Notes for Quantum Mechanics I, Phys 701, Fall 2023, University of Waterloo

J. D. D. Martin

`last commit hash: a08dd21        compiled: 2023-12-06, 17:02 EST`

I update these notes frequently. For the most recent version, please see: this link.

The symbols in the section titles are clickable links to video lectures.

Please let me know of any errors — I can easily correct and repost these notes.

Contents

1 Correspondence between lectures and topics

1) 2023-09-07 Lecture: Generators, transformation groups, Stone's theorem, He_2 and matter wave interference

2) 2023-09-12 Lecture: Postulates of QM, relationship between the position operator and the generator of spatial translations

3) 2023-09-14 Lecture: Heisenberg inequality, application to He_2

4) 2023-09-19 Lecture: Explicit form of the momentum operator in position space, minimum uncertainty wave-functions

5) 2023-09-21 Lecture: Momentum eigenfunctions in position space, time-evolution, review of Lagrangian and Hamiltonian classical dynamics

6) 2023-09-26 Lecture: Making the connection between CM and QM

7) 2023-09-28 Lecture: Adding magnetic fields to the Schrödinger equation

8) 2023-10-03 Lecture: Bound-state Aharanov-Bohm (AB) effect

9) 2023-10-05 Lecture: Experimental observation of the AB effect

10) 2023-10-17 Lecture: Intro to relativistic one-particle quantum mechanics, the Klein-Gordon equation (KGE)

11) 2023-10-19 Lecture: SDE and KGE for Coulomb potential

12) 2023-10-24 Lecture: SDE and KGE for Coulomb potential continued

13) 2023-10-26 Lecture: Continuity equation for the Schrödinger and Klein-Gordon equations

14) 2023-10-31 Lecture: Dirac equation

15) 2023-11-02 Lecture: Pauli equation from the Dirac equation

16) 2023-11-07 Lecture: angular momentum in the hydrogen atom, Introduction to scattering, cross-sections

17) 2023-11-09 Lecture: Natural units (for problems set), elastic scattering

18) 2023-11-14 Lecture: Elastic scattering cont.'d, hard-sphere scattering cross-sections

19) 2023-11-16 Lecture: Scattering amplitudes from phase shifts, Ramsauer-Townsend minima

20) 2023-11-21 Lecture: Lecture cancelled

21) 2023-11-23 Lecture: Relationship between scattering length and the low-energy s-wave phase shift, Born approximation

22) 2023-11-28 Lecture: Born approximation, proton-Ca nucleus scattering

23) 2028-11-30 Lecture: Resonant scattering and the Breit-Wigner formula; the H-Kr example

24) 2028-12-05 Lecture: Derivation of formulae for numerically solving the one-dimensional Schrödinger equation (Cooley)

2 Lectures

2.1 2023-09-07 Lecture

Lecture based on [1, 2]. For a mathematically “respectable” presentation see: Ref. [3].

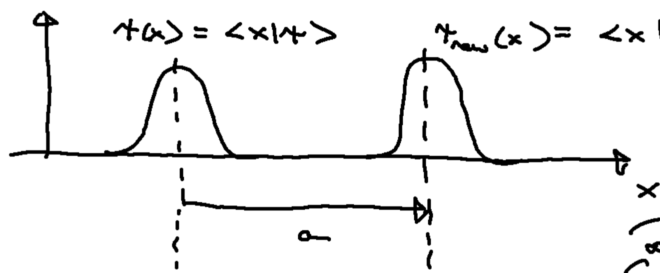
①

Generators and Transformation Groups

- start by discussing unitary transformations.

e.g. spatial translations

$\psi(x) = \langle x|\psi\rangle$ $\qquad$ $\psi_{new}(x) = \langle x|\underbrace{\mathcal{J}(a)}_{\text{spatial translation operator.}}|\psi\rangle$



$$\overbrace{\int_{-\infty}^{\infty} dx\, |\psi(x)|^2 = 1}^{\text{normalization}}$$

$$\langle\psi|\psi\rangle = 1$$

Properties of $\mathcal{J}(a)$:

① $\mathcal{J}(0) = \mathbb{1}$

②

② $\mathcal{J}(a)$ is unitary.

An operator $\mathcal{U}$ is <u>unitary</u> if

$$\underbrace{\mathcal{U}^{\dagger}}_{\substack{\text{Hermitian}\\\text{conjugate of}\\\mathcal{U}}} = \underbrace{\mathcal{U}^{-1}}_{\text{inverse of }\mathcal{U}}$$

<u>Inverse</u> of A is denoted by A^{-1}, and satisfies

$$A^{-1}A = AA^{-1} = \mathbb{1}$$

<u>Hermitian conjugate</u> of A is denoted by $A^{\dagger}$ and satisfies

$$\langle\Phi|A|\psi\rangle = \langle\psi|A^{\dagger}|\Phi\rangle^{*}$$

for all Φ and ψ.

③

$\mathcal{G}(a)$ unitary means it preserves normalization.

Start with $\langle \psi | \psi \rangle = 1$

$$\langle \mathcal{G}(a)\psi \,|\, \mathcal{G}(a)\psi \rangle = \langle \psi | \mathcal{G}^{+}(a)\,\mathcal{G}(a) | \psi \rangle$$

$$= 1 \quad \text{if} \quad \mathcal{G}^{+}(a)\,\mathcal{G}(a) = \mathbb{1}$$

or equivalently $\mathcal{G}(a)$ is unitary.

③ $\mathcal{G}(a)\,\mathcal{G}(b) = \mathcal{G}(a+b)$

④

Consider consequences of the properties ①, ② and ③ for $\mathcal{G}(a)$:

$$\mathcal{G}(a+\delta a) = \mathcal{G}(\delta a)\,\mathcal{G}(a)$$

$$= \left(\mathbb{1} + \delta a \left.\frac{d\mathcal{G}(a)}{da}\right|_{a=0} \right) \mathcal{G}(a)$$

Define $T := \underbrace{-i \left.\frac{d\mathcal{G}(a)}{da}\right|_{a=0}}$

So that

$$\mathcal{G}(a+\delta a) = (\mathbb{1} + i\,\delta a\,T)\,\mathcal{G}(a) \qquad (\#)$$

T must be Hermitian. Why?

(5)

Since $\mathcal{J}(\delta a)$ is unitary:

$$\begin{aligned}\mathbb{1} &= \mathcal{J}(\delta a)\,\mathcal{J}^{+}(\delta a)\\ &= (\mathbb{1} + i\delta a T)(\mathbb{1} - i\delta a T^{+})\\ &= \mathbb{1} + i\delta a \underbrace{(T - T^{+})}_{=0}\end{aligned}$$

$$T = T^{+}$$

From (‡), we have the DE:

$$\frac{d\mathcal{J}(a)}{da} = iT\,\mathcal{J}(a)$$

with "initial conditions" $\mathcal{J}(0) = \mathbb{1}$

A solution is $\boxed{\mathcal{J}(a) = e^{iTa}}$

(6)

We have just given a heuristic justification of Stone's theorem:

"Given a set of unitary operators (forming a group) depending continuously on a parameter and satisfying $U(\alpha_1 + \alpha_2) = U(\alpha_1)U(\alpha_2)$ and $U(0) = \mathbb{1}$,

then there exists an operator T called the infinitesimal generator of the transformation group such that

$$U(\alpha) = e^{i\alpha T}$$

with $T = T^{+}$ (T hermitian)."

⑦

Next: for $g(\omega)$ can we give a physical interpretation for T?

First experimental demonstration of *matter* wave interference

- known for photons since $E = h\nu$:

$$p = \frac{h}{\lambda}$$

- de Broglie hypothesized this relationship to hold for particles with mass:
- de Broglie (1923):

  "a stream of electrons passing through a sufficiently narrow hole should also exhibit diffraction phenomena" ... "it is in this direction where one has probably to look for experimental confirmations of our ideas"

  (Jammer, "The conceptual development of quantum mechanics", pg 246)

- more or else directly observed by Davisson and Germer in 1927, Phys. Rev. 30, 705 (1927).
- nice summary in Trigg's *Crucial Experiments in Modern Physics*

Peaks emerge in monogenergetic electron scattering of a "clean" surface

- scattering occurs preferentially into certain angles:

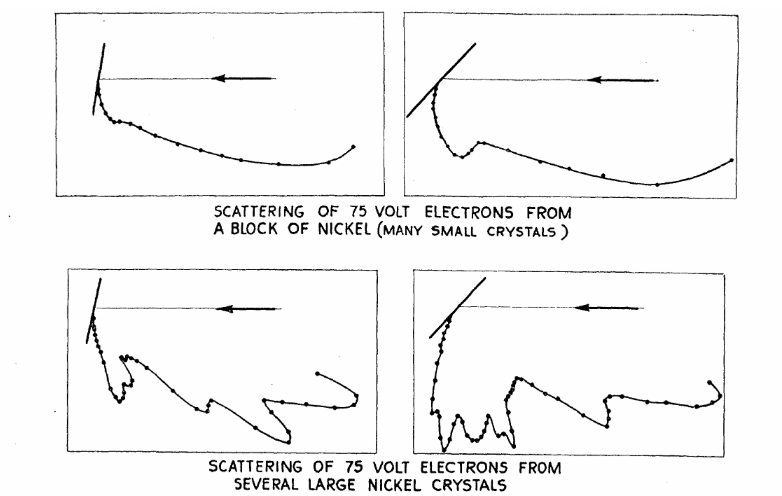


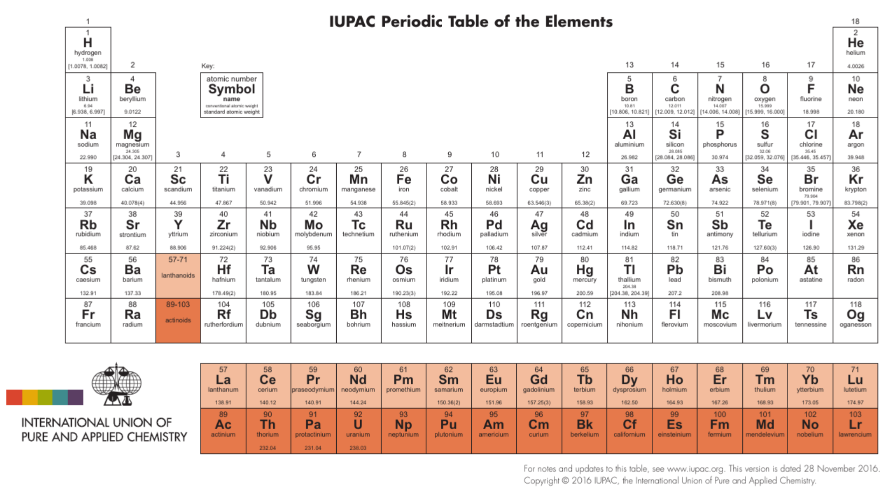
Fig. 1. Scattering curves from nickel before and after crystal growth had occurred.

from Davisson and Germer, Phys. Rev. 30, 705 (1927).

An surprising application of matter wave interference

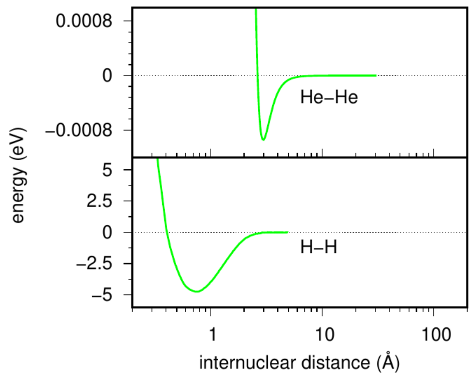
- matter wave interference is now a probe of the properties of surfaces (low energy electron scattering) and solids (neutron scattering), in the same way that x-ray diffraction is.
- but we can also use matter wave interference to learn about the “particle” being scattered.

The “lazy” gases do not form chemical bonds



He_2 controversy

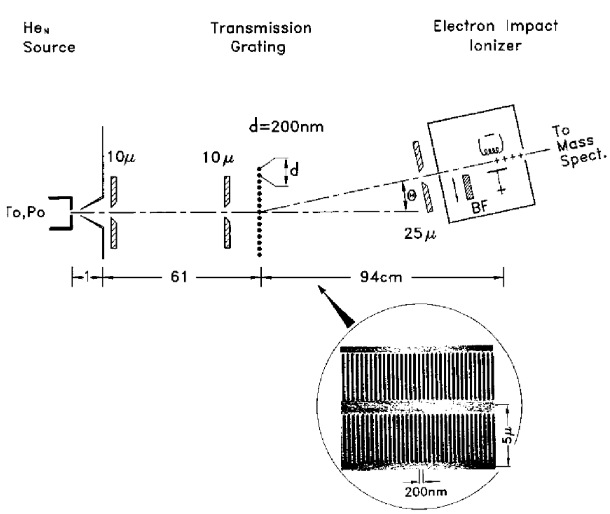
- does He_2 exist ? If so, it is very weakly bound. Comparison with H_2 (Born-Oppenheimer):



- weak attraction, at 300 K, $kT \approx 0.03$ eV.
- in *principle* these curves can be calculated, but with "theoretical uncertainty".

We can learn about the "particle" using its wave properties

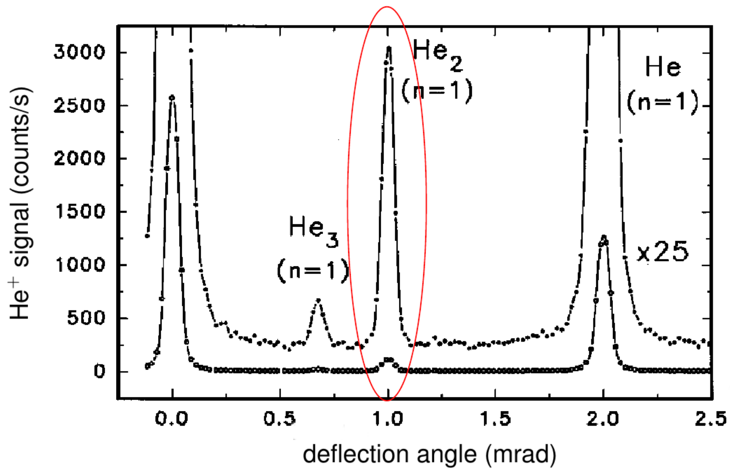
- W. Schöllkopf and J. Peter Toennies, J. Chem. Phys. 104, 1155 (1996):



- any He_2 in the beam will be moving at the same speed as the He atoms, thus will have 1/2 the de Broglie wavelength.

Observation of *extra* diffraction peak shows existence of He_2

- W. Schöllkopf and J. Peter Toennies, J. Chem. Phys. 104, 1155 (1996):



①

For spatial translations, let us write:

$$\mathcal{J}(a) = e^{-iaK} \quad \left(\text{let's use } -K \text{ instead of } T\right)$$

Hermitian $(K^{+} = K)$

What is K?

Postulates of QM (Shankar's PQM wording)

1) The state of a system is represented by a normalized vector $\left(\langle \psi(t) | \psi(t) \rangle = 1 \right)$ in a Hilbert space.

$$\int_{-\infty}^{\infty} dx \; \psi^{*}(x) \psi(x) = \int_{-\infty}^{\infty} dx \; |N|^2$$

②

2) Physical observables (position, angular momentum, etc...) correspond to Hermitian operators.

3) If a system is in a state $|\psi\rangle$, then measurement of an observable Ω will yield one of its eigenvalues ω, with probability:

$$P(\omega) = |\langle \omega | \psi \rangle|^2$$

and the state will change from $|\psi\rangle$ to $|\omega\rangle$.

4) The state vector obeys the Schrödinger equation:

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H \, |\psi(t)\rangle$$

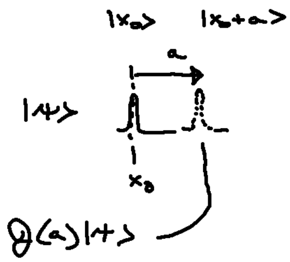
Hermitian so that state stays normalized.

