Quantum Mechanics I

Quantum Mechanics

Momentum Representation: Definition and Application; Linear Potentials and Dual Space

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Pink Floyd: "Another Brick in the Wall (Pt. II)"

Momentum Rep

The Story so Far...

- Any problem with piecewise constant potential:
  - Subdivide space into regions where $W(x)$ is constant
    - (so $W(x)$ crosses the E-level *dis*continuously)
  - Solve the Schrödinger equation in each region
    - ...using boundary conditions for (ultimate) normalizability
  - Match the solutions between regions
  - using that $\Delta\psi(x)=0$ and $\Delta\psi'(x)=0$.
- Include also $\lambda\,\delta(x-a)$-type singularities
  - using that $\Delta\psi(a)=0$ but now $\Delta\psi'(a)=2M\lambda\,\psi(a)/\hbar$.
- All of this presupposes the <u>*choice*</u>
  - of the coordinate representation:

$$\Psi(\vec{r},t) := \langle\vec{r}\,|\Psi(t)\rangle \qquad\qquad Q_\alpha\,|\vec{r}\rangle = x_\alpha\,|\vec{r}\rangle$$

  - No reason not to use some other observable instead of Q_α.

Momentum Rep

Definitions

- So, use P_α instead, for the momentum representation

$$\Psi(\vec{p},t) := \langle\vec{p}|\Psi(t)\rangle \qquad P_\alpha|\vec{p}\rangle = p_\alpha|\vec{p}\rangle$$

- Just as with the coordinate representation,
  - p_α may well be a continuously varying eigenvalue
  - orthonormality requires that $\langle\vec{p}'|\vec{p}\rangle = \delta^{(3)}(\vec{p}-\vec{p}')$
- Relation to the coordinate representation:

$$\frac{\hbar}{i}\frac{\partial}{\partial x^\alpha}\langle\vec{r}|\vec{p}\rangle = \left\langle\vec{r}\left|\frac{\hbar}{i}\frac{\partial}{\partial x^\alpha}\right|\vec{p}\right\rangle = \left\langle\vec{r}\left|P_\alpha\right|\vec{p}\right\rangle = \left\langle\vec{r}\left|p_\alpha\right|\vec{p}\right\rangle = p_\alpha\langle\vec{r}|\vec{p}\rangle$$

  - Solve this differential equation, treating p_α as a parameter:

$$\langle\vec{r}|\vec{p}\rangle = N_{\vec{p}}\,e^{i\vec{p}\cdot\vec{r}/\hbar}$$

the Fourier transform kernel!

  - transforms coordinate ↔ momentum representation

Momentum Rep

Definitions

$$\langle \vec{r} | \vec{p} \rangle = N_{\vec{p}}\, e^{i\vec{p}\cdot\vec{r}/\hbar}$$

- The transform kernel is normalized:

$$\delta^{(3)}(\vec{p}-\vec{p}') \stackrel{!}{=} \langle \vec{p}' | \vec{p} \rangle = \langle \vec{p}' | \mathbb{1} | \vec{p} \rangle = \langle \vec{p}' | \int \mathrm{d}^3\vec{r}\, |\vec{r}\rangle \langle \vec{r}| | \vec{p} \rangle$$

$$= \int \mathrm{d}^3\vec{r}\, \langle \vec{p}' | \vec{r} \rangle \langle \vec{r} | \vec{p} \rangle = N^*_{\vec{p}'} N_{\vec{p}} \int \mathrm{d}^3\vec{r}\, e^{-i\vec{p}'\cdot\vec{r}/\hbar} e^{i\vec{p}\cdot\vec{r}/\hbar}$$

$$= N^*_{\vec{p}'} N_{\vec{p}} \int \mathrm{d}^3\vec{r}\, e^{i(\vec{p}-\vec{p}')\cdot\vec{r}/\hbar} = |N_{\vec{p}}|^2 (2\pi\hbar)^3 \delta^{(3)}(\vec{p}-\vec{p}')$$

$$N_{\vec{p}} = \frac{1}{\sqrt{(2\pi\hbar)^3}} \qquad \boxed{\langle \vec{r} | \vec{p} \rangle = \frac{1}{\sqrt{(2\pi\hbar)^3}} e^{i\vec{p}\cdot\vec{r}/\hbar}}$$

