = n\log 3}\varphi)(x) = 3^{-\frac{3n}{2}}\varphi(3^{-n}x)$

$$\left.\begin{array}{l} \Rightarrow \|\varphi_n\|_{L^2} = \|U_{s_n}^*\varphi\|_{L^2} = \|\varphi\|_{L^2} = 1 \\ \operatorname{supp}\varphi_n \subset B_{2\cdot 3^n}(0)\setminus B_{3^n}(0) \Rightarrow \operatorname{supp}\varphi_n \cap \operatorname{supp}\varphi_m = \emptyset \text{ if } n\neq m \end{array}\right\} \Rightarrow \{\varphi_n\}_{n\in\mathbb{N}} \text{ orthonormal}$$

$\Rightarrow \langle\varphi_n, H_r\varphi_m\rangle = 0$ if $n\neq m$ and $\langle\varphi_n, H_r\varphi_n\rangle = \langle U_{s_n}^*\varphi, H_r U_{s_n}^*\varphi\rangle < 0$ for $n \ge n_0 \gg 1$.

$\Rightarrow \operatorname{span}\{\varphi_{n_0}, \dots, \varphi_{n_0+k}\} \subset \operatorname{ran}(P_\lambda(H_r)|_{\lambda=0}) = \operatorname{ran}(P_{[E_1,0]}(H_r))$ $\forall k\ge 0$ $(E_1 = \inf\sigma(H_r))$.

- The thesis ultimately follows from the above arguments recalling that

$$\lambda\in\sigma_{disc}(H_r) \Leftrightarrow P_{\{\lambda\}}(H_r) \neq 0$$
$$\psi \text{ eigenvector} \Leftrightarrow \psi\in\operatorname{ran}(P_{\{\lambda\}}(H_r))$$

In particular: $P_{[E_1,0]}(H_r) = P_{\bigcup_n\{E_n\}} = \sum_n P_{\{E_n\}}$, $\dim(\operatorname{ran}(P_{[0,\infty)}(H_r))) = +\infty$ $\blacksquare$

Proposition:
- $E_1 = \inf\sigma(H_r) = -\frac{\mu}{2\hbar^2}(ke^2)^2$
- Ground state: $\psi_1(x) = \frac{1}{\sqrt{\pi}R_B^{3/2}} e^{-|x|/R_B}$ $\left(R_B = \frac{\hbar^2}{\mu k e^2} = \text{Bohr's radius}\right)$

Proof: The previous proposition ensures that $E_1 = \inf\sigma(H_r)$ is an eigenvalue. In order to determine the related eigenfunction, we consider trial functions of the form

$$\psi_\lambda(x) = c_\lambda e^{-\lambda|x|/2} \quad (\lambda>0,\ c_\lambda>0)$$

$1 = \|\psi_\lambda\|^2_{L^2} = c_\lambda^2\int_{\mathbb{R}^3} dx\, e^{-\lambda|x|} = 4\pi c_\lambda^2\int_0^\infty dr\, r^2 e^{-\lambda r} = \frac{8\pi c_\lambda^2}{\lambda^3} \Rightarrow c_\lambda = \frac{\lambda^{3/2}}{\sqrt{8\pi}}$;

Upper bound

$E_1 = \inf_{\|\psi\|=1}\langle\psi, H_r\psi\rangle \le \langle\psi_\lambda, H_r\psi_\lambda\rangle = \int_{\mathbb{R}^3} dx\left[\frac{\hbar^2}{2\mu}|\nabla\psi_\lambda|^2 - \frac{ke^2}{|x|}|\psi_\lambda|^2\right] = 4\pi c_\lambda^2\int_0^\infty dr\, r^2\left[\frac{\hbar^2}{2\mu}\left(\frac{\lambda}{2}\right)^2 - \frac{e^2}{r}\right]e^{-\lambda r}$

$= 4\pi c_\lambda^2\left[\frac{\hbar^2}{4\mu\lambda} - \frac{ke^2}{\lambda^2}\right] = \frac{\hbar^2\lambda^2}{8\mu} - \frac{ke^2}{2}\lambda$

Minimizing w.r.t. $\lambda \Rightarrow E_1 \le \min_{\lambda>0}\left[\frac{\hbar^2\lambda^2}{8\mu} - \frac{ke^2}{2}\lambda\right] = -\frac{\mu(ke^2)^2}{2\hbar^2}$, $\psi_{\lambda_*}(x) = \frac{1}{\sqrt{\pi}R_B^{3/2}}e^{-|x|/R_B}$

Lower bound

Coulomb estimate (see below)

$E_1 = \inf_{\|\psi\|=1}\langle\psi, H_r\psi\rangle = \inf_{\|\psi\|=1}\int_{\mathbb{R}^3} dx\left[\frac{\hbar^2}{2\mu}|\nabla_x\psi|^2 - \frac{ke^2}{|x|}|\psi|^2\right] \ge \inf_{\|\psi\|=1}\left[\frac{\hbar^2}{2\mu}\|\nabla\psi\|^2_{L^2} - ke^2\|\nabla\psi\|_{L^2}\overset{1}{\cancel{\|\psi\|_{L^2}}}\right]$

$\ge \inf_{\eta>0}\left[\frac{\hbar^2}{2\mu}\eta^2 - ke^2\eta\right] = -\frac{\mu(ke^2)^2}{2\hbar^2}$ (lower bound = upper bound)