③

Is k a physical observable?

$$\underbrace{\psi(x)}_{\text{wavefcn in position space.}} = \langle x|\psi\rangle$$

$$\underbrace{\psi_{new}(x)}_{\text{after translation}} = \langle x|\mathcal{T}(a)|\psi\rangle$$
$$= \langle \mathcal{T}^{\dagger}(a)x|\psi\rangle$$
$$= \langle \mathcal{T}^{-1}(a)x|\psi\rangle$$
$$= \langle x-a|\psi\rangle$$
$$= \psi(x-a)$$



$$\mathcal{T}^{-1}(a) = \mathcal{T}(-a) \; (*)$$
$$\mathcal{T}^{-1}(a)\,\mathcal{T}(a) = \mathbb{1}$$
$$\mathcal{T}(a)\,\mathcal{T}(b) = \mathcal{T}(a+b)$$
$$\mathcal{T}(0) = \mathbb{1}$$

Suppose a particle has a well-defined momentum p', then by de Broglie:

④

$$\langle x|\psi\rangle = \langle x|p'\rangle$$
$$= N e^{ip'x/\hbar} \qquad \left(\lambda = \frac{h}{p'}\right)$$
$$= N e^{i\left(\frac{hx}{\lambda}\frac{1}{\hbar}\right)}$$
$$= N e^{i\left(\frac{2\pi x}{\lambda}\right)} = N\left(\cos\left(\frac{2\pi x}{\lambda}\right) + i\sin\left(\frac{2\pi x}{\lambda}\right)\right)$$

$$\langle x|\mathcal{T}(a)|\psi\rangle = \langle x-a|p'\rangle$$
$$= N e^{ip'(x-a)/\hbar}$$
$$= N e^{-ip'a/\hbar}\underbrace{e^{ip'x/\hbar}}_{\langle x|p'\rangle/N}$$
$$= \langle x|e^{-\frac{ipa}{\hbar}}|p'\rangle$$
$$= e^{-\frac{ip'a}{\hbar}}\langle x|p'\rangle$$

Suggests that $k = p/\hbar$ where p is the momentum operator.

5

Proceed, assuming this is the case, checking for logical consistency.

Relationship between the position operator and the generator of spatial translations

The expectation value of an operator Ω representing an observable is: $\langle \Omega \rangle_\psi := \langle \psi | \Omega | \psi \rangle$

Why is this of interest?

Expand $|\psi\rangle$ in an orthonormal basis with basis vectors corresponding to the eigenkets of Ω:

$$|\psi\rangle = \underbrace{\sum_\omega |\omega\rangle\langle\omega|}_{\mathbb{1}} \psi\rangle \qquad \text{where: } \Omega|\omega\rangle = \omega|\omega\rangle$$

"resolution of identity" $\qquad \langle\omega|\omega'\rangle = \delta_{\omega,\omega'}$

6

That this expansion can be done for any Hermitian Ω ($\Omega = \Omega^\dagger$) is known as the "spectral decomposition theorem".

[for notational convenience I am assuming a discrete, non-degenerate spectrum, but this doesn't change anything in an essential way]

$$\begin{aligned}
\langle \Omega \rangle_\psi &= \langle \psi | \Omega | \psi \rangle \\
&= \langle \psi | \mathbb{1} \Omega \mathbb{1} | \psi \rangle \\
&= \langle \psi | \sum_{\omega'} |\omega'\rangle\langle\omega'| \Omega | \sum_{\omega''} |\omega''\rangle\langle\omega''| \psi \rangle \\
&= \sum_{\omega',\omega''} \langle\psi|\omega'\rangle\langle\omega'|\omega''|\omega''\rangle\langle\omega''|\psi\rangle \\
&= \sum_{\omega',\omega''} \omega'' \langle\psi|\omega'\rangle \underbrace{\langle\omega'|\omega''\rangle}_{\delta_{\omega',\omega''}} \langle\omega''|\psi\rangle
\end{aligned}$$

(7)

$$\langle \Omega \rangle_\psi = \sum_{\omega'} \omega' \langle \psi | \omega' \rangle \langle \omega' | \psi \rangle$$

$$\boxed{\langle \Omega \rangle_\psi = \sum_{\omega'} \omega' \underbrace{|\langle \omega' | \psi \rangle|^2}_{\text{the probability of being in } |\omega'\rangle \text{ according to our postulates.}}}$$

Thus $\langle \Omega \rangle_\psi$ is the average value of Ω that we expect to measure for state ψ.

Apply expectation value to spatial translations.

$$\langle \mathcal{T}(a)\psi | x | \mathcal{T}(a)\psi \rangle = \underbrace{\langle \psi | x | \psi \rangle} + a$$

$$\langle \psi | \underbrace{\mathcal{T}^+(a)\, x\, \mathcal{T}(a)} | \psi \rangle = \langle \psi | x | \psi \rangle + a.$$

(8)

This will be true if

$$\mathcal{T}^+(a)\, x\, \mathcal{T}(a) = x + a\mathbb{1} \qquad (*)$$

$$\mathcal{T}(a) = e^{-ipa/\hbar} \qquad \Big\{\; e^A = \mathbb{1} + A + \frac{1}{2!}A^2 \ldots$$

$$\left(\mathbb{1} + \frac{ipa}{\hbar} + \ldots\right) x \left(\mathbb{1} - \frac{ipa}{\hbar} + \ldots\right) = x + a\mathbb{1}$$

$$\left(x + \frac{ipax}{\hbar} - x\frac{ipa}{\hbar} + O(a^2)\right) = x + a\mathbb{1}$$

$$\frac{i\cancel{a}}{\hbar}(px - xp) = \cancel{a}$$

$$(xp - px) = i\hbar$$

$$\boxed{[x, p] = i\hbar}$$

$[A, B] := AB - BA$ is the commutator of operators A and B.

(9)

Addendum : (added 2023-09-14)

$$\left(x + \frac{ipax}{\hbar} - x\,\frac{ipa}{\hbar} + \underbrace{O(a^2)}_{} \right) = x + a\mathbb{1}$$

we ignored possible non-zero terms because they don't appear on RHS. Was this valid?

Could be problematic because there is no guarantee that

$$\mathcal{J}^{+}(a)\, x\, \underbrace{\mathcal{J}(a)}_{e^{-ipa/\hbar}} = x + a\mathbb{1}$$

it would be good to show that this Eqn $\Rightarrow [x,p] = i\hbar$

Useful mathematical result:

If X and Y (two generic Hermitian operators) commute with $[X,Y]$

$$e^{X} Y e^{-X} = Y + \underbrace{[X,Y]}_{}$$

[See Baker - Campbell - Hausdorff formula wikipedia page]

2.3 2023-09-14 Lecture

This is generic material. I follow notation of Ref. [2].

Post-lecture: In the lecture, someone asked about wavefunctions that "saturate" the Heisenberg inequality; i.e., satisfy the *equality*. We will derive the form of these wavefunctions (Gaussian; e.g., see page 290 of Ref. [4].) once we consider the form that the momentum operator takes in position space.

①

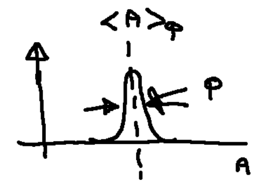
Heisenberg inequality

"Had this celebrated Heisenberg uncertainty principle instead been called the "principle of non-commuting operators" we would see it less frequently invoked to describe matters having nothing to do with quantum mechanics".
J.D. Jackson.

- consider two physical observables corresponding to the operators A and B.

- "dispersion" of A for a state φ is:

$$\Delta_\varphi A := \sqrt{\langle (A - \langle A\rangle_\varphi \mathbb{1})^2 \rangle_\varphi}$$



②

- to condense our derivation, define:

$$A_0 := A - \langle A\rangle_\varphi \mathbb{1}$$

so that

$$\Delta_\varphi A = \sqrt{\langle A_0^2\rangle_\varphi}$$

and similarly for B_0.

- we will derive general version of $\Delta_\varphi x \, \Delta_\varphi p \geq \frac{\hbar}{2}$ (which is a consequence of $[x, p] = i\hbar$)

- note that $[A, B]$ is anti-Hermitian.
  i.e. $O = -O^+$ then O is anti-Hermitian.
  note: $-iO$ is Hermitian. Why?

$$-(iO)^\dagger = -(-i)(-O) = -iO$$

Thus we will define $C := -i[A, B]$, so that C is Hermitian.

$$\Rightarrow [A, B] = iC$$

(3)

Follows that $[A_0, B_0] = iC$ (*)

Take $|\psi\rangle = (A_0 + i\lambda B_0)|\varphi\rangle$

real.

$\langle\psi|\psi\rangle \geqslant 0$ (true for all ψ in a Hilbert space)

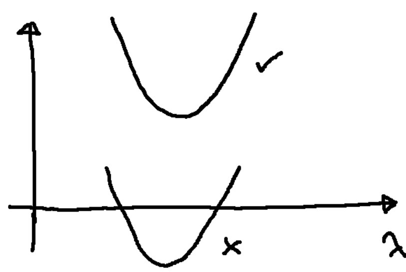
$$\langle\varphi|(A_0 - i\lambda B_0)(A_0 + i\lambda B_0)|\varphi\rangle \geqslant 0$$

$$\langle\varphi|A_0^2 + \lambda^2 B_0^2 - i\lambda B_0 A_0 + A_0 i\lambda B_0|\varphi\rangle \geqslant 0$$

$$\langle A_0^2\rangle_\varphi + \lambda^2\langle B_0^2\rangle_\varphi + i\lambda\underbrace{\langle A_0B_0 - B_0A_0\rangle_\varphi}_{iC \quad (\text{from } *)} \geqslant 0$$

$$\underbrace{\langle B_0^2\rangle_\varphi}_{\text{"a"}}\lambda^2 \underbrace{- \langle C\rangle_\varphi}_{\text{"b"}}\lambda + \underbrace{\langle A_0^2\rangle_\varphi}_{\text{"c"}} \geqslant 0 \qquad (\ddagger)$$

(4)



$\underbrace{b^2 - 4ac}$

To satisfy ($\ddagger$) we need $b^2 - 4ac \leqslant 0$

$$(\langle C\rangle_\varphi)^2 - 4\langle B_0^2\rangle_\varphi\langle A_0^2\rangle_\varphi \leqslant 0$$

Rearrange to give:

$$\langle B_0^2\rangle_\varphi\langle A_0^2\rangle_\varphi \geqslant \frac{(\langle C\rangle_\varphi)^2}{4}$$

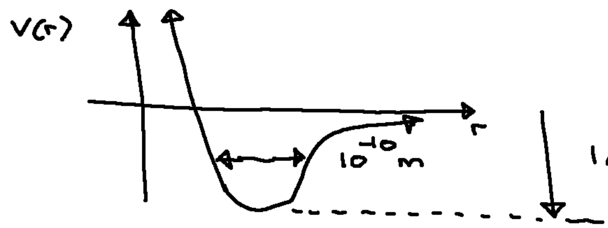
$$\Delta_\varphi A \;\Delta_\varphi B \geqslant \frac{1}{2}\left|\langle [A, B]\rangle_\varphi\right|$$

(5)

For x and p, $[x,p] = i\hbar$, so that

$$\Delta_\varphi x \, \Delta_\varphi p \geq \frac{\hbar}{2}$$

Let's use the uncertainty relation to estimate if He – He potential supports a bound state.



1 meV "well-depth".

$\Delta_\varphi x \simeq 10^{-10}$ m

$\langle p \rangle_\varphi = 0$ for a bound-state (you will be asked to prove)

(6)

$$\langle p_o^2 \rangle_\varphi = \underbrace{\langle p^2 \rangle_\varphi}_{2m \langle KE \rangle_\varphi}$$

$$\langle p^2 \rangle_\varphi \geq \frac{(\hbar/2)^2}{(\Delta_\varphi x)^2}$$

$$\langle KE \rangle_\varphi \geq \frac{1}{2m} \frac{(\hbar/2)^2}{(\Delta_\varphi x)^2}$$

$$\gtrsim \frac{(10^{-34}\, J.s)^2}{2\left(\frac{1}{2} 4 * 1.66 * 10^{-27}\, kg\right)} \frac{1}{(10^{-10}\, m)^2}$$

$$\geq 3.8 * 10^{-23} \frac{J}{kg \cdot m^2/s^2} J \Big/ 1.6 * 10^{-19} \frac{J}{eV}$$

$\gtrsim 0.2$ meV   about 1/5 of well-depth. Probably a bound-state exists.

2.4 2023-09-19 Lecture

Pre-lecture:

Lecture based on Ref. [1] and Ref. [4].

1

The explicit form of the momentum operator in position space (Sakurai)

$$\mathcal{J}(a)|\psi\rangle = \mathcal{J}(a)\underbrace{\int dx\, |x\rangle\langle x|}_{\mathbb{1}}\psi\rangle$$

$$= \int dx\, |x+a\rangle \underbrace{\langle x|\psi\rangle}_{=:\,\psi(x)} \quad \text{wave-fcn in position space}$$

$$= \int dx\, |x\rangle \psi(x-a)$$

Expand both sides in powers of a, using $\mathcal{J}(a) = e^{-ipa/\hbar}$

$$\left(1 - \frac{ipa}{\hbar} + O(a^2)\right)|\psi\rangle = \int dx\, |x\rangle \left(\underbrace{\psi(x)}_{\langle x|\psi\rangle} - a\psi'(x) + O(a^2)\right) \quad (*)$$

0th order agrees.

2

1st order agreement requires:

$$-\frac{ip}{\hbar}|\psi\rangle = \int dx\, |x\rangle (-1)\, \psi'(x)$$

Equivalently:

$$p|\psi\rangle = -i\hbar \int dx\, |x\rangle \frac{d}{dx}\langle x|\psi\rangle$$

You can verify that this form of p, satisfies $(*)$ to all orders of a.

Suppose that we want to evaluate a matrix element of p using 2 arb. position space wave-fcns.

③

$$\langle \varphi | p | \psi \rangle = -i\hbar \int dx \, \langle \varphi | x \rangle \frac{d}{dx} \langle x | \psi \rangle$$

$$= \int dx \, \varphi(x)^* (-i\hbar) \frac{d}{dx} \psi(x)$$

Use explicit form of p in position space to derive the "minimum uncertainty wavefunctions".

From Hilbert-space axioms: $\langle \psi | \psi \rangle = 0 \Rightarrow |\psi\rangle = |\vec{0}\rangle$

Thus using expression from Heisenberg inequality section of notes $(A_0 + i\lambda B_0)|\varphi\rangle = |\vec{0}\rangle$

$$\lambda_0 = \frac{-b \pm \sqrt{\cancel{b^2 - 4ac}}}{2a} = \frac{-b}{2a} = \sqrt{\frac{c}{a}} = \frac{\Delta_\varphi x}{\Delta_\varphi p}$$

$= 0$

$\pm\sqrt{4ac}$

④

$A \to x$, $B \to p$

$$[(x - \langle x \rangle) + i\lambda_0 (p - \langle p \rangle)] |\varphi\rangle = |\vec{0}\rangle$$

Fold with $\langle x|$

$$x \underbrace{\langle x | \varphi \rangle}_{=: \, \varphi(x)} - \langle x \rangle \langle x | \varphi \rangle + i\lambda_0 \langle x | p | \varphi \rangle - i\lambda_0 \langle p \rangle \langle x | \varphi \rangle = 0$$

$$x\varphi(x) - \langle x \rangle \varphi(x) + i\lambda(-i\hbar) \frac{d}{dx} \varphi(x) - i\lambda_0 \langle p \rangle \varphi(x) = 0 \quad (*)$$

Use a substitution to simplify solving

$$\varphi(x) = e^{ix\langle p \rangle / \hbar} \, \Theta(x - \langle x \rangle)$$

new function

(5)

$$\frac{d}{dx}\varphi(x) = \frac{i\langle p\rangle}{\hbar} e^{ix\langle p\rangle/\hbar}\,\Theta(x-\langle x\rangle) + e^{ix\langle p\rangle/\hbar}\,\Theta'(x-\langle x\rangle)$$

(*) can be rewritten using the substitution as:

$$(x-\langle x\rangle)\,\Theta(x-\langle x\rangle) + \cancel{i\lambda_0\langle p\rangle\,\Theta(x-\langle x\rangle)} - \cancel{i\lambda_0\langle p\rangle\,\Theta(x-\langle x\rangle)} + \lambda_0\hbar\,\Theta'(x-\langle x\rangle) = 0$$

Shift x by $\langle x\rangle$: $\quad \lambda_0\hbar\,\Theta'(x) + x\,\Theta(x) = 0$

$$\int\frac{d\Theta}{\Theta} = \frac{-1}{\lambda_0\hbar}\int dx\, x \qquad\qquad \lambda_0\hbar\,\frac{d\Theta(x)}{dx} = -x\,\Theta(x)$$

$$\ln\Theta + C = \frac{-x^2}{2\lambda_0\hbar} \qquad\qquad \int\frac{d\Theta(x)}{\Theta(x)} = -\frac{1}{\lambda_0\hbar}\int x\,dx$$

(6)

$$\Theta(x) = A\, e^{-\frac{x^2}{2\lambda_0\hbar}}$$

$$\varphi(x) = e^{ix\langle p\rangle/\hbar}\, A\, e^{-\frac{(x-\langle x\rangle)^2}{2\lambda_0\hbar}}$$

Let's get rid of λ_0. $\left(= \dfrac{\Delta_\varphi x}{\Delta_\varphi p} \text{ from (3)}\right)$

But also $\Delta_\varphi x\,\Delta_\varphi p = \hbar/2$; i.e. minimum uncertainty, so

$$\lambda_0 = \frac{(\Delta_\varphi x)^2}{\hbar/2}$$

$$\boxed{\psi(x) = A\, e^{ix\langle p\rangle/\hbar}\, e^{-\frac{(x-\langle x\rangle)^2}{4(\Delta_\varphi x)^2}}} \qquad e^{-\frac{x^2}{2\sigma^2}}$$

2.5 2023-09-21 Lecture

Pre-lecture:

Determination of the form of the momentum eigenkets in position space follows Ref. [1]. For a nice review of CM in the QM context, see Ref. [5].