- Thus:

$$\tilde{\Psi}(\vec{p},t) := \langle \vec{p} | \Psi(t) \rangle = \int \mathrm{d}^3\vec{r}\, \langle \vec{p} | \vec{r} \rangle \langle \vec{r} | \Psi(t) \rangle$$

$$\left.\begin{aligned} \tilde{\Psi}(\vec{p},t) &= \frac{1}{\sqrt{(2\pi\hbar)^3}} \int \mathrm{d}^3\vec{r}\, e^{-i\vec{p}\cdot\vec{r}/\hbar}\, \Psi(\vec{r},t) \\ \Psi(\vec{r},t) &= \frac{1}{\sqrt{(2\pi\hbar)^3}} \int \mathrm{d}^3\vec{p}\, e^{+i\vec{p}\cdot\vec{r}/\hbar}\, \tilde{\Psi}(\vec{p},t) \end{aligned}\right\}$$ Fourier transform!

Momentum Rep

Definitions

- Typical operators in momentum representation:
  - The momentum operator itself:
    $$P_\alpha \widetilde{\Psi}(\vec{p},t) = \langle\vec{p}|\overleftarrow{P}_\alpha|\Psi(t)\rangle = p_\alpha \widetilde{\Psi}(\vec{p},t)$$
  - The coordinate operator:
    $$Q_\alpha \widetilde{\Psi}(\vec{p},t) = \langle\vec{p}|Q_\alpha|\Psi(t)\rangle = \int \mathrm{d}^3\vec{r}\,\langle\vec{p}|\vec{r}\rangle\langle\vec{r}|\overleftarrow{Q}_\alpha|\Psi(t)\rangle$$
    $$= \frac{1}{\sqrt{(2\pi\hbar)^3}} \int \mathrm{d}^3\vec{r}\; \underbrace{e^{-i\vec{p}\cdot\vec{r}/\hbar}\, x_\alpha}\; \Psi(\vec{r},t)$$
    $$= \frac{1}{\sqrt{(2\pi\hbar)^3}} \int \mathrm{d}^3\vec{r}\big(i\hbar\tfrac{\partial}{\partial p_\alpha} e^{-i\vec{p}\cdot\vec{r}/\hbar}\big)\Psi(\vec{r},t)$$
    $$= i\hbar\tfrac{\partial}{\partial p_\alpha}\Big(\frac{1}{\sqrt{(2\pi\hbar)^3}} \int \mathrm{d}^3\vec{r}\, e^{-i\vec{p}\cdot\vec{r}/\hbar}\, \Psi(\vec{r},t)\Big) = i\hbar\tfrac{\partial}{\partial p_\alpha}\widetilde{\Psi}(\vec{p},t)$$
  - That is, in the momentum representation, $Q_\alpha = i\hbar\frac{\partial}{\partial p_\alpha}$
  - just as in the coordinate representation, $P_\alpha = \frac{\hbar}{i}\frac{\partial}{\partial x^\alpha}$

Momentum Rep

Applications

- Thus, in the momentum representation

$$P_\alpha \widetilde{\Psi}(\vec{p},t) = p_\alpha \widetilde{\Psi}(\vec{p},t) \quad \text{and} \quad Q_\alpha \widetilde{\Psi}(\vec{p},t) = i\hbar \frac{\partial}{\partial p_\alpha} \widetilde{\Psi}(\vec{p},t)$$

- Then, the Hamiltonian is

quadratic function *operator function*

$$H = \frac{1}{2M}\vec{P}^2 + W(\vec{Q}) = \frac{1}{2M}\vec{p}^2 + W\left(i\hbar\frac{\partial}{\partial p_\alpha}\right)$$