Lemma (Coulomb estimate): $\psi\in H^1(\mathbb{R}^d) \Rightarrow \int_{\mathbb{R}^3} dx\,\frac{|\psi(x)|^2}{|x|} \le \|\nabla\psi\|_{L^2}\|\psi\|_{L^2}$

Let us prove the estimate for $\psi \in \mathcal{C}_c^\infty(\mathbb{R}^3)$. We preliminarily notice the identity

$$\sum_{j=1}^3 \left[\partial_{x_j}, \frac{x_j}{|x|}\right]\psi = \sum_{j=1}^3 \left(\partial_{x_j} \frac{x_j}{|x|}\right)\psi = \sum_{j=1}^3 \left(\frac{1}{|x|} - \frac{x_j x_j}{|x|^2}\right)\psi = \frac{2}{|x|}\psi$$

We then obtain

$$\langle \psi, \tfrac{2}{|x|}\psi\rangle = \langle \psi, \sum_{j=1}^3\left[\partial_{x_j}, \tfrac{x_j}{|x|}\right]\psi\rangle = \sum_j \left[\langle \psi, \partial_{x_j}\left(\tfrac{x_j}{|x|}\psi\right)\rangle - \langle \psi, \tfrac{x_j}{|x|}\partial_{x_j}\psi\rangle\right] = (\text{integrating by parts})$$

$$= \sum_j\left[-\langle \partial_{x_j}\psi, \tfrac{x_j}{|x|}\psi\rangle - \langle \tfrac{x_j}{|x|}\psi, \partial_{x_j}\psi\rangle\right] \leq 2\sum_j \|\partial_{x_j}\psi\|_{L^2}\left\|\tfrac{x_j}{|x|}\psi\right\|_{L^2} \leq 2\left(\sum_j\|\partial_{x_j}\psi\|^2\right)^{1/2}\left(\sum_j\left\|\tfrac{x_j}{|x|}\psi\right\|^2\right)^{1/2} = 2\|\nabla\psi\|\,\|\psi\|$$

Since $\mathcal{C}_c^\infty(\mathbb{R}^3)$ is dense in $H^1(\mathbb{R}^3)$, the thesis ultimately follows by standard density arguments. ∎

Decomposition in angular harmonics

To characterize the spectrum $\sigma(H_r)$ more explicitly, it is convenient to exploit the rotational symmetry of the model.

Def: the angular momentum operator $L_i := \sum_{j,k=1}^3 \varepsilon_{ijk} Q_j P_k$, $D(L_i) = \mathcal{C}_c^\infty(\mathbb{R}^3)$ $(i=1,2,3)$; $L^2 = L_1^2 + L_2^2 + L_3^2$

Rmk: ε_{ijk} = Levi-Civita symbol selects commuting components Q_j, P_k $\Rightarrow$ no ordering ambiguity.

Rmk: L_1, L_2, L_3 are unbounded symmetric operators (in fact, essentially self-adjoint)

Lemma: $[L_i, L_j] = i\hbar \sum_{k=1}^3 \varepsilon_{ijk} L_k$, $\quad [L_i, L^2] = 0 \quad$ in $\mathcal{C}_c^\infty(\mathbb{R}^3)$.

Proof: $[L_1, L_2] = [Q_2P_3 - Q_3P_2, Q_3P_1 - Q_1P_3] = Q_2[P_3, Q_3]P_1 + Q_1[Q_3, P_3]P_2 = -i\hbar Q_2P_1 + i\hbar Q_1P_2 = i\hbar L_3$

$[L_1, L^2] = [L_1, \cancel{L_1^2} + L_2^2 + L_3^2] = [L_1, L_2]L_2 + L_2[L_1, L_2] + [L_1, L_3]L_3 + L_3[L_1, L_3] = i\hbar(L_3L_2 + L_2L_3 - L_2L_3 - L_3L_2) = 0$

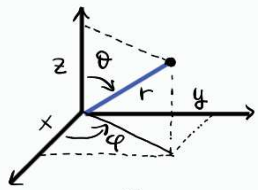
Rmk: $[L_i, L_j] \neq 0 \Rightarrow L_i, L_j$ are not compatible observables $\Rightarrow \nexists$ joint spectral decomposition
$\Rightarrow$ Heisenberg uncertainty relations. Exercise

Rmk: L_i = generator of rotations around the i-th axis in $\mathbb{R}^3 \to$ unitary group $U_\theta = e^{i\theta L_i}$

Exercise Compute the analogous classical Poisson brakets for $M_i = \sum_{j,k=1}^3 \varepsilon_{ijk} x_j p_k$

Let us now proceed to examine the relative Hamiltonian H_r in polar coordinates. To this avail, consider the standard change of coordinates

$$\begin{cases} x = r\sin\theta\cos\varphi \\ y = r\sin\theta\sin\varphi \\ z = r\cos\theta \end{cases} \Leftrightarrow \begin{cases} r = \sqrt{x^2+y^2+z^2} \in (0,\infty) \\ \theta = \arccos\left(\frac{z}{\sqrt{x^2+y^2+z^2}}\right) \in (0,\pi) \\ \varphi = \operatorname{arctg}\left(\frac{y}{x}\right) \in [0, 2\pi) \end{cases}$$