①

The momentum eigenfunctions in position space i.e. $\langle x'|p'\rangle = ?$

↖ state of well-defined momentum.

$$p\,|p'\rangle = -i\hbar \int dx''\,|x''\rangle \frac{d}{dx''}\langle x''|p'\rangle$$

$$p'\,|p'\rangle = \quad ''$$

better notations!!! $\left.\frac{d}{dx} f(x)\right|_{x=x''}$ or $f'(x'')$

Fold from left with $\langle x'|$

$$\langle x'|p'|p'\rangle = -i\hbar \int dx''\,\underbrace{\langle x'|x''\rangle}\,\frac{d}{dx''}\langle x''|p'\rangle \qquad (\ddagger)$$

Aside: $|\psi\rangle = \underbrace{\int dx'\,|x'\rangle\langle x'|}_{\mathbb{1}}\psi\rangle$ fold from left with $\langle x''|$ ⤳

②

$$\underbrace{\langle x''|\psi\rangle} = \int dx'\,\underbrace{\langle x''|x'\rangle}_{\delta(x''-x')}\,\underbrace{\langle x'|\psi\rangle} \qquad (*)$$

Recall definition of δ-"fcn":

$$\int f(x)\,\delta(x-a)\,dx = f(a)$$

By defining $\langle x''|x'\rangle$ to be $\delta(x''-x')$, $(*)$ becomes

$$\langle x''|\psi\rangle = \langle x''|\psi\rangle$$

as req'd. //

Going back to $(\ddagger)$, we have

$$p'\,\underbrace{\langle x'|p'\rangle} = -i\hbar\,\frac{d}{dx'}\,\underbrace{\langle x'|p'\rangle}_{=:\,f(x')}$$

③

$$\underset{(\,:=\, ip'/\hbar)}{\alpha}\, f(x') = \frac{d f(x')}{dx'}$$

Has the solution:

$$f(x') = \underbrace{c}_{\text{arb. const.}}\, e^{\alpha x'}$$

So $\underbrace{\langle x'|p'\rangle}_{\text{wavefcn in position space of momentum eigenstate.}} = c\, e^{ip'x'/\hbar}$ (x)

Is there a meaningful choice for c?

$$\underset{\text{arb. state}}{|\alpha\rangle} = \underbrace{\int dp'\, |p'\rangle\langle p'|}_{\mathbb{1}\text{, "resolution of the identity".}}\alpha\rangle$$

Fold from left with $\langle p''|$

$$\langle p''|\alpha\rangle = \int dp'\ \langle p''|p'\rangle\langle p'|\alpha\rangle$$

④

This will work out if $\langle p''|p'\rangle = \delta(p''-p')$

Use this constraint to determine c.

$$\begin{aligned}
\delta(p''-p') &= \langle p''|p'\rangle \\
&= \langle p''|\ \underbrace{\int dx'\, |x'\rangle\langle x'|}_{\mathbb{1}}\ |p'\rangle \\
&= \int dx'\ \langle p''|x'\rangle\langle x'|p'\rangle \\
&= \int dx'\ \langle x'|p''\rangle^{*}\langle x'|p'\rangle \\
&= \int dx'\ c^{*}e^{-ip''x'/\hbar}\ c\, e^{ip'x'/\hbar} \\
&= |c|^2 \underbrace{\int dx'\, e^{ix'(p'-p'')/\hbar}}_{\text{standard result}} \qquad (xx)
\end{aligned}$$

use (x) from previous page.

⑤

Purely mathematical : $\int_{-\infty}^{\infty} dx\, e^{ikx} = 2\pi\,\delta(k)$ (o)

Define $\theta := x'/\hbar$, so that

$$\delta(p''-p') = |c|^2 \int_{-\infty}^{\infty} d\theta\, \hbar\, e^{i\theta(p'-p'')}$$, using (o)

$$= |c|^2 \hbar\, 2\pi\, \delta(p'-p'')$$

$$1 = |c|^2 \hbar\, 2\pi$$

Thus $c = \frac{1}{\sqrt{2\pi\hbar}}$ (to within a phase)

So $$\boxed{\langle x''|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{ip'x''/\hbar}}$$

⑥

$$J\cdot s \rightarrow kg\cdot\frac{m^2}{s^2}\cdot s \rightarrow \frac{kg\cdot m^2}{s}$$

Units of c are $\sqrt{\frac{s}{kg\cdot m^2}}$.

Do these dimensions make sense?

Go back to (xx) on pg 4.

LHS has units of 1/momentum $\rightarrow \frac{s}{kg\cdot m}$

RHS has units $m\cdot\frac{s}{kg\cdot m^2} \rightarrow \frac{s}{kg\cdot m}$

⑦

Time evolution

- recall postulate: $i\hbar \frac{d}{dt} |\psi(t)\rangle = H\,|\psi(t)\rangle$

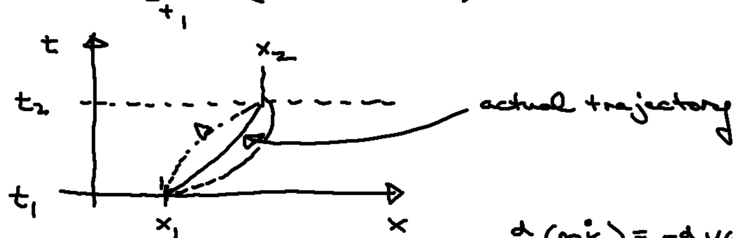
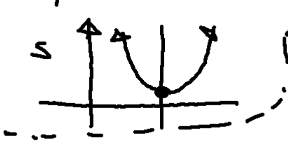
How do we determine H? Two major approaches:

1) "canonical quantization"
   adapting the classical equations of motion.
2) use invariance principles (more modern).

Look at both, starting with 1).

⑧

Lagrangian and Hamiltonian classical dynamics

General idea	1-d example, conservative force.
Start with a Lagrangian: $\mathcal{L}(q, \dot{q}, t)$	$\mathcal{L} = T - U$ $= \frac{1}{2} m \dot{x}^2 - V(x)$
Action: $S := \int_{t_1}^{t_2} dt\, \mathcal{L}(q, \dot{q}, t)$ must be "stationary" to first-order in deviations gives Euler-Lagrange (EL) eqns: $\underbrace{\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}}\right) = \frac{\partial \mathcal{L}}{\partial q}}_{\text{for each generalized coord.}}$	$S = \int_{t_1}^{t_2} dt \left(\frac{1}{2} m \dot{x}^2 - V(x)\right)$  

$\frac{d}{dt}(m\dot{x}) = -\frac{d}{dx} V(x)$

$m\ddot{x} = -\frac{d}{dx} V(x)$

(9)

Define canonical momenta:

$$p_i := \frac{\partial \mathcal{L}}{\partial \dot{q}_i}$$

$$p = m\dot{x}$$

Define Hamiltonian

$$H := -\mathcal{L} + \sum_i \dot{q}_i p_i$$

$$H = -\frac{1}{2}m\dot{x}^2 + V(x) + \dot{x}m\dot{x}$$

$$= \underbrace{\frac{1}{2}m\dot{x}^2}_{p^2/2m} + V(x)$$

The EL eqns can be used to establish:

$$\frac{d}{dt} A(q,p,t) = \underbrace{\{A,H\}}_{\text{Poisson bracket}} + \frac{\partial A}{\partial t}$$

$$\{A,B\} := \sum_i \left[\frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i} \right]$$

$$\frac{dx}{dt} = \{x,H\}$$

$$= \frac{\partial x}{\partial x}\frac{\partial H}{\partial p} - \underbrace{\cancel{\frac{\partial x}{\partial p}}}_{=0}\frac{\partial H}{\partial x}$$

$$\boxed{\frac{dx}{dt} = \frac{p}{m}}$$

(10)

$$\frac{dp}{dt} = \{p,H\}$$

$$= \underbrace{\cancel{\frac{\partial p}{\partial x}}}_{=0}\frac{\partial H}{\partial p} - \frac{\partial p}{\partial p}\frac{\partial H}{\partial x}$$

$$\frac{dp}{dt} = -\frac{\partial H}{\partial x}$$

$$\boxed{\frac{dp}{dt} = -\frac{dV(x)}{dx}}$$

Connection with QM ??

Recipe for CM → QM, replace every Poisson bracket relationship: $\{\ldots,\ldots\} = \ldots$

$$\frac{1}{i\hbar}[\ldots,\ldots] = \ldots$$

2.6 2023-09-26 Lecture

Pre-lecture:

Note that we will be using the SI system for electromagnetic units, in contrast to Sakurai and Napolitano [1] which use the Gaussian system (see their Appendix A for an explanation of the different electromagnetic unit systems). Because of this difference, many of the expressions that we derive will look slightly different from those in other sources (factors of c, $4\pi\epsilon_0$, etc ...).

1

A way to make a connection between CM and QM

Consider how expectation values change as a fcn of time. e.g. position.

$$\langle x \rangle_{\psi(t)} = \langle \psi(t) | x | \psi(t) \rangle$$

Write $|\psi(t)\rangle = \underbrace{U(t)}_{\text{unitary time evolution operator.}} |\psi(0)\rangle$

[Aside. If we satisfy conditions of Stone's theorem then

$$U(t) = e^{-iHt/\hbar}$$

Straightforward to show TDSE follows.

Conditions of Stone's theorem: U unitary ✓

$U(0) = \mathbb{I}$ ✓

$U(t_1 + t_2) = U(t_1) U(t_2)$? not always true!]

2

$$\langle x \rangle_{\psi(t)} = \langle U(t)\psi(0) | x | U(t)\psi(0) \rangle$$
$$= \langle \psi(0) | \underbrace{U^\dagger(t) x U(t)}_{x_H(t)} | \psi(0) \rangle$$

Suggests the Heisenberg picture in which the operators that represent the observables change with time.

e.g. $x_H(t) := U^\dagger(t)\, x_S\, U(t)$

but state vector stays constant in time.

e.g. $|\psi(0)\rangle$

For an arb. operator in Schrödinger picture, define corresponding Heisenberg version as:

$$A_H(t) := U^\dagger(t) A_S(t) U(t)$$

3

Let's look at $\frac{d}{dt} A_H(t)$:

$$\frac{d}{dt} A_H(t) = \frac{d}{dt}\left(\mathcal{U}^{\dagger}(t) A_S(t) \mathcal{U}(t) \right)$$

$$= \left(\frac{d}{dt}\mathcal{U}^{\dagger}(t)\right) A_S(t)\, \mathcal{U}(t) + \underbrace{\mathcal{U}^{\dagger}(t)\left(\frac{d}{dt} A_S(t)\right)\mathcal{U}(t)}_{(*) \qquad \left(\frac{dA_S(t)}{dt}\right)_H}$$

$$+ \mathcal{U}(t) A_S(t)\left(\frac{d}{dt}\mathcal{U}(t)\right)$$

What is $d\mathcal{U}/dt$?

Start from

$$|\psi(t)\rangle = \mathcal{U}(t)|\psi(0)\rangle$$

take derivative wrt time:

$$\frac{d}{dt}|\psi(t)\rangle = \frac{d}{dt}\mathcal{U}(t)\, |\psi(0)\rangle$$

4

$$\frac{d}{dt}|\psi(t)\rangle = \frac{d}{dt}\mathcal{U}(t)\,|\psi(0)\rangle$$

$$\frac{1}{i\hbar} H |\psi(t)\rangle = \frac{d}{dt}\mathcal{U}(t)|\psi(0)\rangle$$

$$\frac{1}{i\hbar} H\, \mathcal{U}(t)|\psi(0)\rangle = \frac{d}{dt}\mathcal{U}(t)|\psi(0)\rangle$$

Since $|\psi(0)\rangle$ is arb. state vector than

$$\frac{1}{i\hbar} H_S(t)\mathcal{U}(t) = \frac{d}{dt}\mathcal{U}(t)$$

$$\frac{d}{dt}\mathcal{U}(t) = \frac{1}{i\hbar} H_S(t)\mathcal{U}(t)$$

$$\frac{d}{dt}\mathcal{U}^{\dagger}(t) = -\frac{1}{i\hbar}\mathcal{U}^{\dagger}(t) H_S(t)$$

5

Now that we have $\frac{d\mathcal{U}(t)}{dt}$ and $\frac{d\mathcal{U}^+(t)}{dt}$ we can proceed with rewriting (*) on pg 3:

$$\frac{dA_H(t)}{dt} = -\frac{1}{i\hbar}\mathcal{U}^+(t)H_S(t)A_S(t)\mathcal{U}(t)$$

$\mathcal{U}(t)\mathcal{U}^+(t) = \mathbb{1}$

$$+ \quad \mathcal{U}^+(t)A_S(t)\frac{1}{i\hbar}H_S(t)\mathcal{U}(t)$$

$$+ \left(\frac{dA_S(t)}{dt}\right)_H$$

$$= -\frac{1}{i\hbar}H_H(t)A_H(t) + \frac{1}{i\hbar}A_H(t)H_H(t) + \left(\frac{dA_S(t)}{dt}\right)_H$$

$$\boxed{\frac{dA_H(t)}{dt} = \frac{1}{i\hbar}\left[A_H(t), H_H(t)\right] + \left(\frac{dA_S}{dt}\right)_H}$$

$\frac{dA}{dt} = \{A, H\} + \frac{\partial A}{\partial t}$

Poisson bracket. in CM

e.g. $\frac{dx_H}{dt} = \frac{1}{i\hbar}\left[x_H(t), H_H(t)\right]$

notice similarity with

6

A recipe for CM → QM:

replace every Poisson bracket relationship

$$\{\cdots, \cdots\} = \cdots$$

$\downarrow \quad \downarrow \quad \downarrow$ c#'s to q#'s.

by $\frac{1}{i\hbar}[\cdots, \cdots] = \cdots$

classical quantities

operators

e.g. $\{x, p\} = 1 \Rightarrow \frac{1}{i\hbar}\left[x_H(t), p_H(t)\right] = \mathbb{1}$

$$\mathcal{U}^+(t)x_S\cancel{\mathcal{U}(t)\mathcal{U}^+(t)}p_S\mathcal{U}(t) - \mathcal{U}^+(t)p_S\cancel{\mathcal{U}(t)\mathcal{U}^+(t)}x_S\mathcal{U}(t) = i\hbar$$

$$x_Sp_S - p_Sx_S = i\hbar$$

$$[x_S, p_S] = i\hbar.$$

(7)

We are going to use this recipe to figure out how to "add" magnetic fields to Hamiltonians.