- Beneficial when $W(Q)$ is constant or a linear function!
- Consider first $W(Q) = 0$ $(= const.)$:

$$i\hbar\frac{\partial}{\partial t}\widetilde{\Psi}(p,t) = \frac{p^2}{2M}\widetilde{\Psi}(p,t) \quad \Rightarrow \quad \widetilde{\Psi}(p,t) = e^{-i(p^2/2M\hbar)t}\,\widetilde{\Psi}(p,0)$$

  - and by Fourier-transforming back:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int \mathrm{d}p\, e^{i(kx-\omega t)}\,\widetilde{\Psi}(p,0) \quad k := \frac{p}{\hbar} \quad \omega = \frac{p^2}{2M\hbar}$$

since we are ***mostly*** interested in space distributions

negotiable

Momentum Rep

$$k := \frac{p}{\hbar} \qquad \omega = \frac{p^2}{2M\hbar}$$

Constant Potential

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int \mathrm{d}p\, e^{i(kx-\omega t)}\, \widetilde{\Psi}(p,0)$$

- For states with a specific energy, i.e., stationary states,
  - in constant potential, momentum is also constant
  - Then

$$\widetilde{\Psi}(p,0) = N\,\delta(p-p_0) \quad \Rightarrow \quad \Psi(x,t) = \frac{N}{\sqrt{2\pi\hbar}}\, e^{-i(\omega_0 t - k_0 x)}$$

  - just as we had used (as solutions of the coord. representation Schrödinger PDE, 1st order in time & 2nd order in space).
- For a gaussian “packet” at rest,

$$\Psi(x,0) = \frac{1}{\sqrt[4]{2\pi a^2}}\, e^{-(\frac{x}{2a})^2} \qquad \widetilde{\Psi}(p,0) = \sqrt[4]{\frac{2a^2}{\pi\hbar^2}}\, e^{-(\frac{ap}{\hbar})^2}$$

$$\Psi(x,t) = \sqrt[4]{\frac{a^2}{2\pi^3\hbar^2}} \int \mathrm{d}p\, \exp\Big\{ i\frac{px}{\hbar} - \underbrace{\Big(\frac{a^2}{\hbar^2} + \frac{i\,t}{2M\hbar}\Big)}_{\alpha^2/\hbar^2} p^2 - \Big\}$$

$$\Psi(x,t) = \frac{1}{\sqrt[4]{2\pi\,\alpha(t)^2}}\, e^{-(\frac{x}{2\alpha(t)})^2} \qquad \alpha(t) = a\sqrt{1 + \frac{i\hbar t}{2Ma^2}}$$

Newton’s 1st law!

Momentum Rep

Linear Potential

- If $W(Q)$ is linear, the Schrödinger equation becomes

$$i\hbar\frac{\partial}{\partial t}\widetilde{\Psi}(p,t) = \left[\frac{p^2}{2M} - FQ\right]\widetilde{\Psi}(p,t) = \left[\frac{p^2}{2M} - i\hbar F\frac{\partial}{\partial p}\right]\widetilde{\Psi}(p,t)$$