This identifies the unitary operator

$$U: L^2(\mathbb{R}^3, d^3x) \simeq L^2(\mathbb{R}, dx)\otimes L^2(\mathbb{R}, dy)\otimes L^2(\mathbb{R}, dz) \longrightarrow L^2((0,\infty), r^2dr)\otimes \underbrace{L^2((0,\pi), \sin\theta\, d\theta)\otimes L^2([0,2\pi), d\varphi)}_{L^2(S^2, d\Omega)}$$

$$\psi(x) \equiv \psi(x,y,z) \longmapsto \psi(r\sin\theta\cos\varphi, r\sin\theta\sin\varphi, r\cos\theta)$$

By explicit computations we derive the following

Lemma $UL_1U^* = i\hbar\left(\sin\varphi\,\partial_\theta + \frac{\cos\varphi}{\tan\theta}\partial_\varphi\right)$, $\quad UL_2U^* = i\hbar\left(-\cos\varphi\,\partial_\theta + \frac{\sin\varphi}{\tan\theta}\partial_\varphi\right)$, $\quad UL_3U^* = -i\hbar\,\partial_\varphi$

$UL^2U^* = -\hbar^2\left[\frac{1}{\sin\theta}\partial_\theta(\sin\theta\,\partial_\theta\,\cdot) + \partial_{\varphi\varphi}\right] = -\hbar^2\Delta_{S^2}^{(LB)}$ (Laplace-Beltrami operator on S^2)

$UH_rU^* = -\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\partial_r(r^2\partial_r\,\cdot) + \frac{1}{r^2\sin\theta}\partial_\theta(\sin\theta\,\partial_\theta\,\cdot) + \frac{1}{r^2}\partial_{\varphi\varphi}\right] - \frac{ke^2}{r} = -\frac{\hbar^2}{2\mu}\frac{1}{r^2}\partial_r(r^2\partial_r\,\cdot) + \frac{L^2}{2\mu r^2} - \frac{ke^2}{r}$

Rmk: In the sequel, the unitary operators U will be omitted, though working in polar coordinates.

Proposition:
- $L_3 = -i\hbar\partial_\varphi$ is essentially self-adjoint on
$D(L_3) = \{\psi \in L^2(0,2\pi)\cap \mathcal{C}^1(0,2\pi) \mid \psi(0) = \psi(2\pi),\ \psi'(0) = \psi'(2\pi)\}$
- $\sigma(L_3) = \sigma_{disc}(L_3) = \sigma_{pp}(L_3) = \{\hbar m \mid m \in \mathbb{Z}\}$

Proof: the Fourier family $\left\{\frac{e^{im\varphi}}{\sqrt{2\pi}}\right\}_{m\in\mathbb{Z}}$ is an orthonormal basis of $L^2(0,2\pi)$ consisting of eigenvectors of L_3, i.e., $L_3\frac{e^{im\varphi}}{\sqrt{2\pi}} = \hbar m\frac{e^{im\varphi}}{\sqrt{2\pi}}$.

Rmk: the observable values of the z-component of the angular momentum are discrete.

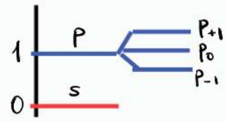
Proposition:
- $L^2 = -\hbar^2 \Delta_{S^2}^{(LB)}$ is essentially self-adjoint on $D(L^2) = \mathcal{C}^\infty(S^2)$
- $\sigma(L^2) = \sigma_{disc}(L^2) = \sigma_{pp}(L_2) = \{\hbar^2 \ell(\ell+1) \mid \ell \in \mathbb{N}_0\}$
- $\exists \{Y_{\ell m}(\theta,\varphi)\}_{\substack{\ell\in\mathbb{N}_0 \\ m\in\mathbb{Z}}}$ orthonormal basis of $L^2([0,\pi), \sin\theta\, d\theta) \otimes L^2([0,2\pi) d\varphi) = L^2(S^2, d\Omega)$:

$$L_3 Y_{\ell m} = \hbar m Y_{\ell m} \qquad L^2 Y_{\ell m} = \hbar^2 \ell(\ell+1) Y_{\ell m}, \qquad \|Y_{\ell m}\|_{L^2(S^2, d\Omega)} = 1$$

Rmk: the eigenspace associated to the eigenvalue $\hbar^2\ell(\ell+1)$ has dimension $\sum_{m=-\ell}^{\ell} 1 = 2\ell+1$

$\ell = 0$: "s-wave" ($s \equiv$ sharp) $\to \exists!\ Y_{00}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}} \rightsquigarrow$ ground state

$\ell = 1$: "p-wave" ($p \equiv$ principal) $\to Y_{10}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}} \cos\theta, \quad Y_{1,\pm1}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}} \cos\theta\, e^{\pm i\varphi}$



Rmk: Explicit expressions for the spherical harmonics

$$Y_{\ell m}(\theta,\varphi) = (-1)^{\frac{m+|m|}{2}} \sqrt{\frac{(2\ell+1)(\ell-|m|)!}{2(\ell+m)!}}\, P_\ell^{|m|}(\cos\theta)\, \frac{e^{im\varphi}}{\sqrt{2\pi}} \qquad (-\ell \le m \le \ell)$$

$$P_\ell^{|m|}(t) := \frac{1}{2^\ell \ell!} (1-t^2)^{m/2} \frac{d^{\ell+m}}{dt^{\ell+m}} (1-t^2)^\ell \qquad t = \cos\theta \in [-1,1]$$ "generalized Legendre polynomials"