In CM we are use to Lorentz force law:

$$\frac{m}{e}\ddot{\vec{x}} = \vec{E} + \dot{\vec{x}} \times \vec{B} \qquad (*)$$

Procedure is to get Lagrangian for which EL eqns give the Lorentz force law.
Then get Hamiltonian.

(8)

Recall Maxwell's eqns: (SI)

$$\nabla\cdot\vec{E} = \rho/\epsilon_0 \,, \quad \nabla\times\vec{E} = -\frac{\partial\vec{B}}{\partial t}$$

$$\nabla\cdot\vec{B} = 0 \,, \quad \nabla\times\vec{B} = \mu_0\vec{J} + \mu_0\epsilon_0\frac{\partial\vec{E}}{\partial t}$$

Introduce the vector potential $\vec{A}$, such that $\boxed{\vec{B} = \nabla\times\vec{A}}$
(automatically satisfies $\nabla\cdot\vec{B} = 0$)

$$\nabla\times\vec{E} = -\frac{\partial}{\partial t}(\nabla\times\vec{A}) \Rightarrow \nabla\times\underbrace{\left(\vec{E} + \frac{\partial\vec{A}}{\partial t}\right)}_{\text{represent by } -\nabla\varphi} = 0$$

scalar field.

$$\vec{E} + \frac{\partial\vec{A}}{\partial t} = -\nabla\varphi \Rightarrow \boxed{\vec{E} = -\nabla\varphi - \frac{\partial\vec{A}}{\partial t}}$$

2.7 2023-09-28 Lecture

Pre-lecture:

(1)

There is a degree of arbitrariness in repres. $\vec{E}$ and $\vec{B}$ using $\vec{A}$ and φ:

$$\vec{B} = \nabla \times \underbrace{\vec{A}}_{?}$$

arb. fcn. known as "gauge" fcn.

$$\vec{A}' = \vec{A} + \nabla\Lambda$$

$$\underbrace{\varphi'}\, = \varphi - \frac{\partial \Lambda}{\partial t}$$

these give the same $\vec{E}$ and $\vec{B}$ as $\vec{A}$ and φ.

$A, \varphi \longleftrightarrow A', \varphi'$ is known as a "gauge transformation"

Aside!

$\underbrace{\nabla \cdot \vec{A} = 0}$ "Coulomb gauge"

$\underbrace{\nabla \cdot \vec{A} = -\frac{\partial \varphi}{\partial t}}$ "Lorenz gauge"

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \qquad \vec{B} = \nabla \times \vec{A}$$

$$\vec{E} = -\nabla\varphi - \frac{\partial \vec{A}}{\partial t} \qquad (*)$$

$$= -\nabla\varphi - \left(\frac{\partial}{\partial t}(\vec{A}' - \nabla\Lambda)\right)$$

$$= -\nabla\underbrace{\left(\varphi - \frac{\partial \Lambda}{\partial t}\right)}_{\varphi' = \varphi - \frac{\partial \Lambda}{\partial t}} - \frac{\partial \vec{A}'}{\partial t}$$

(2)

Equations of motion with magnetic fields

$$\mathcal{L} = \frac{1}{2} m \vec{v} \cdot \vec{v} + e \underbrace{\vec{v}}_{\dot{\vec{x}}} \cdot \vec{A} - e\varphi$$

("best" justification is as non-relativistic approximation to the relativistic Lagrangian, which you can motivate by through Lorentz invariance of the action ($\int dt\, \mathcal{L}$).)

EL equations:

$$\frac{d}{dt}\left(m\vec{v} + e\vec{A}\right) = -e\vec{\nabla}\varphi + e\vec{\nabla}(\vec{v} \cdot \vec{A})$$

Be careful! We want $\frac{d\vec{A}}{dt}$ and $\underline{\text{not}}$ $\frac{\partial \vec{A}}{\partial t}$.

"total derivative" accounts for motion in field.

(3)

$$\frac{d\vec{A}}{dt} = \frac{\partial \vec{A}}{\partial t} + (\vec{v}\cdot\vec{\nabla})\vec{A}$$

$$m\frac{d\vec{v}}{dt} + \underbrace{e\frac{\partial\vec{A}}{\partial t}} + e(\vec{v}\cdot\vec{\nabla})\vec{A} = \underbrace{-e\vec{\nabla}\varphi} + e\vec{\nabla}(\vec{v}\cdot\vec{A})$$

recognize expression for $\vec{E}$ in terms of φ and $\vec{A}$.

$$m\frac{d\vec{v}}{dt} = e\vec{E} + \left(e\vec{\nabla}(\vec{v}\cdot\vec{A}) - e(\vec{v}\cdot\nabla)\vec{A}\right) \quad (*)$$

Purely mathematical result:

For any vector field $\vec{y}$ and constant vector $\vec{c}$

$$\rightarrow \vec{c}\times(\nabla\times\vec{y}) = \nabla(\vec{c}\cdot\vec{y}) - (\vec{c}\cdot\nabla)\vec{y}$$

Recognize this form in $(*)$

$$\vec{v}\times\underbrace{(\nabla\times\vec{A})}_{\vec{B}} = \nabla(\vec{v}\cdot\vec{A}) - (\vec{v}\cdot\nabla)\vec{A}$$

(4)

$$\boxed{\frac{m}{e}\frac{d\vec{v}}{dt} = \vec{E} + \vec{v}\times\vec{B}}$$ as req'd.

Thus $\mathcal{L} = \frac{1}{2}m\vec{v}\cdot\vec{v} + e\vec{v}\cdot\vec{A} - e\varphi$ is correct.

What Hamiltonian does this Lagrangian give?

$$p_i := \frac{\partial\mathcal{L}}{\partial\dot{q}_i}$$

In this case $\vec{p} = m\vec{v} + e\vec{A}$

$$H := -\mathcal{L} + \sum \dot{q}_i p_i$$

In this case $H = -\frac{1}{2}m\vec{v}\cdot\vec{v} + e\varphi - e\vec{v}\cdot\vec{A} + \vec{v}\cdot\vec{p}$

(5)

$$H = e\varphi + \vec{v}\cdot\left(\vec{p} - e\vec{A} - \tfrac{1}{2}m\vec{v}\right)$$

express in term of p. i.e. $\vec{v} = \dfrac{\vec{p}-e\vec{A}}{m}$

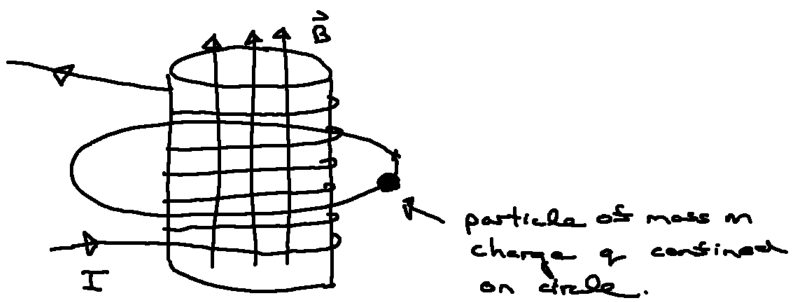
$$H = e\varphi + \left(\frac{\vec{p}-e\vec{A}}{m}\right)\cdot\left(\vec{p} - e\vec{A} - \tfrac{1}{2}(\vec{p}-e\vec{A})\right)$$

$$\boxed{H = e\varphi + \frac{(\vec{p}-e\vec{A})^2}{2m}}$$

For QM we will have $[x_j, p_k] = i\hbar\,\delta_{jk}$

To keep p as generator of translations, we keep $\vec{p} = -i\hbar\nabla$ in position space.

(6)



The spectrum (energy levels) change with I even though $\vec{B} = \vec{0}$ outside solenoid.!!!

Aharanov - Bohm effect.

2.8 2023-10-03 Lecture

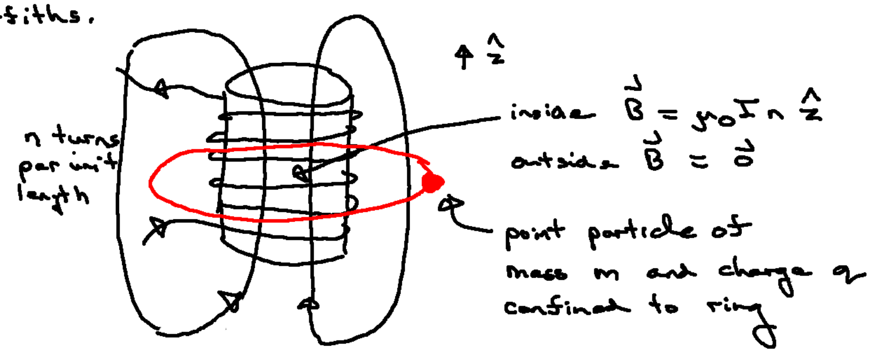
Pre-lecture:

Lecture is based on section in Ref. [6].

① Example of $H = \dfrac{(\vec{p} - e\vec{A})^2}{2m}$

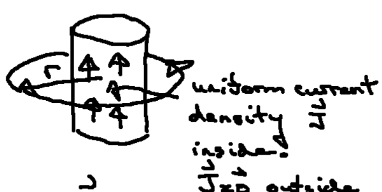
(also illustration of Aharonov – Bohm effect)

Griffiths.

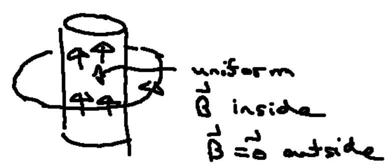


We will find that although $\vec{B} = \vec{0}$ on ring the presence of magnetic flux through ring changes energy levels of particle.

② First determine $\vec{A}$. Use an analogy.



$\vec{B}$?



A ?

$\nabla \cdot \vec{B} = 0$, $\nabla \times \vec{B} = \mu_0 \vec{J}$

$\nabla \cdot \vec{A} = 0$, $\vec{B} = \nabla \times \vec{A}$

Use Stoke's theorem (for arb. $\vec{v}$)

$$\oint \vec{v} \cdot d\vec{\ell} = \int_S \nabla \times \vec{v} \cdot d\vec{a}$$

$$\oint \vec{B} \cdot d\vec{\ell} = \underbrace{\int_S \mu_0 \vec{J} \cdot d\vec{a}}_{\mu_0 I_{enclosed}}$$

Biot-Savart tells us $\vec{B}$ only points in $\hat{\phi}$ direction. $B_\phi 2\pi r = \mu_0 I_{enclosed}$

$\vec{A}$

(3)

$$\vec{B} = \hat{\phi}\, \frac{\mu_0 I_{enclosed}}{2\pi r} \qquad \Bigg| \qquad \vec{A} = \hat{\phi}\, \frac{\overbrace{\Phi_{enclosed}}^{B_z \pi r^2 \leftarrow \mu_0 I n}}{2\pi r} \leftarrow$$

in Coulomb gauge ($\nabla\cdot\vec{A} = 0$)

$$H = \frac{1}{2m}(\vec{p} - e\vec{A})^2$$

these are not the same in QM.

$$= \frac{1}{2m}\left(p^2 + e^2A^2 - \overbrace{e\vec{p}\cdot\vec{A} - e\vec{A}\cdot\vec{p}} \right)$$

Work in position space: $\vec{p}\cdot\vec{A}\psi = -i\hbar\, \nabla\cdot(\vec{A}\psi)$

General identity: $\nabla\cdot(\vec{v} f) = (\nabla\cdot\vec{v}) f + \vec{v}\cdot\nabla f$

any vector field ($\vec{v}$), any scalar field (f)

(4)

$$\vec{p}\cdot\vec{A}\psi = -i\hbar\left[\underbrace{(\nabla\cdot\vec{A})}_{=0 \text{ in Coulomb gauge}}\psi + \vec{A}\nabla\psi\right]$$

$$= -i\hbar\, \vec{A}\cdot\nabla\psi$$

$$= \vec{A}\cdot\vec{p}\,\psi$$

$$H = \frac{1}{2m}p^2 + \frac{e^2}{2m}A^2 - \frac{e}{m}\vec{A}\cdot\vec{p}$$ in Coulomb gauge!!!

What form do $\vec{p}$ and p^2 take on the ring?

$$\nabla\psi = \frac{1}{r}\frac{\partial\psi}{\partial\phi}\hat{\phi}$$

$$\nabla^2\psi = \frac{1}{r^2}\frac{\partial^2\psi}{\partial\phi^2}$$

time indep. SE

Solve eigenvalue problem: $H\psi(\phi) = E\psi(\phi)$. with periodic BC's.

⑤

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d^2\psi(\phi)}{d\phi^2}+\frac{e^2}{2m}\left(\frac{\Phi}{2\pi r}\right)^2\psi(\phi)$$

$$+\frac{e}{m}\left(\frac{\Phi}{2\pi r}\right)i\hbar\frac{1}{r}\frac{d\psi(\phi)}{d\phi}=E\psi(\phi)$$

Divide $\hbar^2/(2mr^2)$

$$-\frac{d^2\psi(\phi)}{d\phi^2}+\frac{2m\cancel{r^2}}{\hbar^2}\frac{e^2}{\cancel{2m}}\frac{\Phi^2}{(2\pi)^2\cancel{r^2}}\psi(\phi)$$

$$+\frac{2\cancel{m}\cancel{r^2}}{\hbar^2}\frac{e}{\cancel{m}}\frac{\Phi}{2\pi\cancel{r}}i\hbar\frac{1}{\cancel{r}}\frac{d\psi(\phi)}{d\phi}=\frac{E}{(\hbar^2/2mr^2)}\psi(\phi)$$

Define $\beta := \frac{e\Phi}{2\pi\hbar}$

$$-\frac{d^2\psi(\phi)}{d\phi^2}+\beta^2\psi(\phi)+2i\beta\frac{d\psi(\phi)}{d\phi}=\frac{E}{(\hbar^2/2mr^2)}\psi(\phi)$$

⑥

$$\epsilon := \frac{E}{\hbar^2/(2mr^2)}-\beta^2$$

$$\frac{d^2\psi(\phi)}{d\phi^2}+\epsilon\psi(\phi)-2i\beta\frac{d\psi(\phi)}{d\phi}=0$$

Try trial solution $\psi(\phi)=C e^{i\lambda\phi}$

$$-\lambda^2 C\cancel{e^{i\lambda\phi}}-2i\beta(i\lambda)\cancel{e^{i\lambda\phi}}+\epsilon C\cancel{e^{i\lambda\phi}}=0$$

$$\lambda^2-2\beta\lambda-\epsilon=0$$

$$\lambda=\beta\pm\sqrt{\beta^2+\epsilon}\qquad(*)$$

Apply periodic BC's: $\psi(0)=\psi(2\pi)\to C=Ce^{i\lambda 2\pi}$

$\Rightarrow\ \lambda=0,\pm1,\pm2,\pm3,\ldots$

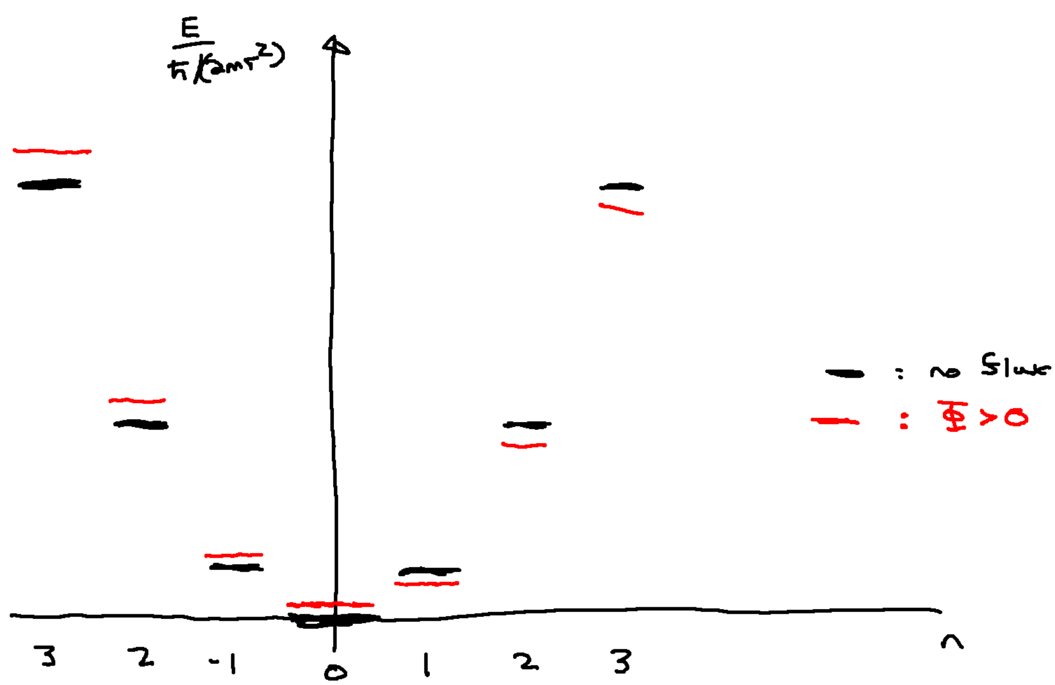
Sub into $(*)$ and solve for ϵ.