  - This still separates, producing

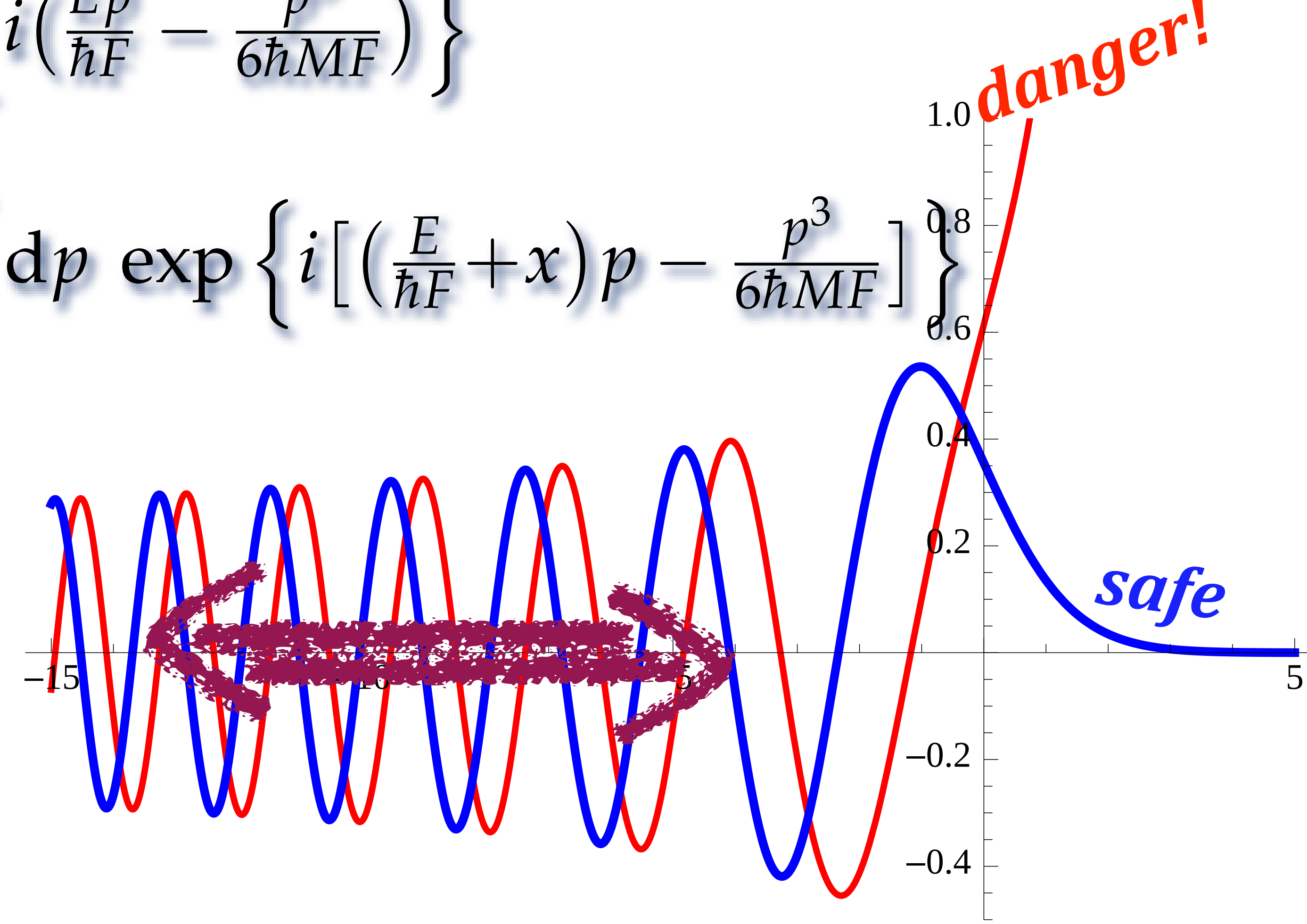
$$\widetilde{\Psi}_E(p,t) = A\,e^{-iEt/\hbar}\exp\left\{i\left(\frac{Ep}{\hbar F} - \frac{p^3}{6\hbar MF}\right)\right\}$$

E is "merely" the separation constant

  - The Fourier transform

$$\Psi_E(x,t) = \frac{A}{\sqrt{2\pi\hbar}}e^{-iEt/\hbar}\int \mathrm{d}p\,\exp\left\{i\left[\left(\frac{E}{\hbar F}+x\right)p - \frac{p^3}{6\hbar MF}\right]\right\}$$

  - cannot be expressed via simpler functions in closed form,
  - is an Airy function.