Proof: Let us introduce the raising/lowering operators $L_\pm := L_1 \pm i L_2$, $D(L_\pm) = \mathcal{C}^\infty(S^2)$

Lemma 1: a) $L_\pm^* = L_\mp$; b) $[L_+, L_-] = 2\hbar L_3$, $[L_3, L_\pm] = \pm\hbar L_\pm$, $[L^2, L_\pm] = 0$;
c) $L^2 = L_+ L_- - \hbar L_3 + L_3^2 = L_- L_+ + \hbar L_3 + L_3^2$

Proof: Explicit computation using $L_\pm = \hbar e^{\pm i\varphi}(\pm \partial_\theta + i \cot\theta\, \partial_\varphi)$

Lemma 2: Let $Y_{\lambda,m} \in L^2(S^2)$ be s.t. $L^2 Y_{\lambda m} = \hbar^2 \lambda Y_{\lambda m}$, $L_3 Y_{\lambda m} = \hbar m Y_{\lambda m}$, $\|Y_{\lambda m}\| = 1$. Then, for $\lambda \ge m(m\pm1)$,

$$L^2(L_\pm Y_{\lambda m}) = \hbar^2\lambda (L_\pm Y_{\lambda m}), \quad L_3(L_\pm Y_{\lambda m}) = \hbar(m\pm1) L_\pm Y_{\lambda m}, \quad \|L_\pm Y_{\lambda m}\| = \hbar(\lambda - m(m\pm1))$$

Proof: $L^2(L_\pm Y_{\lambda m}) = (\cancel{[L^2, L_\pm]} + L_\pm L^2) Y_{\lambda m} = \hbar^2 \lambda L_\pm Y_{\lambda m}$;

$L_3(L_\pm Y_{\lambda m}) = ([L_3, L_\pm] + L_\pm L_3) Y_{\lambda m} = (\pm\hbar L_\pm + \hbar m L_\pm) Y_{\lambda m} = \hbar(m\pm1) L_\pm Y_{\lambda m}$;

$\|L_\pm Y_{\lambda m}\|^2 = \langle Y_{\lambda m}, L_\pm^* L_\pm Y_{\lambda m}\rangle = \langle Y_{\lambda m}, L_\mp L_\pm Y_{\lambda m}\rangle = \langle Y_{\lambda m}, (L^2 \mp \hbar L_3 - L_3^2) Y_{\lambda m}\rangle$

$= (\hbar^2\lambda \mp \hbar(\hbar m) - (\hbar m)^2) \langle Y_{\lambda m}, Y_{\lambda m}\rangle = \hbar^2(\lambda - m(m\pm1)) \ge 0$ (norm)

Lemma 3: $L^2 Y_{\lambda m} = \hbar^2 \lambda Y_{\lambda m} \Rightarrow \lambda = \ell(\ell+1)$ with $-\ell \le m \le \ell$, $\ell \in \mathbb{N}_0$

Proof: $0 \le \|L_\pm Y_{\lambda m}\|^2 = \hbar^2(\lambda - m(m\pm1)) \Rightarrow m(m\pm1) \le \lambda$ with $m \in \mathbb{Z} \Rightarrow \lambda \ge 0$, $m_\pm = \frac{-(\pm1) - \sqrt{1+4\lambda}}{2}$

Setting $\ell := -\frac{1}{2} + \frac{1}{2}\sqrt{1+4\lambda} \in \mathbb{R} \Rightarrow \lambda = \ell(\ell+1)$, $(\ell+\frac{1}{2})^2 = \lambda + \frac{1}{4} \ge m(m\pm1) + \frac{1}{4} = (m\pm\frac{1}{2})^2 \Rightarrow -\ell \le m \le \ell$

By contradiction, assume $\ell \in \mathbb{R}\setminus\mathbb{N}$. Then $\exists k \in \mathbb{N}$ s.t. $m+k < \ell < m+k+1$

$\phi := \phi_{\ell(\ell+1), m+k} \Rightarrow L^2\phi = \hbar^2\ell(\ell+1)\phi$, $L_3\phi = \hbar(m+k)\phi \Rightarrow L_3 L_+ \phi = \hbar(m+k+1)\phi$

$\Rightarrow L_+\phi$ is an eigenvector of L_3 which does not fulfill $-\ell \le m+k+1 \le \ell$ ↯

Taking the above Lemmas into account, the proof can now be completed retracing the same arguments discussed for the harmonic oscillator

Let $Y_{\lambda m} \in L^2(S^2)$ s.t. $L_3 Y_{\lambda m} = \hbar m Y_{\lambda m}$, $L^2 Y_{\lambda m} = \hbar^2 \lambda Y_{\lambda m}$, $\|Y_{\lambda m}\| = 1$ (*)

Lemma 3 + $\{\frac{e^{im\varphi}}{\sqrt{2\pi}}\}$ orthonormal basis of $L^2(0,2\pi) \Rightarrow Y_{\ell m}(\theta,\varphi) = \Lambda_{\ell m}(\theta) \frac{e^{im\varphi}}{\sqrt{2\pi}}$ $(-\ell \le m \le \ell)$