⑦

$$\epsilon = (\underset{:=n}{n} - \beta)^2 - \beta^2$$

$$\frac{E}{\hbar^2/2mr^2} = \left(n - \frac{e\Phi}{2\pi\hbar}\right)^2$$

⑧



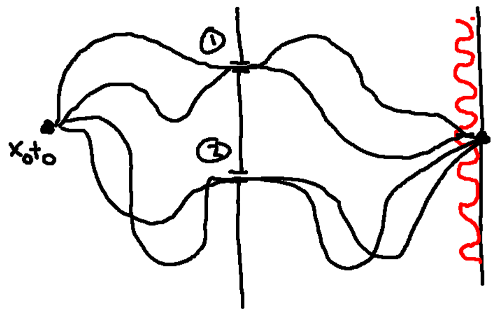
2.9 2023-10-05 Lecture

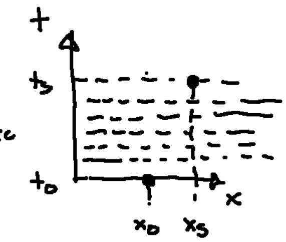
Pre-lecture:

(1)

Experimental observation of the Aharonov-Bohm effect

- "double slit interference" (with no magnetic field)





"action" $S := \int \mathcal{L}\, dt$

$$\langle x_s t_s | x_0 t_0 \rangle = \int \mathcal{D}[x(t)]\, e^{\frac{i\, S[x(t)]}{\hbar}}$$

} path integral

(2)

$$\langle x_s t_s | x_0 t_0 \rangle = \overbrace{\left\{ \int \mathcal{D}[x_1(t)]\, e^{\frac{i\, S[x_1(t)]}{\hbar}} \right\}}^{A_1} \quad \text{paths that pass through slit 1}$$

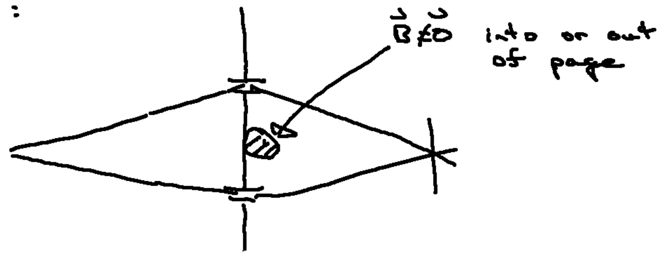
$$\overbrace{\left\{ + \int \mathcal{D}[x_2(t)]\, e^{\frac{i\, S[x_2(t)]}{\hbar}} \right\}}^{A_2} \quad \text{" slit 2}$$

Destructive interference: $\frac{A_1}{A_2} = e^{i n \pi}$ $\quad n = 1, 3, 5, \ldots$

Constructive interference $\frac{A_1}{A_2} = e^{i n 2\pi}$ $\quad n = 0, 1, 2, 3, \ldots$

(3)

Put magnetic flux in region between the 2 slits:



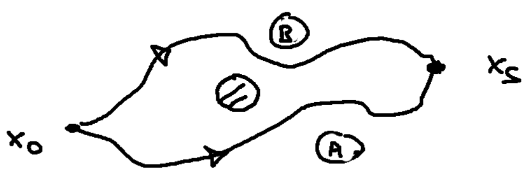
$$\mathcal{L} = \frac{1}{2} m v^2 - \cancel{e\phi} + e\,\vec{v}\cdot\vec{A},$$

All paths have additional phases $\left(\frac{\text{action}}{\hbar}\right)$

$$\Delta\phi = \frac{1}{\hbar}\int_{t_0}^{t_s} e\,\vec{v}\cdot\vec{A}\,dt \qquad \vec{v} = \frac{d\vec{x}}{dt}$$

$$= \frac{1}{\hbar}\int_{x_0}^{x_s} e\,\vec{A}\cdot d\vec{x}$$

(4)



$$\Delta\phi_{A,B} = \frac{e}{\hbar}\left[\int_{x_0 \,(A)}^{x_s} \vec{A}\cdot d\vec{x} - \int_{x_0 \,(B)}^{x_s} \vec{A}\cdot d\vec{x}\right]$$

$$= \frac{e}{\hbar}\oint \vec{A}\cdot d\vec{x}$$

Remember Stoke's theorem:

For any vector field $\vec{w}$: $\quad \oint \vec{w}\cdot d\vec{l} = \int_S (\nabla\times\vec{w})\cdot d\vec{a}$

$$\Delta\phi_{A,B} = \frac{e}{\hbar}\int_S \vec{B}\cdot d\vec{a} = \frac{e\Phi}{\hbar}$$

$\vec{B} = \nabla\times\vec{A}$; Φ = enclosed magnetic flux

⑤

Choosing $\frac{e\Phi}{\hbar} = \pi \mod 2\pi$

allows constructive $\leftrightarrow$ destructive.

Aharonov-Bohm free particle interference experiment

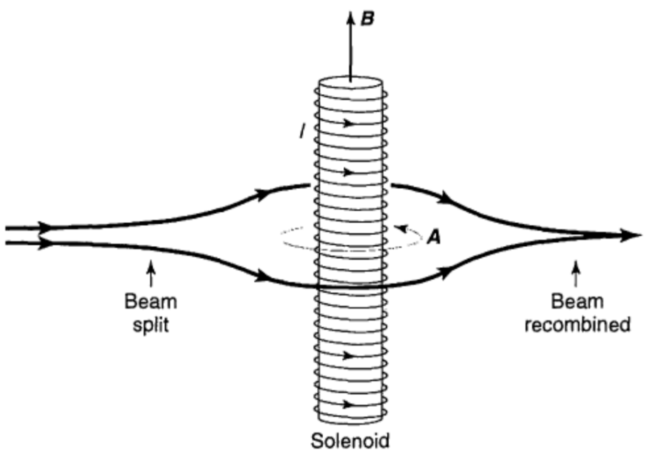


Fig. 4.17 from Griffiths and Schroeter, *Introduction to Quantum Mechanics, 3rd ed.*

Experimental observation by Chambers

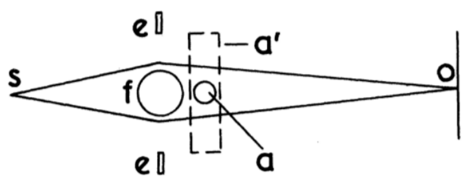
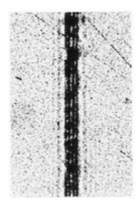
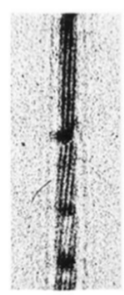


FIG. 1. Schematic diagram of interferometer, with source s, observing plane o, biprism e, f, and confined and extended field regions a and a'.



with no enclosed flux



enclosed flux varying ↕

from Chambers, Phys. Rev. Lett., 5, 3 (1960)

With magnetic field confined using superconductor

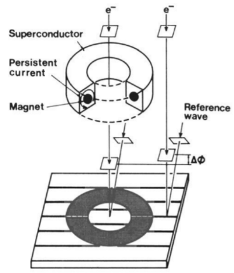
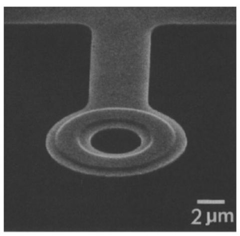


FIG. 1. Conceptual diagram of the experiment. A Cu layer for shielding from an electron wave is not shown.



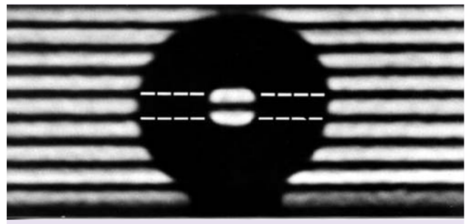


Figure 3. Electron interference pattern demonstrating the magnetic Aharonov–Bohm effect in an experiment that strictly excludes all stray fields.[4] A coherent electron beam traveling normal to the page is made to pass around a toroidal magnet (seen as a shadow) or through its 4-μm-diameter hole. The magnet's superconducting cladding prevents all stray fields. Having threaded or passed around the magnet, the beam is made to interfere with a reference plane wave. The resulting pattern, with the interference fringe inside the hole offset by half a cycle from those outside whenever the magnet flux is an odd multiple of $h/2e$, indicates an AB phase shift of π (modulo 2π) between the threading and bypassing electrons.

from Osakabe *et al.* , *Phys. Rev. A, 34, 815 (1986), and Batelaan and Tonomura, Physics Today, Sept. 2009*

Aharonov-Bohm: a semi-classical argument

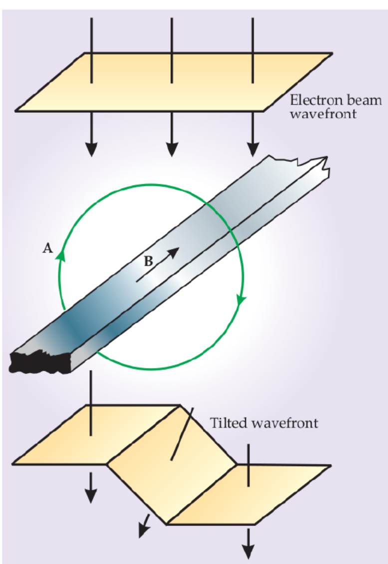


Figure 2. Semiclassical argument for the magnetic Aharonov–Bohm effect. Consider the plane wavefront of a coherent electron beam passing through and around a uniformly magnetized bar. Electrons going through the bar are deflected by the Lorentz force, tilting their sector of the wavefront. Electrons passing outside the bar see no magnetic field, so their sectors remain untilted. But because continuity requires the three sectors of the constant-phase front to remain contiguous, the two untilted sectors are now displaced along the beam direction, which implies a corresponding phase shift across a cross section of the beam. The phase shift thus calculated in terms of the Lorentz force is the same as that predicted by the AB effect in terms of the vector potential **A** circling the bar.

from Batelaan and Tonomura,
Physics Today, Sept. 2009

2.10 2023-10-17 Lecture

Pre-lecture:

There is one topic I was not sorry to skip: the relativistic wave equation of Dirac. It seems to me that the way this is usually presented in books on quantum mechanics is profoundly misleading. Dirac thought that his equation is a relativistic generalization of the non-relativistic time-dependent Schrödinger equation that govems the probability amplitude for a point particle in an external electromagnetic field. For some time after, it was considered to be a good thing that Dirac's approach works only for particles of spin one half, in agreement with the known spin of the electron, and that it entails negative-energy states, states that when empty can be identified with the electron's antiparticle. Today we know that there are particles like the $\mathrm{W}^{\pm}$ *that are every bit as elementary as the electron, and that have distinct antiparticles, and yet have spin one, not spin one half. The right way to combine relativity and quantum mechanics is through the quantum theory of fields, in which the Dirac wave function appears as the matrix element of a quantum field between a one-particle state and the vacuum, and not as a probability amplitude.*

From introduction to S. Weinberg, *Lectures on quantum mechanics*, Second edition (Cambridge University Press, Cambridge, United Kingdom ; New York, NY, 2015).

Well here we go, hehehe :)

(1)

Relativistic one-particle quantum mechanics

What is wrong with the time-dep Schrödinger eqn (TDSE)?
(from special relativity (SR) point of view).

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right)\psi(\vec{r},t) = i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}$$

order disagrees, so TDSE will not be covariant.
i.e. have the same form in different inertial ref. frames,

Remember from SR:

$$E = \sqrt{(pc)^2 + (mc^2)^2}$$

(2)

What about

$$\sqrt{(cp)^2 + (mc^2)^2}\ \psi(\vec{r},t) = i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t}\ ?$$

$\vec{p} = -i\hbar\nabla$

Problem: how do we take $\sqrt{\ }$ of operator?
Can we use power series to define?

$$H = m\sqrt{(p/m)^2+1} \qquad (c=1)$$

$$= m\left(1 + \underbrace{\frac{1}{2}\left(\frac{p}{m}\right)^2} - \frac{1}{8}\left(\frac{p}{m}\right)^4 + \dots\right)$$

We have same problem!!! Orders of spatial and time derivatives don't match. Not covariant!!!

(3)

Instead "square" both sides. $(\hbar=1)$

$$(\underbrace{p^2}_{-\nabla^2 \,=\, -\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)} + m^2)\,\psi(\vec{r},t) = -\frac{\partial^2}{\partial t^2}\psi(\vec{r},t)$$

Slightly rearrange to give:

$$\boxed{\left(\frac{\partial^2}{\partial t^2} - \nabla^2 + m^2\right)\psi(r,t) = 0}$$

Klein-Gordon equation KGE

Is this equation consistent with SR?

④

Use Lorentz 4-vector tensor notation -.

contravariant components : $\tilde{a}^{\mu} = \dfrac{d\tilde{x}^{\mu}}{dx^{\nu}} a^{\nu}$ — Einstein summation convention

covariant components : $\tilde{a}_{\mu} = \underbrace{\dfrac{dx^{\nu}}{d\tilde{x}^{\mu}}}_{\text{Lorentz transformation between the two inertial reference frames}} a_{\nu}$ — old inertial ref. frame.

new "~" inertial ref. frame

Suppose I have two 4-vectors, a and b :

$$a^{\mu} b_{\mu} = a^0 b_0 + a^1 b_1 + a^2 b_2 + a^3 b_3$$
$$= a^0 b^0 - a^1 b^1 - a^2 b^2 - a^3 b^3 \quad \Big\} \text{ using rule on next page.}$$

To get some insight we have remember to convert between covariant and contravariant components.

⑤

$$a_{\mu} = \eta_{\mu\nu} a^{\nu}$$

$$\eta_{\mu\nu} = \begin{bmatrix} 1 & & & 0 \\ & -1 & & \\ & & -1 & \\ 0 & & & -1 \end{bmatrix}$$

time part

space part

$a^{\mu} b_{\mu}$ is invariant (stays the same) under transformations between different inertial reference frames.

e.g. $x^{\mu} x_{\mu} = (ct)^2 - x^2 - y^2 - z^2$

$$\partial_{\mu} \partial^{\mu} = \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2}$$

invariant under Lorentz transformations!

$\left(\frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$ $\left(\frac{\partial}{\partial t}, -\frac{\partial}{\partial x}, -\frac{\partial}{\partial y}, -\frac{\partial}{\partial z}\right)$

⑥

KGE rewritten is just

$$(\underbrace{\partial_\mu \partial^\mu}_{\frac{\partial^2}{\partial t^2}-\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}-\frac{\partial^2}{\partial z^2}} + m^2)\,\underbrace{\psi(\vec{r},t)} = 0$$

In another inertial ref. frame.

$$(\underbrace{\tilde{\partial}_\mu \tilde{\partial}^\mu}_{} + m^2)\,\underbrace{\psi(\tilde{\vec{r}},\tilde{t})}_{\text{same wavefunction.}} = 0$$

Since this is Lorentz invariant, KGE is covariant.

All of this is for free particles. How do we incorporate "potentials"?

⑦

Remember that $A^\mu = (\varphi, \vec{A})$ is a 4-vector.

Scalar pot. vector potential

$$p_\mu := (i\partial_t, i\nabla), \quad p^\mu = (i\partial_t, -i\nabla)$$

KGE: $$(-p^\mu p_\mu + m^2)\psi(\vec{r},t) = 0$$

Using non-relativistic $H = \frac{(\vec{p}-e\vec{A})^2}{2m}$ as motivation, to replace p^μ by $p^\mu - eA^\mu$

KGE with EM field

$$\boxed{\left[-(p^\mu - eA^\mu)(p_\mu - eA_\mu) + m^2\right]\psi(\vec{r},t) = 0}$$

Next lecture: see what energy levels this gives for H-atom.