- Note: $\Psi_E^*(x,t) = \Psi_E(x,t)$
  standing wave

QMI

Momentum Rep

Linear Potential

- The strange homogeneous force field $W(Q) = -FQ$

$$H\,|\Psi_E(t)\rangle = \left[\frac{P^2}{2M} - FQ\right]|\Psi_E(t)\rangle = E\,|\Psi_E(t)\rangle$$

- Consider translating $Q \to Q + a$:

$$\left[\frac{P^2}{2M} - F(Q+a)\right]|\Psi_E(t)\rangle = \left[\frac{P^2}{2M} - FQ\right]|\Psi_E(t)\rangle - Fa\,|\Psi_E(t)\rangle$$

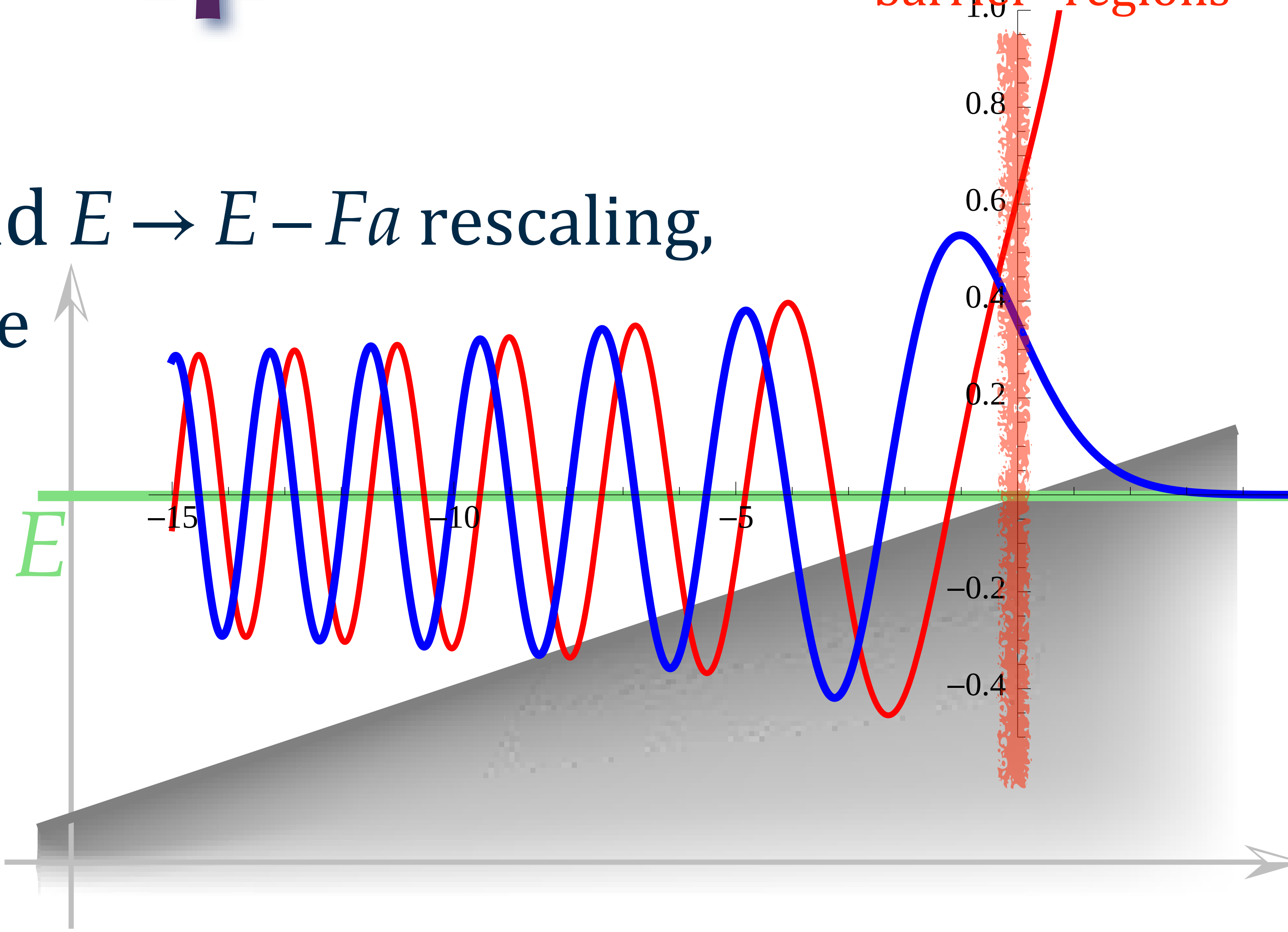
$$= (E - Fa)\,|\Psi_E(t)\rangle$$

  - It is equivalent to shifting the energy $E \to E - Fa$.
  - So, if the potential $W(Q) = -FQ$ were to extend to $x \to \infty$,
  - there would have to exist a stationary state with $E = -\infty$
  - ...no lowest-energy (a.k.a. ground) state
  - Potentials that allow this are "unbounded from below."
  - Typically, such potentials are valid in very limited regions (e.g., the hydrogen atom Coulomb potential $\to -\infty$ @ $r = 0$.)

Momentum Rep

Linear Potential

- Using the $Q \to Q + a$ and $E \to E - Fa$ rescaling,
  - The Airy functions solve differential equation
    $$y''(x) - x{\cdot}y(x) = 0$$
  - Interpolate between the oscillatory and the non-oscillatory regime
  - The transition occurs where $x = 0$, *i.e.*, in our case, when $W(Q) = E$



- This then provides an *exact interpolation* between
  - the classically allowed (oscillatory) region