- $m = -\ell$: $m(m-1) = \ell(\ell+1) = \lambda \overset{\text{Lemma 2}}{\Rightarrow} \|L_- Y_{\ell m}\|^2 = \hbar^2(\lambda - m(m-1)) = 0 \Rightarrow L_- Y_{\ell,-\ell} = 0$

$\Rightarrow (\partial_\theta - \frac{\ell}{\tan\theta}) \Lambda_{\ell,-\ell} = 0 \Rightarrow \Lambda_{\ell,-\ell}(\theta) = c_\ell (\sin\theta)^\ell$ $\left(\|Y_{\ell,-\ell}\| = 1 \Rightarrow c_\ell = \sqrt{\frac{(2\ell+1)!}{2^{2\ell+1}(\ell!)^2}}\right)$

- $m = -\ell+1$: Lemma 2 $\Rightarrow Y_{\ell,-\ell+1} = \frac{L_+ Y_{\ell,-\ell}}{\hbar\sqrt{2\ell}}$ is a solution of (*) and it can be shown by contradiction that it is the only one.
(for fixed $\ell \in \mathbb{N}_0$, $m = -\ell+1$)

- $-\ell\leq m\leq \ell$: By iteration, we get that $Y_{\ell m}=\frac{1}{\hbar^{\ell+m}}C_{\ell m}L_+^{\ell+m}Y_{\ell,-\ell}$ is the unique solution of (*)
  $\hookrightarrow$ Legendre polynomials $P_\ell^{|m|}$ by algebraic computations.

Finally, notice the following facts:
- $Y_{\ell m}$ are eigenfunctions of L^2, L_3 associated to different eigenvalues $\Rightarrow \{Y_{\ell m}\}$ orthogonal
- Stone-Weierstrass theorem: $\{P_\ell^{|m|}\}$ dense in $L^2(-1,1) \Rightarrow \{Y_{\ell m}\}$ complete system.

$\Rightarrow \{Y_{\ell m}\}$ orthonormal basis consisting of eigenvectors.

Corollary: $\forall \psi\in L^2(\mathbb{R}^3)\ \exists \{f_{\ell m}\}_{\ell m}\subset L^2((0,\infty),r^2dr)$ s.t. $\psi(r,\theta,\varphi)=\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} f_{\ell m}(r)\,Y_{\ell m}(\theta,\varphi)$

Energy levels and bound states

The following result is self-evident, working in polar coordinates

Lemma: $[L_3,H_r]=0,\ \ [L^2,H_r]=0$

Rmk: $H_r=-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\partial_r(r^2\partial_r\,\cdot)+\frac{L^2}{2\mu r^2}-\frac{ke^2}{r}=\bigoplus_{\ell=0}^{+\infty} h_\ell\otimes\Pi_\ell$ acting on $L^2((0,\infty),r^2dr)\otimes L^2(S^2,d\Omega)$

with $\Pi_\ell=$ projector on $\mathrm{span}(\{Y_{\ell,-\ell},\dots,Y_{\ell,\ell}\})=\sum_{m=-\ell}^{\ell}|Y_{\ell m}\rangle\langle Y_{\ell m}|$ on $L^2(S^2,d\Omega)$

$h_\ell=-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\partial_r(r^2\partial_r\,\cdot)+\frac{\hbar^2\ell(\ell+1)}{2\mu r^2}-\frac{ke^2}{r}$ on $L^2((0,\infty),r^2dr)$

It is then natural to look for common eigenfunctions of L_3, L^2, H_r of the form

$$\psi_{E,\ell,m}(r,\theta,\varphi)=f_{E,\ell}(r)\,Y_{\ell m}(\theta,\varphi)$$

s.t. $L_3\psi_{E\ell m}=\hbar m\,\psi_{E\ell m},\ L^2\psi_{E\ell m}=\hbar^2\ell(\ell+1)\psi_{E\ell m},\ H_r\psi_{E\ell m}=E\psi_{E\ell m}\Rightarrow h_\ell f_{E\ell}=E f_{E\ell}$

Rmk: The natural unit of measure for lengths is $R_{Bohr}=\frac{\hbar^2}{\mu k e^2}$. We henceforth refer to the dimensionless radial coordinate $\rho:=r/R_{Bohr}$ and consider the associated unitary operator

$$U_{Bohr}: L^2((0,\infty),r^2dr)\to L^2((0,\infty),d\rho),\quad (U_{Bohr}f)(\rho):=R_{Bohr}^{3/2}\rho\, f(R_{Bohr}\rho)\equiv\tilde f(\rho)$$

$$\Rightarrow \tilde h_\ell=U_{Bohr}h_\ell U^*_{Bohr}=\frac{\mu(ke^2)^2}{\hbar^2}\left(-\frac{1}{2}\frac{d^2}{d\rho^2}+\frac{\ell(\ell+1)}{2\rho^2}-\frac{1}{\rho}\right)\quad\text{acting on } L^2((0,\infty),d\rho)$$

$$D(\tilde h_\ell)=U_{Bohr}D(h_\ell)=U_{Bohr}\{f\in L^2((0,\infty),r^2dr)\mid h_\ell f\in L^2((0,\infty),r^2dr)\}$$
$$=\{\tilde f\in L^2((0,\infty),d\rho)\mid \tilde f(0)=0,\ \tilde h_\ell\tilde f\in L^2((0,\infty),d\rho)\}=H_0^2((0,\infty)).$$

Proposition: $\forall \ell\in\mathbb{N}_0\ \exists\{\tilde f_{n\ell}\}_{n\geq \ell+1}\subset L^2((0,\infty),d\rho)$ orthonormal system of eigenfunctions of $\tilde h_\ell$:

$$\tilde h_\ell\tilde f_{n\ell}=-\frac{1}{2n^2}\tilde f_{n\ell}\qquad (\|\tilde f_{n\ell}\|_{L^2((0,\infty),d\rho)}=1)$$

Rmk: the eigenvalues of the radial Hamiltonian are negative and independent of the angular momentum number $\ell\in\mathbb{N}_0$.