2.11 2023-10-19 Lecture

Pre-lecture:

The treatment of the KGE for the Coulomb potential in this section is based on Section 8.1.2 of Ref. [8].

The treatement of SDE for the Coulomb potential in this section is based on Section 6.3 of Ref. [9].

(1)

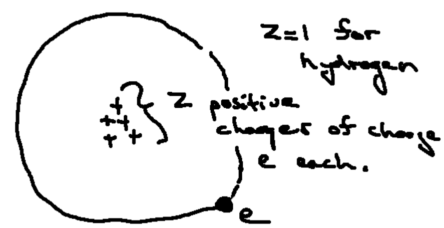
Stationary solutions of KGE

$$\psi(\vec{r},t) = \psi(\vec{r})\, e^{-iEt} \qquad (\hbar = 1)$$

KGE becomes:

$$(E - e\varphi)^2 \psi(\vec{r}) - (-i\nabla - e\vec{A})^2 \psi(\vec{r}) - m^2 \psi(\vec{r}) = 0$$

Consider a purely electrostatic field described by $\vec{A} = \vec{0}$, and $\varphi = -\frac{Ze}{4\pi\epsilon_0 r}$



(2)

$$(E - e\varphi)^2 \psi(\vec{r}) = (-\nabla^2 + m^2)\psi(\vec{r})$$

Because of spherical symmetry, hypothesize eigenfcns of form:

$$\psi(\vec{r}) = R(r)\, \underbrace{Y_{\ell,m}(\theta,\phi)}_{\text{spherical harmonics}}$$

For the radial part we get:

$$\left[-\frac{d^2}{dr^2} + \frac{1}{r^2}\left(-\frac{Z^2e^4}{(4\pi\epsilon_0)^2} + \ell(\ell+1)\right) - \frac{2ZEe^2}{4\pi\epsilon_0 r} + (m^2 - E^2)\right] \underbrace{rR(r)}_{=:\, u(r)} = 0$$

Surprise!!! Has the "same mathematical form" as the radial equation for hydrogen that arises from the Schrödinger eqn.

③

Radial equation that arises from the SDE has form:

$$\left[\frac{\hbar^2}{2m}\left(-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}\right)-\frac{Z\alpha\hbar c}{r}-E\right]\underbrace{rR(r)}_{=:u(r)}=0$$

α : "fine structure constant"

$\frac{e^2}{4\pi\epsilon_0} \to$ energy · length $\Big\}$ $\hbar c \to$ energy · length

$$\alpha := \frac{e^2}{4\pi\epsilon_0}\frac{1}{\hbar c} \text{ SI } \left(\frac{e^2}{\hbar c} \text{ Gaussian}, \ \frac{e^2}{4\pi\hbar c} \text{ HL}\right)$$

$$\simeq \frac{1}{137}$$

④

Aside, energy levels of hydrogen atom

in atomic units $\quad E = -\frac{1}{2n^2}$

in "real units": $\quad E = -\frac{1}{2n^2}\underbrace{\underbrace{mc^2}_{0.5\,\text{MeV}}\alpha^2}_{\left(\frac{1}{137}\right)^2 \ \to\ 27\,\text{eV}}$

$$E \approx -\frac{1}{2n^2}\,13.5\,\text{eV}$$

5

To simplify, introduce a dimensionless length:

$$\rho := \frac{r}{\frac{1}{\frac{1}{\hbar}\sqrt{2m(-E)}}}$$

$$\left[-\frac{d^2}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2} - \frac{1}{\rho}\underbrace{\frac{\sqrt{2m(-E)}}{\hbar|E|}\, Z\alpha\hbar c}_{=:\rho_0} - \frac{E}{|E|}\right]u(\rho) = 0$$

$$\boxed{\left[\frac{d^2}{d\rho^2} - \frac{\ell(\ell+1)}{\rho^2} + \frac{\rho_0}{\rho} - 1\right]u(\rho) = 0}$$

Examine solutions next lecture.

2.12 2023-10-24 Lecture

Pre-lecture:

The treatment of the KGE for the Coulomb potential in this section is based on Section 8.1.2 of Ref. [8].

The treatement of SDE for the Coulomb potential in this section is based on Section 6.3 of Ref. [9].

①

Cont'd from last lecture.

Analyze for small and large ρ.

<u>Small ρ</u>: $\left[\frac{d^2}{d\rho^2} - \frac{\ell(\ell+1)}{\rho^2}\right]u(\rho) = 0$

hypothesize $u(\rho) = \rho^k$, plug in gives $\underbrace{k=-\ell}_{\text{blows up at small } \rho}$ or $\ell+1$.

$u(\rho) \propto \rho^{\ell+1}$ for small ρ.

<u>Large ρ</u> $\left[\frac{d^2}{d\rho^2} - 1\right]u(\rho) = 0$

$u(\rho) \propto e^{\pm\rho}$ are solutions. $u(\rho) \propto e^{-\rho}$

②

Hypothesize solution of form:

$$u(\rho) \stackrel{?}{=} \rho^{\ell+1} e^{-\rho} \underbrace{w(\rho)}_{\text{power series (yet to be determined)}} \qquad (*)$$

$$w(\rho) = \sum_{k=0}^{\infty} a_k \rho^k$$

Substitute $(*)$ into $\left[\frac{d^2}{d\rho^2} - \frac{\ell(\ell+1)}{\rho^2} + \frac{\rho_0}{\rho} - 1\right]u(\rho) = 0$

hefty amount of tedious algebra

$$\frac{a_{k+1}}{a_k} = \frac{2(\ell+k+1) - \rho_0}{(k+1)(2(\ell+1)+k)}$$

At large k: $\frac{a_{k+1}}{a_k} \simeq \frac{2}{k}$

③

For comparison

$$f(\rho) = e^{2\rho}$$
$$= \sum_{k=0}^{\infty} \frac{1}{k!}(2\rho)^k$$
$$= \sum_{k=0}^{\infty} a_k \rho^k \quad a_k = \frac{2^k}{k!}$$

$$\frac{a_{k+1}}{a_k} = \left(\frac{2^{k+1}}{(k+1)k!}\right) / (2^k / k!)$$

$$\simeq \frac{2}{k} \text{ at large } k.$$

This shows us that our solutions won't be normalizable unless $a_k = 0$ for some k.

④

Thus $2(l+k+1) - \rho_0 = 0$
so that series terminates.

Define N such that $2(l+\underset{0,1,2,3,\ldots}{N}+1) - \rho_0 = 0$

Remember $\rho_0 = \frac{\sqrt{2m(-E)}}{\hbar |E|} Z \alpha \hbar c$

$$\rho_0^2 = \frac{2m}{|E|} Z^2 \alpha^2 c^2$$

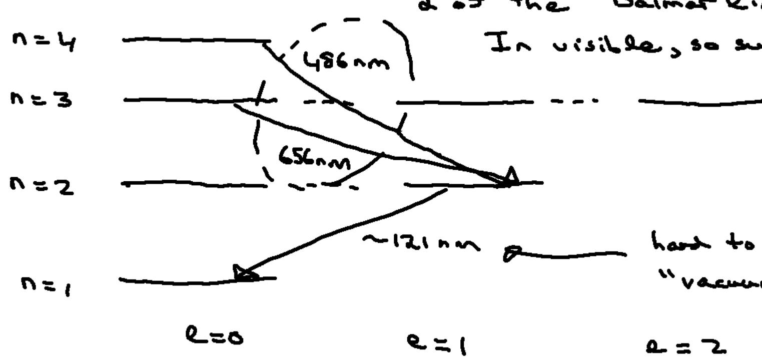
$$E = -2mc^2 Z^2 \alpha^2 / [2(l+N+1)]^2$$

Define principal quantum number $n := l+N+1$

(5)

$$\boxed{E = -\frac{1}{2} m c^2 Z^2 \alpha^2 \frac{1}{n^2}}$$

2 of the "Balmer lines". In visible, so suitable for testing theory.



hard to work with. In "vacuum ultraviolet".

(6)

Solving the KGE "for the hydrogen atom"

$$\underbrace{\left[-\frac{d^2}{dr^2} + \frac{1}{r^2}\left(-Z^2\alpha^2 + l(l+1)\right) - \frac{2EZ\alpha}{r} + (m^2 - E^2)\right]}_{\text{radial KGE}} u(r) = 0$$

$$* \quad \underbrace{\left[\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + \frac{\rho_0}{\rho} - 1 \right] u(\rho) = 0}_{\text{radial SDE}}$$

Define: $\sigma^2 := 4(m^2 - E^2)$, $\rho := \sigma r$, $\gamma := Z\alpha$, $\lambda := 2\gamma E/\sigma$

to rewrite KGE as:

$$* \quad \left[\frac{d^2}{d(\rho/2)^2} - \frac{1}{(\rho/2)^2}\left(l(l+1) - \gamma^2\right) + \frac{2\lambda}{(\rho/2)} - 1 \right] u(\rho/\sigma) = 0$$

⑦

SOE	KGE
ρ	$\rho/2$
$\ell(\ell+1)$	$\ell(\ell+1)-\gamma^2 =: \ell'(\ell'+1)$
ρ_0	2χ

$$\ell' = -\frac{1}{2} \pm \sqrt{\left(\ell+\frac{1}{2}\right)^2-\gamma^2}$$

$$2(\ell' + \underbrace{N}_{0,1,2,3,\dots} + 1) - 2\chi = 0 \quad \longrightarrow \quad 2(\ell'+N+1) - \frac{2\,2\gamma E}{4(m^2-E^2)} = 0$$

$$E = \frac{m}{\sqrt{1+\left(\frac{\gamma}{\ell'+N+1}\right)^2}}$$

rearrange to solve for E

⑧

$$\boxed{E = m\left\{1+\left[\frac{Z\alpha}{\underbrace{n-\ell-1}_{N}+\frac{1}{2}+\sqrt{\left(\ell+\frac{1}{2}\right)^2-(Z\alpha)^2}}\right]^2\right\}^{-1/2}}$$

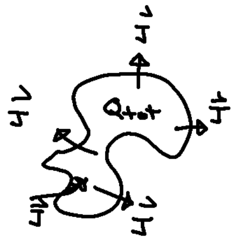
energy levels of "hydrogen" according to KGE

Expand in powers of $(Z\alpha)$

$$E = mc^2 - \frac{1}{2n^2}(Z\alpha)^2mc^2\left[1+\frac{(Z\alpha)^2}{n}\left(\frac{1}{(\ell+\frac{1}{2})}-\frac{3}{4n}\right) + O((Z\alpha)^4)\right]$$

2.13 2023-10-26 Lecture

① **Continuity Equation**



Remember from Electricity and Magnetism (E&M) the charge continuity equation:

$$\oint \vec{J}\cdot d\vec{a} = -\frac{dQ_{tot}}{dt}$$

$$= -\int dV \frac{\partial \rho}{\partial t} \qquad (*)$$

charge density

divergence theorem

For any vector field $\vec{w}$: $\left\{ \oint \vec{w}\cdot d\vec{a} = \int dV\, \nabla\cdot\vec{w} \right\}$

For (*) to be consistent with the divergence theorem:

$$\nabla\cdot\vec{J} = -\frac{\partial \rho}{\partial t} \quad \Big\}\ \text{"charge continuity equation"}$$

② Back to QM, starting with the normal non-relativistic SDE.

$$\frac{\partial}{\partial t}\underbrace{|\psi|^2}_{\psi\psi^*} = \psi^* \underbrace{\frac{\partial \psi}{\partial t}} + \psi \underbrace{\frac{\partial}{\partial t}\psi^*}$$

Use:

$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi \quad \Big\}\ \text{NRSDE}$$

to get:

$$\underbrace{\frac{\partial}{\partial t}|\psi|^2} = \psi^*\left[\frac{1}{i\hbar}\left(-\frac{\hbar^2\nabla^2}{2m} + V\right)\psi\right] + \psi\left[\frac{-1}{i\hbar}\left(-\frac{\hbar^2\nabla^2}{2m} + V\right)\psi^*\right]$$

$$= -\frac{\hbar}{2im}\left[\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right] \qquad (Y)$$

Suppose $\vec{v} := \psi^*\nabla\psi - \psi\nabla\psi^*$

③

Take $\nabla\cdot$ of $\vec{v}$:

use
$$\underbrace{\nabla\cdot(f\vec{g})} = \nabla f\cdot\vec{g} + f\,\nabla\cdot\vec{g}$$
vector calc identity.

$$\nabla\cdot\vec{v} = \cancel{\nabla\psi^*\cdot\nabla\psi} + \psi^*\nabla^2\psi - \cancel{\nabla\psi\cdot\nabla\psi^*} - \psi\nabla^2\psi^* \qquad (X)$$

Based on (X) and (Y) we can write:

$$\frac{\partial}{\partial t}|\psi|^2 = -\nabla\cdot\underbrace{\left(-\frac{i\hbar}{2m}\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right]\right)}_{=:\,\vec{J}}$$

④

<u>Continuity equation for KGE</u>

Since KGE is consistent with SR, we want a continuity eqn consistent with SR.

Remember from E&M, that $\nabla\cdot\vec{J} = -\frac{\partial\rho}{\partial t}$ can be written as

$$\partial_\mu J^\mu = 0$$

where $J^\mu = (\underbrace{\rho c}_{4}, \vec{J})$

Let's try to use a generalized form of current density that we found for SDE:

(5)

$$j^\mu = A\left[\psi^* \partial^\mu \psi - \psi \partial^\mu \psi^*\right]$$

$$\partial_\mu J^\mu = A\left[\cancel{(\partial_\mu \psi^*)(\partial^\mu \psi)} + \psi^* \partial_\mu \partial^\mu \psi - \cancel{(\partial_\mu \psi)(\partial^\mu \psi^*)} - \psi \partial_\mu \partial^\mu \psi^*\right] \qquad (\omega)$$

Remember KGE (for free particle) : $(\partial_\mu \partial^\mu + m^2)\psi = 0$

$$\partial_\mu \partial^\mu \psi = -m^2 \psi$$

$$\partial_\mu \partial^\mu \psi^* = -m^2 \psi^*$$

Then we may write (ω) as:

$$\partial_\mu J^\mu = A\left[\psi^* \cancel{(-m^2\psi)} - \psi \cancel{(-m^2\psi^*)}\right]$$

$$= 0 \qquad \checkmark \quad \text{continuity.}$$

(6)

The "time part" of j^μ is:

$$j^0 = A\,\underbrace{\left(\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t}\right)}_{\text{not a positive real number in general}}$$

whereas $|\psi|^2$ is.

e.g. $\psi(x,t) = N e^{i(px - Et)}$

Apply KGE :

$$\underbrace{-E^2 + p^2}_{\partial^\mu \partial_\mu \psi} + m^2 = 0$$

$$E^2 = p^2 + m^2 \qquad (\text{remember } c=1)$$

7

$$\underbrace{j^0}_{} = A\left(\cancel{e^{-i(px-Et)}}(-iE)\cancel{e^{i(px-Et)}} - \cancel{e^{i(px-Et)}}(+iE)\cancel{e^{-i(px-Et)}}\right);$$

NN^*

$$= \underbrace{-2iA\,\underbrace{E}_{\text{real}}\,\underbrace{NN^*}_{\text{real}}}_{}$$

no obvious reason why this should be real and positive.

- Dirac developed his equation with motivation of finding a corresponding continuity eqn with real positive probability densities.

2.14 2023-10-31 Lecture

1

Dirac equation

- motivated by finding a continuity equation with a positive probability density, Dirac proposed avoiding 2nd order time derivatives with:

$$i\frac{\partial}{\partial t}\underbrace{|\psi\rangle}_{n\times 1} = (\underbrace{\vec{\alpha}}_{}\cdot\underbrace{\vec{p}}_{-i\nabla} + \underbrace{\beta}_{}\overbrace{m}^{\text{mass of particle}})\underbrace{|\psi\rangle}_{n\times 1} \qquad \begin{pmatrix}\hbar = 1,\\ c = 1\end{pmatrix}$$

yet to be determined $n\times n$, constant square matrices.