  - the classically forbidden (non-oscillatory) region
  - for the cases where $W(Q)$ crosses the E-level continuously

Momentum Rep

"Box Quantization"

- Pretend that space is a big $L \times L \times L$ box
  - B.C.: $\Psi_E(\text{boundary}, t) = 0$
  - Then $\psi_E(\text{boundary}) = A \sin(\boldsymbol{k} \cdot \boldsymbol{r})$ where $k_\alpha = n_\alpha (2\pi / L)$ and

$${}_L\langle \vec{p} | \vec{p}' \rangle_L = \delta_{p'_x, p_x} \delta_{p'_y, p_y} \delta_{p'_z, p_z} \qquad \langle \vec{p} | \vec{p}' \rangle = \delta^{(3)}(\vec{p}' - \vec{p})$$

  - and expectation values

$$\langle f(\vec{p}) \rangle_L = \sum_{\vec{p}} f(\vec{p})\, {}_L\langle \vec{p} | \left(\hat{\rho} = |\Psi\rangle \langle \Psi| \right) | \vec{p} \rangle_L = \sum_{\vec{p}} f(\vec{p}) \left| {}_L\langle \vec{p} | \Psi \rangle_L \right|^2$$

$$\langle f(\vec{p}) \rangle = \int \mathrm{d}^3\vec{p}\, f(\vec{p})\, \langle \vec{p} | \left(\hat{\rho} = |\Psi\rangle \langle \Psi| \right) | \vec{p} \rangle = \int \mathrm{d}\vec{p}\, f(\vec{p}) \left| \langle \vec{p} | \Psi \rangle \right|^2$$

  - should coincide in the $L \to \infty$ limit

    setting $\langle f(\vec{p}) \rangle_L = \left(\frac{2\pi\hbar}{L} \right)^3 \langle f(\vec{p}) \rangle$ suffices:
  - calculate expectation values, then take the limit. ("$0 \cdot \infty$" form)
  - Often a useful in research practice; sums done numerically