Rmk: explicit expressions for the radial eigenfunctions:

$$\tilde f_{n\ell}(\rho)=-\frac{1}{n}\sqrt{\frac{(n-\ell-1)!}{((n+\ell)!)^3}}\left(\frac{2\rho}{n}\right)^{\ell+1}L_{n+\ell}^{2\ell+1}\left(\frac{2\rho}{n}\right)e^{-\rho/n}\qquad (n,\ell\in\mathbb{N}_0 \text{ s.t. } n\geq\ell+1\geq 1)$$

$$L_k^j(t):=(-1)^j\frac{k!}{(k-j)!}t^{-j}e^t\frac{d^{k-j}}{dt^{k-j}}(t^ke^{-t})\quad\begin{pmatrix}0\leq j\leq k\\ t\in[0,\infty)\end{pmatrix}\quad \text{generalized Laguerre polynomials}$$

Proof: Consider the raising/lowering operators $A_\ell^{\pm}=\frac{1}{\sqrt2}\left(\mp\frac{d}{d\rho}+\frac{\ell+1}{\rho}-\frac{1}{\ell+1}\right)$, $D(A_\ell^\pm)=H_0^2((0,\infty),d\rho)$

Lemma 1: a) $(A_\ell^\pm)^*=A_\ell^\mp$ b) $[A_\ell^+,A_\ell^-]=\frac{\ell+1}{\rho^2}\mathbb{1}$; c) $\tilde h_\ell=A_\ell^-A_\ell^+-\frac{1}{2(\ell+1)^2}$; $\tilde h_{\ell+1}=A_\ell^+A_\ell^--\frac{1}{2(\ell+1)^2}$

proof: explicit computation.

Lemma 2: Let $\tilde{f}_{e n}$ be such that $\tilde{h}_e \tilde{f}_{en} = \eta \tilde{f}_{en}$ $(\eta<0)$, $\|\tilde{f}_{ne}\| = 1$. Then:

a) If $\eta > -\frac{1}{2(\ell+1)^2}$: $\tilde{h}_{e+1}(A_e^+ \tilde{f}_{en}) = \eta (A_e^+ \tilde{f}_{en})$, $\|A_e^+ \tilde{f}_{ne}\|^2 = \frac{1}{2(\ell+1)^2} + \eta$;

b) If $\eta > -\frac{1}{\ell^2}$, $\ell>0$: $\tilde{h}_{e-1}(A_e^- \tilde{f}_{en}) = \eta (A_e^- \tilde{f}_{en})$, $\|A_e^- \tilde{f}_{ne}\|^2 = \frac{1}{2\ell^2} + \eta$.

proof: the thesis follows from Lemma 1 with the usual argument on the norms.

Lemma 3: $\eta = -\frac{1}{2n^2}$, $n \geq \ell+1$

proof: $0 \leq \|A_e^+ \tilde{f}_{en}\|^2 = \eta + \frac{1}{2(\ell+1)^2} \Rightarrow \eta \geq -\frac{1}{2(\ell+1)^2}$ Then, the thesis follows by contradiction.

Assume $\exists \gamma \in \mathbb{R}\setminus\mathbb{N}$, $\gamma > \ell+1$ s.t. $\eta = -\frac{1}{2\gamma^2} > -\frac{1}{2(\ell+1)^2} \Rightarrow \exists k \in \mathbb{N}$ s.t. $\ell+k < \gamma < \ell+k+1$

On the other hand, by Lemma 2, $\tilde{h}_{e+k}(A_e^+)^k \tilde{f}_{en} = \eta (A_e^+)^k \tilde{f}_{en}$ and

$\|(A_e^+)^k \tilde{f}_{en}\|^2 = \frac{1}{2(\ell+k+1)^2} + \eta \geq 0$ with $\eta = -\frac{1}{2\gamma^2} \Rightarrow \gamma \geq \ell+k+1$ ↯

Next, we retrace the same arguments outlined for the harmonic oscillator Hamiltonian and for the angular momentum operator.