For connection with SR: $E = \sqrt{(pc)^2 + (mc^2)^2}$

$$\boxed{(\vec{\alpha}\cdot\vec{p} + \beta m)^2 = \underbrace{p^2 + m^2}_{(cp)^2 + (mc^2)^2} \qquad (c=1)}$$

(2)

$$(\vec{\alpha}\cdot\vec{p} + \beta m)^2 = \alpha_x^2 p_x^2 + \alpha_y^2 p_y^2 + \alpha_z^2 p_z^2 \quad \checkmark$$
$$+ \alpha_x p_x \alpha_y p_y + \alpha_y p_y \alpha_x p_x$$
$$+ \cdots$$
$$+ \alpha_x p_x \beta + \beta \alpha_x p_x$$
$$+ \cdots$$
$$+ \beta^2 m^2 \quad \checkmark$$

If I want this to be $= p^2 + m^2$, we require

$$\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = I$$

and

$$\alpha_x \alpha_y + \alpha_y \alpha_x = 0 \quad , \text{etc...}$$

or $\quad [\alpha_i, \alpha_j]_+ = 0 \quad$ for $i \neq j$

$$[\alpha_i, \beta]_+ = 0$$

$\left(\begin{array}{l}\text{anti-commutator:} \\ [A,B]_+ = AB+BA\end{array}\right)$

(3)

For unitary time evolution,

$$\vec{\alpha}\cdot\vec{p} + \beta m$$

has to be Hermitian $(A = A^+)$.

We can satisfy this constraint by requiring that $\vec{\alpha}$ and β be Hermitian.

$$\alpha_i \alpha_i = I$$

$$\left.\begin{array}{l}\alpha_i^{-1} = \alpha_i \\ \alpha_i^{-1} = \alpha_i^+\end{array}\right\} \alpha\text{'s are Hermitian}$$

Thus the α_i's and β are unitary.

Recall:

1) An operator that is Hermitian only has real eigenvalues.
2) An operator that is unitary only has eigenvalues of magnitude one.

④

1) & 2) $\Rightarrow$ eigenvalues have to be +/- 1.

Recall that for any Hermitian matrix A

$$\underbrace{A}_{n\times n} = \mathcal{U}^{+} \underbrace{D}_{n\times n \text{ diagonal matrix}} \underbrace{\mathcal{U}}_{\text{unitary, } n\times n}$$

$\underset{\sim}{\text{Trace}}$ of A is defined as the sum of the diagonal components of a matrix.

$$\mathrm{Tr}(A) = \sum_i A_{ii}$$

$$\mathrm{Tr}(AB) = \sum_{ij} A_{ij} B_{ji}$$

$$= \mathrm{Tr}(BA)$$

more generally

$$\mathrm{Tr}(\underbrace{AB\ldots Y}Z) = \mathrm{Tr}(ZAB\ldots Y)$$

Trace invariant under cyclic permutations of product.

⑤

$$\mathrm{Tr}(A) = \mathrm{Tr}(u^{+} D u)$$
$$= \mathrm{Tr}(\underbrace{u u^{+}}_{I} D)$$
$$= \mathrm{Tr}(D)$$, i.e. sum of eigenvalues

For any Hermitian matrix, its trace is equal to the sum of its eigenvalues.

$$\alpha_i \alpha_j = -\alpha_j \alpha_i \qquad (i \neq j)$$

$$\underbrace{\alpha_i \alpha_i}_{I} \alpha_j = -\alpha_i \alpha_j \alpha_i$$

$$\mathrm{Tr}(\alpha_j) = -\mathrm{Tr}(\alpha_i \alpha_j \alpha_i)$$
$$= -\mathrm{Tr}(\underbrace{\alpha_i^2} \alpha_j)$$
$$\mathrm{Tr}(\alpha_j) = \mathrm{Tr}(-\alpha_j)$$
$$\mathrm{Tr}(\alpha_j) = 0$$

6

Thus the α_j's and β are traceless.

If they are traceless, but yet their eigenvalues are ± 1, then n has to be even. i.e. $\underbrace{2\times 2}_{\text{eliminate easily}}, \underbrace{4\times 4}_{\text{this works.}}$, etc....

Can the α's and β be 2×2?

Pauli spin matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_i\sigma_j = -\sigma_j\alpha_i \quad (j\neq i), \quad \sigma_i^2 = I$$

7

Why can't the σ's be the α's?
We still need a β!!!

The 3 Pauli spin matrices together with the 2×2 identity matrix form a basis for all 2×2 matrices.
Thus if β exists, we will be able to write it as:

$$\beta = c_x\sigma_x + c_y\sigma_y + c_z\sigma_z + c_I I \qquad (*)$$

complex #'s yet TBD.

Apply σ_x from left on both sides.

$$\sigma_x\beta = c_x I + c_y\sigma_x\sigma_y + c_z\sigma_x\sigma_z + c_I\sigma_x \qquad (\times)$$

Apply σ_x from right to $(*)$

$$\beta\sigma_x = c_x I + c_y\sigma_y\sigma_x + c_z\sigma_z\sigma_x + c_I\sigma_x \qquad (\ddagger)$$

8

Add (×) and (≠):

$$[\sigma_x, \beta]_+ = 2c_x I + 2c_I \sigma_x$$
$$0 = c_x I + c_I \sigma_x$$

A basis is a set of $\underbrace{\text{linear indep. vectors}}$ that span a vector space.

Linearly indep means:

$$0 = c_1\vec{v}_1 + c_2\vec{v}_2 + \cdots c_n\vec{v}_n$$

linearly indep.

the only sol^{n} is $c_1 = c_2 = \cdots c_n = 0$.

Thus $c_x = c_I = 0$. Likewise $c_y = c_I = 0$ and $c_z = c_I = 0$ by similar arg. Thus (*) on pg 7 can't give a non-zero β.

9

$\underset{\sim\sim}{3\times3}$ are ruled out because eigenvalues are +/-1 and sum to zero.

$\underset{\sim\sim}{4\times4}$

$$\vec{\alpha} = \underbrace{\begin{bmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{bmatrix}}_{4}\Bigg\}4 , \quad \beta = \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix}$$

$\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ $\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$

satisfy the necessary requirements. (but not unique!!!)

$$\underset{i\neq j}{\alpha_i\alpha_j} = \begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix}\begin{bmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{bmatrix}$$

(10)

$$\alpha_i\alpha_j = \begin{bmatrix} \sigma_i\sigma_j & 0 \\ 0 & \sigma_i\sigma_j \end{bmatrix}$$

Pauli spin matrices anticommute $\sigma_i\sigma_j = -\sigma_j\sigma_i \quad (j\neq i)$

$$= \begin{bmatrix} -\sigma_j\sigma_i & 0 \\ 0 & -\sigma_j\sigma_i \end{bmatrix}$$

$$= -\begin{bmatrix} \sigma_j & 0 \\ 0 & \sigma_j \end{bmatrix}\begin{bmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{bmatrix}$$

$$= -\alpha_j\alpha_i \quad \checkmark$$

Thus α's anti-commute as req'd!

Let's check that the α_i's anti-commute with β.

$$\alpha_i\beta = \begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix}\begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix}$$

(11)

$$\alpha_i\beta = \begin{bmatrix} 0 & -\sigma_i \\ \sigma_i & 0 \end{bmatrix}$$

$$= \begin{bmatrix} -I & 0 \\ 0 & I \end{bmatrix}\begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix}$$

$$= -\beta\alpha_i \quad \checkmark$$

Straightforward to show $\alpha_i^2 = \beta^2 = I$ 4×4.

Note $\alpha_x, \alpha_y, \alpha_z$ and β are not unique.

$\alpha_i^2 = I$, $\beta^2 = I$, $[\alpha_i, \alpha_j]_+ = 0 \ (i\neq j)$, $[\alpha_i, \beta] = 0$

Suppose $\alpha_i' = U\alpha_i U^\dagger$, $\beta' = U\beta U^\dagger$ satisfy thes relationships.

any unitary

(12)

e.g.
$$\begin{aligned}\alpha_i'\alpha_j' &= U\alpha_i \underbrace{U^\dagger U}_{I}\alpha_j U^\dagger \\ &= \\ &= U\alpha_i\alpha_j U^\dagger \\ &= -U\alpha_j\alpha_i U^\dagger \\ &= -\underbrace{U\alpha_j U^\dagger}\,\underbrace{U\alpha_i U^\dagger} \\ &= -\alpha_j'\alpha_i'\end{aligned}$$

etc..... (show all req'd properties)

2.15 2023-11-02 Lecture

(1)

Pauli's Equation

Arises from looking at non-relativistic limit of Dirac equation.

$$i\hbar \frac{\partial \psi}{\partial t} = [c\vec{\alpha}\cdot\vec{p} + \beta mc^2]\psi$$

$\downarrow$ with EM fields (but without justification (!) for which we need covariant form of Dirac's equation)

$$i\hbar\frac{\partial\psi}{\partial t} = [c\vec{\alpha}\cdot\underbrace{(\vec{p}-q\vec{A})}_{=:\vec{\pi}} + \beta mc^2 + q\Phi \underset{\text{4x4 identity}}{I}]\psi \qquad \text{(SI)}$$

② Break up 4×1 ψ into $\begin{bmatrix} \tilde{\chi} \\ \tilde{\varphi} \end{bmatrix} \begin{matrix} \leftarrow 2\times 1 \\ \leftarrow 2\times 1 \end{matrix}$

Dirac's "equation" is now:

$$\left.\begin{aligned} i\hbar \frac{\partial \tilde{\chi}}{\partial t} &= c\,\vec{\sigma}\cdot\vec{\pi}\,\tilde{\varphi} + mc^2\tilde{\chi} + q\Phi\tilde{\chi} \\ i\hbar \frac{\partial \tilde{\varphi}}{\partial t} &= c\,\vec{\sigma}\cdot\vec{\pi}\,\tilde{\chi} - mc^2\tilde{\varphi} + q\Phi\tilde{\varphi} \end{aligned}\right\} (\times)$$

Define χ, φ by

$$\begin{bmatrix} \tilde{\chi} \\ \tilde{\varphi} \end{bmatrix} = e^{-\frac{imc^2 t}{\hbar}} \begin{bmatrix} \chi \\ \varphi \end{bmatrix}$$

Let's write Dirac's "equation" using χ, φ:

③
$$\begin{aligned} i\hbar \frac{\partial \tilde{\chi}}{\partial t} &= i\hbar \frac{\partial}{\partial t}\left(e^{-\frac{imc^2 t}{\hbar}} \chi\right) \\ &= i\hbar \left[-\frac{imc^2}{\hbar} e^{-imc^2 t/\hbar} \chi \right. \\ &\qquad \left. + e^{-\frac{imc^2 t}{\hbar}} \frac{\partial \chi}{\partial t} \right] \\ &= e^{-imc^2 t/\hbar} \left[mc^2 \chi + i\hbar \frac{\partial \chi}{\partial t} \right] \qquad (*) \end{aligned}$$

By similar algebra:

$$i\hbar \frac{\partial \tilde{\varphi}}{\partial t} = e^{-imc^2 t/\hbar} \left[mc^2 \varphi + i\hbar \frac{\partial \varphi}{\partial t} \right] \qquad (\neq)$$

Substitute $(*)$ and $(\neq)$ into $(\times)$:

④

$$i\hbar \frac{\partial \chi}{\partial t} + \cancel{mc^2 \chi} = c\,\vec{\sigma}\cdot\vec{\pi}\,\varphi + \cancel{mc^2 \chi} + q\Phi\chi \quad \text{(YY)}$$

$$i\hbar \frac{\partial \varphi}{\partial t} + mc^2\varphi = c\,\vec{\sigma}\cdot\vec{\pi}\,\chi - mc^2\varphi + q\Phi\varphi$$

$$\underbrace{i\hbar \frac{\partial \varphi}{\partial t}}_{①} + \underset{②}{2mc^2\varphi} - \underbrace{q\Phi\varphi}_{③} = \underset{④}{c\,\vec{\sigma}\cdot\vec{\pi}\,\chi} \quad \text{(xx)}$$

$$\frac{10^{-34}\,\mathrm{J\cdot s}}{\tau} \qquad 10^{-31}\,\mathrm{kg}\;10^{16}\,\frac{\mathrm{m}^2}{\mathrm{s}^2}$$

$$10^{-15}\,\mathrm{J} \rightarrow \underset{\sim\sim}{10\,\mathrm{keV}}$$

much larger than energy scale for "atomic" processes but not nuclear,

as long as τ is much larger than 10^{-19} s than we can ignore $i\hbar \frac{\partial \varphi}{\partial t}$ relative to mc^2.

Ignore ① and ③ and keep ② and ④.

⑤

Rearrange (xx) to solve for χ in terms of φ, to use in (YY):

$$\varphi \simeq \frac{c\,\vec{\sigma}\cdot\vec{\pi}\,\chi}{2mc^2}$$

(YY) becomes:

$$i\hbar \frac{\partial \chi}{\partial t} = \left[\frac{(\vec{\sigma}\cdot\vec{\pi})^2}{2m} + q\Phi\right]\chi \qquad \text{(ZZ)}$$

Two mathematical results:

1) For any $\vec{M}$ and $\vec{N}$ that commute with the σ's
$$(\vec{\sigma}\cdot\vec{M})(\vec{\sigma}\cdot\vec{N}) = \vec{M}\cdot\vec{N} + i\vec{\sigma}\cdot(\vec{M}\times\vec{N})$$

2) $$(\underset{\vec{p}-q\vec{A}}{\vec{\pi}}\times\vec{\pi})\, f(\vec{r}) = q\,i\hbar\,\underset{\nabla\times\vec{A}}{\vec{B}}\, f(\vec{r}) \quad \leftarrow$$

⑥

Using these results in (22) gives:

$$\boxed{i\hbar \frac{\partial \chi}{\partial t} = \left[\frac{1}{2m} (\vec{p} - q\vec{A})^2 - \frac{q}{2m} \hbar \vec{\sigma}\cdot\vec{B} + q\Phi \right] \chi}$$

Pauli's equation

2×1

Remember $\vec{S} = \frac{\hbar}{2} \vec{\sigma}$ (normally seen when introducing spin-1/2)

angular momentum of spin-1/2 system

$$-\frac{q}{2m} \hbar \vec{\sigma}\cdot\vec{B} = -\left(\frac{q}{m}\right) \vec{S}\cdot\vec{B}$$

$\left(-\frac{q}{2m} \vec{L}\cdot\vec{B} \right.$ orbital angular momentum $\left. \right)$

$$= g \left(\frac{-q}{2m}\right) \vec{S}\cdot\vec{B}$$

Pauli's eqn predicts "$g=2$".

⑦

For spin of e^- (compared to $g=1$ for orbital angular momentum).

$$g \simeq 2 \left[1 + \overbrace{\frac{\alpha}{2\pi} + O(\alpha^2)}^{\text{QED.}} \right]$$

But for e^-

$$\alpha \simeq \frac{1}{137} \qquad \frac{\left(\frac{q^2}{4\pi\epsilon_0}\right)}{\hbar c} \begin{array}{l} \text{J.m} \\ \text{J.m} \end{array}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$+\hbar/2$

$-\hbar/2$

2.16 2023-11-07 Lecture

Pre-lecture:

For information on the spectrum of atomic hydrogen, see Chapter 2 of C. J. Foot, *Atomic physics*, Oxford Master Series in Physics 7. Atomic, Optical, and laser physics (Oxford University Press, Oxford ; New York, 2005) (posted to Learn).

(1)

Angular momentum in the hydrogen atom

ℓ : orbital angular momentum of e^-

$s = 1/2$: spin angular momentum of e^-

remember angular momentum coupling (i.e. Clebsch-Gordan coefficients)

j : total (spin and orbital) angular momentum.

j ranges from $|\ell - s|$ to $\ell + s$ in steps of 1.