Momentum Rep

Momentum Distribution

- Momentum distribution within a Hydrogen atom

$$\langle \vec{p} | \psi_g \rangle \propto \int \mathrm{d}^3\vec{r}\, e^{-i\vec{k}\cdot\vec{r}}\, e^{-r/a_0}$$

$$= \int_0^\infty r^2 \mathrm{d}r \int_0^\pi \sin\theta\, \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi\, e^{-i|\vec{k}||\vec{r}|\cos\theta}\, e^{-r/a_0}$$

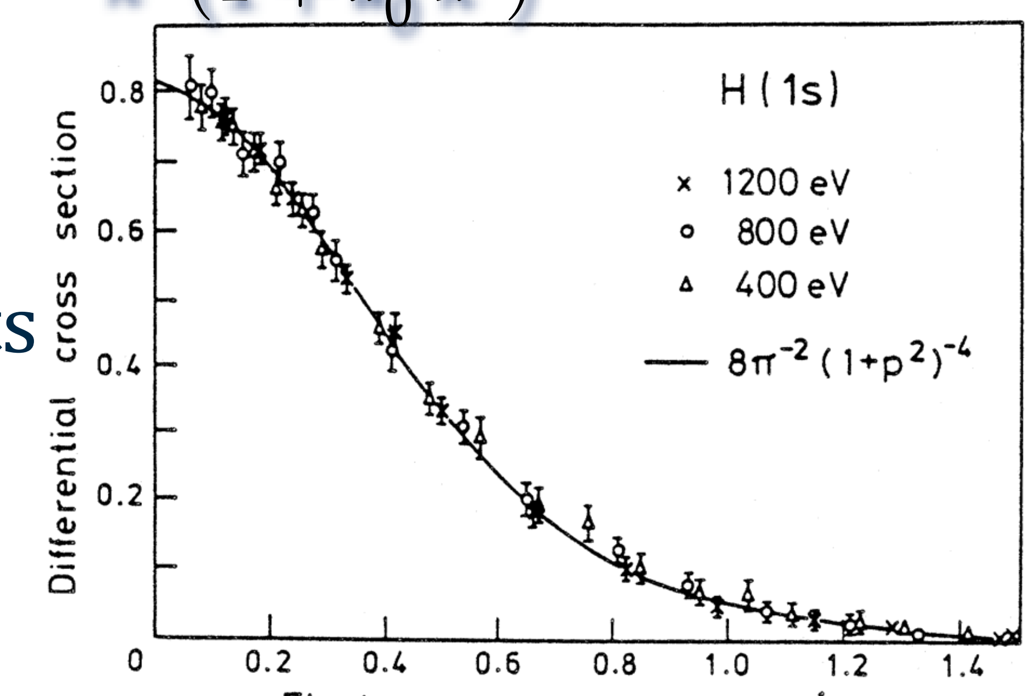
$$= 2\pi \int_0^\infty r^2 \mathrm{d}r\, e^{-r/a_0} \int_{-1}^{1} \mathrm{d}u\, e^{-ikr\,u} = 2\pi \int_0^\infty r^2 \mathrm{d}r\, e^{-r/a_0}\, 2\frac{\sin(kr)}{kr}$$

$$= \tfrac{4\pi}{k} \int_0^\infty r \mathrm{d}r\, e^{-r/a_0} \sin(kr) = \frac{4\pi}{k} \frac{2{a_0}^3 k}{(1+{a_0}^2k^2)^2} \propto (1+{a_0}^2k^2)^{-2}$$

- so that

$$|\langle \vec{p} | \psi_g \rangle|^2 \propto (1+{a_0}^2k^2)^{-4}$$

in agreement with experiments



Q M I

Momentum Rep

Bloch's Theorem

- Spatially periodic potentials (crystals)

$$W(\vec{Q}) = W(\vec{Q} + \vec{R}_{\vec{n}}) \quad \vec{R}_{\vec{n}} := n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