Let $\tilde{f}_{ne}$ be such that $\tilde{h}_e \tilde{f}_{ne} = -\frac{1}{2n^2}\tilde{f}_{ne}$ and $\|\tilde{f}_{ne}\| = 1$. (*)

- $\underline{\ell = n-1}$: $0 = \langle \tilde{f}_{ne}, (\tilde{h}_{n-1} + \frac{1}{2n^2})\tilde{f}_{ne}\rangle = \langle \tilde{f}_{ne}, A_{n-1}^- A_{n-1}^+ \tilde{f}_{ne}\rangle = \|A_{n-1}^+ \tilde{f}_{ne}\|^2$

  $\Rightarrow 0 = A_{n-1}^+ \tilde{f}_{ne} = \frac{1}{\sqrt{2}}\left(-\frac{d}{d\rho} + \frac{n}{\rho} - \frac{1}{n}\right)\tilde{f}_{ne} \Rightarrow \tilde{f}_{n,n-1}(\rho) = c_n \rho^n e^{-\rho/n}$ unique solution

  $\|\tilde{f}_{n,n-1}\| = 1 \Rightarrow c_n = \sqrt{\left(\frac{2}{n}\right)^{2n+1}\frac{1}{(2n)!}}$

- $\underline{\ell = n-2}$: Using lemma 2 $\rightarrow \tilde{f}_{n,n-2} := \sqrt{\frac{2n^2(n-1)^2}{2n-1}}\, A_{n-2}^- \tilde{f}_{n,n-1}$ unique solution of (*)

- $\ell \leq n-1$: By iteration $\rightarrow \tilde{f}_{ne} = \frac{(2n^2)^{\frac{n-1-\ell}{2}}(n-1)!\sqrt{(n+\ell)!}}{\ell!\sqrt{(2n-1)!(n-1-\ell)!}} A_e^- \cdots A_{n-3}^- A_{n-2}^- \tilde{f}_{n,n-1}$ unique solution ■

Theorem: • $\sigma_p(H_r) = \left\{ E_n = -\frac{\mu (ke^2)^2}{2\hbar^2}\frac{1}{n^2} \,\middle|\, n = 1,2,3,\dots \right\}$

• the normalized eigenfunctions are $\psi_{nem}(r,\theta,\varphi) = f_{ne}(r) Y_{em}(\theta,\varphi)$ $(\ell = 0,\dots,n-1,\ |m| \leq \ell)$

$$f_{ne}(r) = -\frac{2}{n^2}\sqrt{\frac{(n-\ell-1)!}{((n+\ell)!\, R_{Bohr})^3}}\left(\frac{2r}{n R_{Bohr}}\right)^{\ell} L_{n+e}^{2\ell+1}\left(\frac{2r}{n R_{Bohr}}\right) e^{-\frac{r}{n R_{Bohr}}} \qquad \left(R_{Bohr} = \frac{\hbar^2}{\mu k e^2}\right)$$

Rmk: $\sigma_p(H_r)$ reproduces the Balmer spectral series (observed experimentally)

↳ It matches the Bohr model (though the latter is wrong in predicting degeneracy)

Rmk: $\{\psi_{nem}\}$ are not a complete system for $L^2(\mathbb{R}^3)$: $\mathrm{span}\{\psi_{nem}\} = \mathcal{H}_{pp} \perp \mathcal{H}_{ac}$

Rmk: A generic element in the eigenspace associated to the eigenvalue $-\frac{\mu(ke^2)^2}{2\hbar^2}\frac{1}{n^2}$ is

$$\psi_n = \sum_{\ell=0}^{n-1}\sum_{m=-\ell}^{\ell} c_{em} f_{ne} Y_{em} \text{ with } \{c_{em}\} \subset \mathbb{C} \text{ s.t. } \sum_{\ell=0}^{n-1}\sum_{m=-\ell}^{\ell}|c_{em}|^2 = 1$$

$\Rightarrow$ the n-th eigenvalue is degenerate $\sum_{\ell=0}^{n-1}\sum_{m=-\ell}^{\ell} 1 = \sum_{\ell=0}^{n-1}(2\ell+1) = n^2$ times

Notably, the ground state $(n=1, \ell=0, m=0)$ is unique: $\psi_{100}(r) = \frac{1}{\sqrt{\pi}R_{Bohr}^{3/2}} e^{-r/R_{Bohr}}$

Rmk: The ground state ψ_{100} is the unique eigenfunction which is invariant under rotations

↳ the probability for an electron in the ground state to be detected in the spherical shell of inner radius R_1 and outher radius R_2 is

$$P_{R_1R_2} = \langle \psi_{100}, \mathbb{1}_{[R_1,R_2]}(|x|)\psi_{100}\rangle = \int_{R_1}^{R_2} dr\, r^2 |\psi_{100}(r)|^2 = \int_{R_1}^{R_2} dr\, \nu(r), \qquad \nu(r) = \frac{r^2}{\pi R_{Bohr}^{3/2}} e^{-\frac{2r}{R_{Bohr}}}$$

$v(r)$ reaches a maximum value for $r = R_{Bohr}$

↳ In the semiclassical limit the electron moves on a circular orbit of radius R_{Bohr}

Rmk: accidental degeneracy: the eigenvalues of H_r do not depend on the angular momentum number $\ell \in \mathbb{N}_0$. This is a manifestation of the SO(4) symmetry proper of the Coulomb potential.