- have finite translation symmetries

$$U(\vec{R}_{\vec{n}}) = \exp\{-i\vec{R}_{\vec{n}}\cdot\vec{P}/\hbar\} \quad U(\vec{R}_{\vec{n}})\, H\, U^{-1}(\vec{R}_{\vec{n}}) = H \quad \left[\, U(\vec{R}_{\vec{n}})\,,\, H\,\right] = 0$$

- But then, they all must have simultaneous eigenstates

$$H\,|\Psi\rangle = E\,|\Psi\rangle \qquad U(\vec{R}_{\vec{n}})\,|\Psi\rangle = c(\vec{R}_{\vec{n}})\,|\Psi\rangle$$

- and the eigenvalues must "concatenate"

$$U(\vec{R}_{\vec{n}'})U(\vec{R}_{\vec{n}}) = U(\vec{R}_{\vec{n}}+\vec{R}_{\vec{n}'}) \quad \Rightarrow \quad c(\vec{R}_{\vec{n}'})c(\vec{R}_{\vec{n}}) = c(\vec{R}_{\vec{n}}+\vec{R}_{\vec{n}'})$$

$$c(\vec{R}_{\vec{n}}) = \exp\{-i\vec{R}_{\vec{n}}\cdot\vec{k}\} \quad \left|c(\vec{R}_{\vec{n}})\right|^2 = 1 \quad \Rightarrow \quad \vec{k} \in \mathbb{R}^3$$

- So, in the coordinate representation,

$$U(\vec{R}_{\vec{n}})\Psi(\vec{r}) := \Psi(\vec{r} - \vec{R}_{\vec{n}}) \quad = e^{-i\vec{R}_{\vec{n}}\cdot\vec{k}}\,\Psi(\vec{r})$$

Momentum Rep

Bloch's Theorem

$$U(\vec{R}_{\vec{n}})\Psi(\vec{r}) := \Psi(\vec{r}-\vec{R}_{\vec{n}}) \quad = e^{-i\vec{R}_{\vec{n}}\cdot\vec{k}}\,\Psi(\vec{r})$$

- Now expand the Bloch wave-function in plane-waves

$$\Psi(\vec{r}) = \sum_{\vec{k}'} a(\vec{k}')\, e^{i\vec{k}'\cdot\vec{r}} \qquad \sum_{\vec{k}'} a(\vec{k}')\, e^{i\vec{k}'\cdot(\vec{r}-\vec{R}_{\vec{n}})} = e^{-i\vec{R}_{\vec{n}}\cdot\vec{k}} \sum_{\vec{k}'} a(\vec{k}')\, e^{i\vec{k}'\cdot\vec{r}}$$

  - from which

$$\sum_{\vec{k}'} a(\vec{k}')\, e^{i\vec{k}'\cdot\vec{r}} = \sum_{\vec{k}'} a(\vec{k}')\, e^{i\vec{k}'\cdot\vec{r}}\, e^{-i\vec{k}'\cdot\vec{R}_{\vec{n}}} e^{i\vec{R}_{\vec{n}}\cdot\vec{k}} = \sum_{\vec{k}'} a(\vec{k}')\, e^{i\vec{k}'\cdot\vec{r}}\, e^{i(\vec{k}-\vec{k}')\cdot\vec{R}_{\vec{n}}}$$

  - and so

$$e^{i(\vec{k}-\vec{k}')\cdot\vec{R}_{\vec{n}}} \stackrel{!}{=} 1 \quad \text{for all } \vec{R}_{\vec{n}} \in \text{ lattice } \Lambda$$

$$\Rightarrow \quad \vec{q} := (\vec{k}-\vec{k}') \in \text{ reciprocal lattice } \Lambda^{-1}$$

  - Finally,

$$\Psi(\vec{r}) = \sum_{\vec{q}\in\Lambda^{-1}} a(\vec{k}+\vec{q})\, e^{i(\vec{k}+\vec{q})\cdot\vec{r}}$$

$\vec{k} := \vec{p}/\hbar$
wave-vector

Quantum Mechanics I

Now, go forth and calculate!!

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