The Laplace-Runge-Lenz (LRL) vector

Classical Mechanics: Consider the Coulomb model with

- Hamiltonian $H(q,p) = \frac{1}{2\mu} p^2 - \frac{ke^2}{|q|}$
- angular momentum $L = q \wedge p$
- LRL vector $A = \frac{1}{\mu k e^2} p \wedge L - \frac{q}{|q|}$

Lemma: i) $|A|^2 = \frac{2}{\mu (ke^2)^2} H |L|^2 + 1, \quad A \cdot L = 0$

ii) $\{A_i, H\}_{PB} = 0 \quad \{A_i, L_j\}_{PB} = \sum_{k=1}^{3} \varepsilon_{ijk} A_k, \quad \{A_i, A_j\} = -\frac{2}{\mu k e^2} \sum_{k=1}^{3} \varepsilon_{ijk} L_k H$

Rmk: H, L, A are constants of motion $\to$ completely integrable system

Lemma: Let $\Omega_- = \{(q,p) \in \mathbb{R}^3 \times \mathbb{R}^3 \mid H(q,p) < 0\}$ = negative energy space and consider the vector fields defined therein

$$B := \sqrt{\frac{\mu (ke^2)^2}{2|H|}} A, \qquad J^{\pm} := \frac{L \pm B}{2}$$

then: a) $\{J_i^{\pm}, H\}_{PB} = 0 \quad \to \quad J^{\pm}$ are constants of motion

b) $\{J_i^{\pm}, J_j^{\pm}\}_{PB} = \sum_{k=1}^{3} \varepsilon_{ijk} J_k^{\pm}, \quad \{J_i^{\pm}, J_j^{\mp}\}_{PB} = 0 \quad \to \quad so(3) \oplus so(3) \simeq so(4)$ algebra

c) $|J^{\pm}|^2 = \frac{\mu (ke^2)^2}{8|H|}$

Quantum Mechanics:

- Hamiltonian $H = \frac{1}{2\mu} P^2 - \frac{ke^2}{|Q|}$
- angular momentum $L = Q \wedge P$

$\Big\}$ canonical quantization

- LRL vector $A = \frac{1}{2\mu k e^2} (P \wedge L - L \wedge P) - \frac{Q}{|Q|} = \frac{1}{\mu k e^2} (P \wedge L - i\hbar P) - \frac{Q}{|Q|}$ symmetrized Jordan quantization

Lemma: i) $|A|^2 = \frac{2}{\mu (ke^2)^2} H (L^2 + \hbar^2) + \mathbb{1}; \quad A \cdot L = L \cdot A = 0;$

ii) $[A_i, H] = 0, \qquad [A_i, A_j] = -\frac{2i\hbar}{\mu k e^2} \sum_{k=1}^{3} \varepsilon_{ijk} L_k H$

Lemma: Let $V_- = \operatorname{ran}(P_{(-\infty,0)}(H))$ = negative energy subspace of $L^2(\mathbb{R}^3)$ and

$$|H| = H \restriction V_-, \qquad B := \sqrt{\frac{\mu (ke^2)^2}{2|H|}} A, \qquad J^{\pm} = \frac{L \pm B}{2}$$

Then: a) $[J_i^{\pm}, H] = 0 \quad \to \quad J^{\pm}$ are constants of motion;

b) $[J_i^{\pm}, J_j^{\pm}] = i\hbar \sum_{k=1}^{3} \varepsilon_{ijk} J_k^{\pm}, \quad [J_i^{\pm}, J_j^{\mp}] = 0;$

c) $|J^{\pm}|^2 = \frac{\mu (ke^2)^2}{8|H|} - \frac{\hbar^2}{4}$

Theorem: $V_- = \bigcup_n \operatorname{ran}\left(P_{\left\{-\frac{\mu (ke^2)^2}{2\hbar^2} \frac{1}{n^2}\right\}}\right) \simeq \bigoplus_n \left(V_{\frac{n-1}{2}} \otimes V_{\frac{n-1}{2}}\right)$ with:

- $|J^{\pm}|^2 \restriction V_\ell = \hbar^2 \ell(\ell+1) \quad \longrightarrow \quad V_\ell \simeq V_\ell \otimes \{1\} \simeq \{1\} \otimes V_\ell$ are invariant subspaces for $|J^{\pm}|^2$
- $H \restriction \left(V_{\frac{n-1}{2}} \otimes V_{\frac{n-1}{2}}\right) = E_n \mathbb{1} = -\frac{\mu (ke^2)^2}{8\hbar^2} \frac{1}{(\ell + 1/2)^2}\Big|_{\ell = \frac{n-1}{2}}$

Exercise (**Zeeman effect**) Consider an hydrogen atom interacting with a homogeneous magnetic field of intensity $\beta = |B| > 0$. Check that the associated Hamiltonian is

$$H = -\frac{\hbar^2}{2\mu}\Delta + \frac{e\beta}{2m}L_3 - \frac{ke^2}{|x|} + \frac{\beta^2}{2m}|x|^2$$

Neglecting the latter term proportional to β^2 (weak-field regime), determine $\sigma_p(H)$ and the degeneracy of the eigenvalues.

Exercise (**Helium atom**) Consider the Hamiltonian operator

$$H = -\frac{\hbar^2}{2\mu}\Delta_{x_1} - \frac{\hbar^2}{2\mu}\Delta_{x_2} - \frac{ke^2}{|x_1|} - \frac{ke^2}{|x_2|} + \frac{ke^2}{|x_1 - x_2|} \quad \text{in } L^2(\mathbb{R}^3, dx_1) \otimes L^2(\mathbb{R}^3, dx_2)$$

Prove that H is bounded from below and find $D(H)$ s.t. H is self adjoint.
Find an estimate for $\sigma(H)$ using Test functions of the form

$$\psi_\alpha \otimes \psi_\alpha \in L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3) \quad \text{with } \psi_\alpha(x) = \frac{\alpha^{3/2}}{\sqrt{8\pi}} e^{-\frac{\alpha}{2}|x|} \quad (\alpha > 0).$$