"s" e.g. $\ell = 0$, $|\ell - s| = 1/2$, $\ell + s = 1/2$, $j = 1/2$

"p" e.g. $\ell = 1$, $|\ell - s| = 1/2$, $\ell + s = 3/2$, $j = 1/2$ or $3/2$

"d" $\ell = 2$, " $3/2$, $\ell + s = 5/2$, $j = 3/2$ or $5/2$

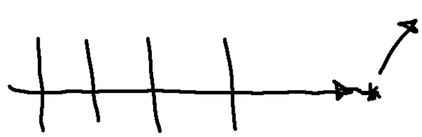
(2)

Scattering

- almost universally described by "cross-sections"* (units of area).

$$R = \sigma F$$

rate (s^{-1}) ; cross-section (m^2) ; flux $\left(\frac{\text{particles}}{s \cdot m^2}\right)$ "luminosity" sometimes.



(3)

- elastic scattering (KE conserved)
  e.g. Rutherford scattering

- inelastic scattering
  e.g.

$$e^- + H_2\underbrace{(v=0)}_{\text{ground vibrational state.}} \rightarrow e^- + H_2\underbrace{(v=1)}_{\text{excited vibrational state}}$$

$$\rightarrow e^- + H + H$$

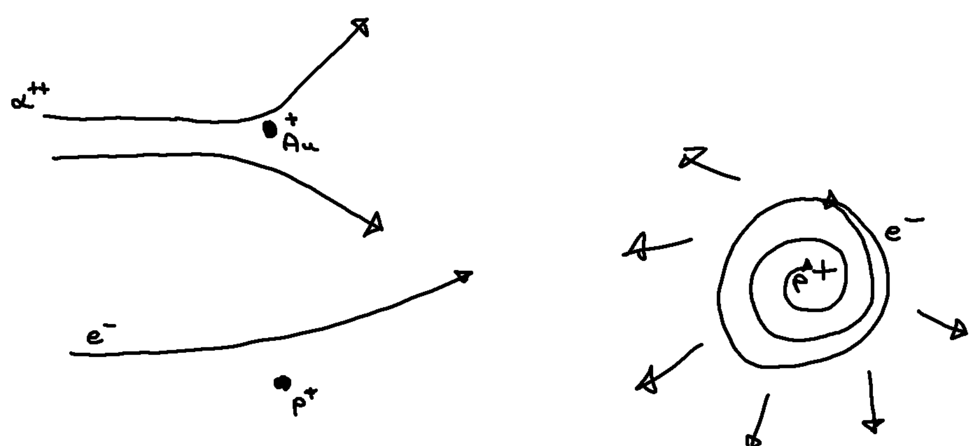
$$\rightarrow e^- + e^- + H_2^+$$

examples of competing "channels" each with its own cross-section "partial cross-sections"

- focus on the elastic channel.

(4)

(Aside: a truly elastic collision is an idealization)



because of radiation that can be emitted in a collision, due to acceleration of charged particles.

2

Cross-sections are frequently referred to. Arxiv: 1310.8214

First results from the LUX dark matter experiment at the Sanford Underground Research Facility

D.S. Akerib,[2] H.M. Araújo,[4] X. Bai,[8] A.J. Bailey,[4] J. Balajthy,[16] S. Bedikian,[19] E. Bernard,[19] A. Bernstein,[6] A. Bolozdynya,[2] A. Bradley,[2] D. Byram,[18] S.B. Cahn,[19] M.C. Carmona-Benitez,[2,14] C. Chan,[1] J.J. Chapman,[1] A.A. Chiller,[18] C. Chiller,[18] K. Clark,[2] T. Coffey,[2] A. Currie,[4] A. Curioni,[19] S. Dazeley,[6] L. de Viveiros,[7] A. Dobi,[16] J. Dobson,[15] E.M. Dragowsky,[2] E. Druszkiewicz,[17] B. Edwards,[19,*] C.H. Faham,[1,5] S. Fiorucci,[1] C. Flores,[13] R.J. Gaitskell,[1] V.M. Gehman,[5] C. Ghag,[11] K.R. Gibson,[2] M.G.D. Gilchriese,[5] C. Hall,[16] M. Hanhardt,[8,9] S.A. Hertel,[19] M. Horn,[19] D.Q. Huang,[1] M. Ihm,[12] R.G. Jacobsen,[12] L. Kastens,[19] K. Kazkaz,[6] R. Knoche,[16] S. Kyre,[14] R. Lander,[13] N.A. Larsen,[19] C. Lee,[2] D.S. Leonard,[16] K.T. Lesko,[5] A. Lindote,[7] M.I. Lopes,[7] A. Lyashenko,[19] D.C. Malling,[1] R. Mannino,[10] D.N. McKinsey,[19] D.-M. Mei,[18] J. Mock,[13] M. Moongweluwan,[17] J. Morad,[13] M. Morii,[3] A.St.J. Murphy,[15] C. Nehrkorn,[14] H. Nelson,[14] F. Neves,[7] J.A. Nikkel,[19] R.A. Ott,[13] M. Pangilinan,[1] P.D. Parker,[19] E.K. Pease,[19] K. Pech,[2] P. Phelps,[2] L. Reichhart,[11] T. Shutt,[2] C. Silva,[7] W. Skulski,[17] C.J. Sofka,[10] V.N. Solovov,[7] P. Sorensen,[6] T. Stiegler,[10] K. O'Sullivan,[19] T.J. Sumner,[4] R. Svoboda,[13] M. Sweany,[13] M. Szydagis,[13] D. Taylor,[9] B. Tennyson,[19] D.R. Tiedt,[8] M. Tripathi,[13] S. Uvarov,[13] J.R. Verbus,[1] N. Walsh,[13] R. Webb,[10] J.T. White,[10,†] D. White,[14] M.S. Witherell,[14] M. Wlasenko,[3] F.L.H. Wolfs,[17] M. Woods,[13] and C. Zhang[18]

[1] *Brown University, Dept. of Physics, 182 Hope St., Providence RI 02912, USA*
[2] *Case Western Reserve University, Dept. of Physics, 10900 Euclid Ave, Cleveland OH 44106, USA*
[3] *Harvard University, Dept. of Physics, 17 Oxford St., Cambridge MA 02138, USA*
[4] *Imperial College London, High Energy Physics, Blackett Laboratory, London SW7 2BZ, UK*
[5] *Lawrence Berkeley National Laboratory, 1 Cyclotron Rd., Berkeley CA 94720, USA*
[6] *Lawrence Livermore National Laboratory, 7000 East Ave., Livermore CA 94550, USA*
[7] *LIP-Coimbra, Department of Physics, University of Coimbra, Rua Larga, 3004-516 Coimbra, Portugal*
[8] *South Dakota School of Mines and Technology, 501 East St Joseph St., Rapid City SD 57701, USA*
[9] *South Dakota Science and Technology Authority, Sanford Underground Research Facility, Lead, SD 57754, USA*
[10] *Texas A & M University, Dept. of Physics, College Station TX 77843, USA*
[11] *University College London, Department of Physics and Astronomy, Gower Street, London WC1E 6BT, UK*
[12] *University of California Berkeley, Department of Physics, Berkeley CA 94720, USA*
[13] *University of California Davis, Dept. of Physics, One Shields Ave., Davis CA 95616, USA*
[14] *University of California Santa Barbara, Dept. of Physics, Santa Barbara, CA, USA*
[15] *University of Edinburgh, SUPA, School of Physics and Astronomy, Edinburgh, EH9 3JZ, UK*
[16] *University of Maryland, Dept. of Physics, College Park MD 20742, USA*
[17] *University of Rochester, Dept. of Physics and Astronomy, Rochester NY 14627, USA*
[18] *University of South Dakota, Dept. of Physics, 414E Clark St., Vermillion SD 57069, USA*
[19] *Yale University, Dept. of Physics, 217 Prospect St., New Haven CT 06511, USA*

(Dated: October 31, 2013)

The Large Underground Xenon (LUX) experiment, a dual-phase xenon time-projection chamber operating at the Sanford Underground Research Facility (Lead, South Dakota), was cooled and filled in February 2013. We report results of the first WIMP search dataset, taken during the period April to August 2013, presenting the analysis of 85.3 live-days of data with a fiducial volume of 118 kg. A profile-likelihood analysis technique shows our data to be consistent with the background-only hypothesis, allowing 90% confidence limits to be set on spin-independent WIMP-nucleon elastic scattering with a minimum upper limit on the cross section of 7.6×10^{-46} cm^2 at a WIMP mass of 33 GeV/c^2. We find that the LUX data are in strong disagreement with low-mass WIMP signal interpretations of the results from several recent direct detection experiments.

PACS numbers: 95.35.+d, 29.40.-n, 95.55.Vj
Keywords: dark matter, direct detection, xenon

Convincing evidence for the existence of particle dark matter is derived from observations of the universe on scales ranging from the galactic to the cosmological [1–3]. Increasingly detailed studies of the Cosmic Microwave Background anisotropies have implied the abundance of dark matter with remarkable precision [4, 5]. One favored class of dark matter candidates, the Weakly Interacting Massive Particle (WIMP), may be amenable to direct detection in laboratory experiments through its interactions with ordinary matter [6, 7]. The WIMPs

* Corresponding Author: blair.edwards@yale.edu
† deceased

3

Example of a cross-section : Fission

"^{235}U is the only isotope found in nature that is fissionable by slow neutrons, although it exists in a small proportion (0.7%) with respect to ^{238}U (99.3%) in a natural uranium sample."

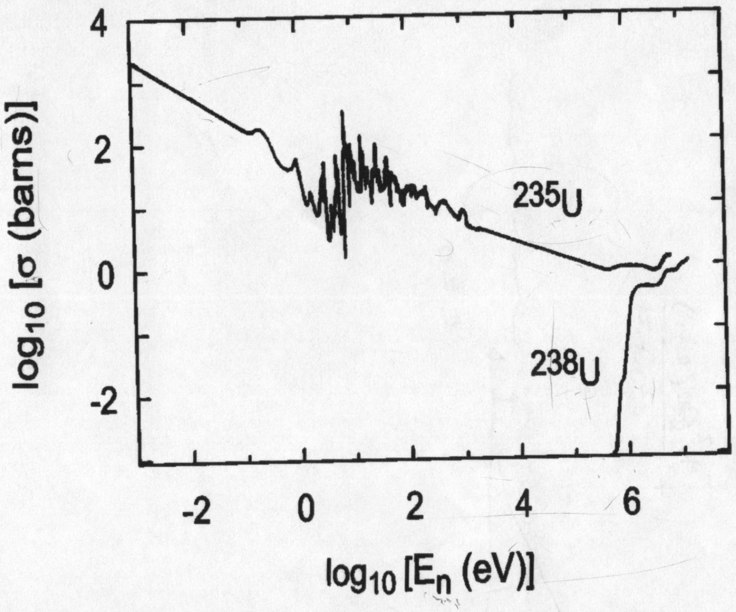


Figure 5.27. Fission cross sections of ^{235}U and ^{238}U bombarded by 0–10 MeV neutrons.

From "Introduction to Nuclear Reactions"
Bertulani and Danielewicz

A fermi (fm) or femtometer $= 10^{-15}$ m

Typical nuclear radii $\simeq 1 \to 10$ fm

$1\,b \simeq 100\,fm^2 \simeq 10^{-28}\,m^2$
"barn"

4

Example of cross-section : Fusion

 , Nucl. Fusion, v.32, 611 (1992).

For a discussion of this notation, see Clayton "Principles of Stellar Evolution..." 1968, pg 284

D+T → α + n

derive better parametrizations for fusion cross-sections and Maxwellian reactivities. The paper is divided into three parts. After a short introduction into the physics of the fusion reactions and R-matrix theory, we compare the data now available with the old parametrizations (to give an idea of their validity and accuracy), and also with the cross-section values resulting from R-matrix calculations. In the third part, we derive new parametrizations based on these R-matrix data for the fusion cross-sections as well as for the reactivities in thermal plasmas.

2. THEORETICAL BACKGROUND

The physics of fusion reactions between light nuclei has been treated in detail elsewhere [7, 8], and detailed information on the states of the intermediate compound systems has been collected in two review papers [9, 10]. Here, we only discuss some basic physics issues that are necessary to understand the parametrization used.

2.1. Parametrization of the cross-section

Fusion reactions between two nuclei can be divided into two parts which are approximately independent of each other, namely the atomic physics of the nuclei approaching each other, and the nuclear physics valid if they are close enough to feel the nuclear forces. The strong energy dependence of the fusion cross-section (see Fig. 1(a)) is mainly due to the repulsive Coulomb potential. As long as the energy available in the centre-of-mass (CM) frame is much smaller than the Coulomb barrier, reactions are possible only because of the tunnelling effect, and the cross-section is proportional to the tunnelling probability:

$$\sigma \sim \exp - \frac{2\pi Z_1 Z_2 e^2}{\hbar v} \tag{1}$$

with v being the relative velocity of the reacting particles [11]. This can be rearranged to give

$$\sigma \sim \exp(-B_G/\sqrt{E}) \tag{2}$$

where

$$B_G = \pi \alpha Z_1 Z_2 \sqrt{2 m_r c^2} \tag{3}$$

is the Gamov constant, expressed in terms of the fine structure constant, $\alpha = e^2/\hbar c = 1/137.03604$, and the reduced mass of the particles, $m_r c^2$, in keV. Throughout this paper, E denotes the energy available in the CM frame. For a particle A with mass m_A striking a stationary particle B, the simple relation $E_A = E(m_A + m_B)/m_B$ holds.

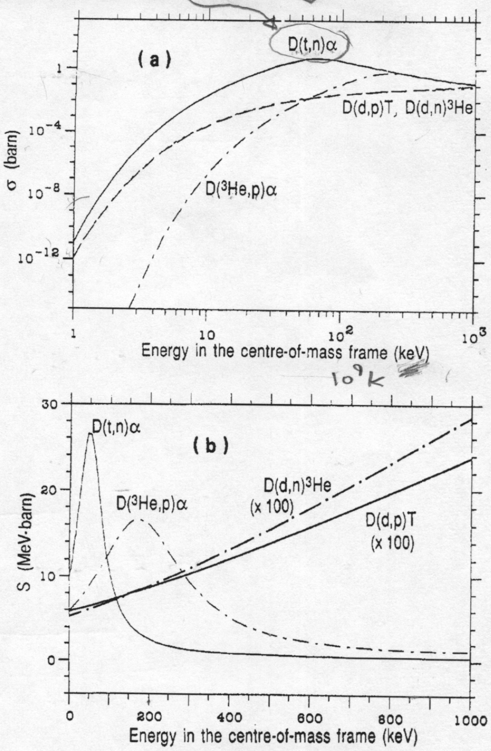


FIG. 1. (a) Fusion cross-sections for the most important fusion reactions as a function of the CM energy of the reacting particles. The curves are calculated from Peres' [3] formula. (b) The S-functions for these reactions as derived from Eq. (4). For the d + d reactions the data have been multiplied by 100 to improve clarity.

Quantum mechanics shows that the fusion reaction probability is also proportional to a geometrical factor $\pi\lambda^2 \sim 1/E$, where λ is the de Broglie wavelength. The strong energy dependences of this factor and the barrier penetrability have prompted the introduction of the astrophysical S-function [12, 13], defined by writing the cross-section as a product of three factors:

$$\sigma = S(E)\,\frac{1}{E}\,\exp(-B_G/\sqrt{E}) \tag{4}$$

The motivation for this definition is that the two well known, strongly energy dependent factors (which describe the Coulombic and phase space parts of the incident channel) are separated, leaving the S-function to represent mainly the presumably slowly varying nuclear part of the fusion reaction probability [13].

2.17 2023-11-09 Lecture

Pre-lecture:

Scattering discussion follows D. J. Griffiths and D. F. Schroeter, *Introduction to quantum mechanics*, 3rd (Cambridge University Press, 2018).

1

Natural units - deduction

Defined "new" lengths, masses and times by:

$$\tilde{\ell} := c_\ell \ell$$
$$\tilde{m} := c_m m$$
$$\tilde{t} := c_t t$$

actual quantities

We need to determine c_ℓ, c_m, and c_t based on some constraints.

For "natural" units we will use the constraints:

1 $\tilde{\hbar} = 1$, 2 $\tilde{c} = 1$, 3 $\tilde{E} = E$

②

Start with ③ $(E = \tilde{E})$

$$\underbrace{E}_{\frac{\text{length}^2}{\text{time}^2}\text{mass}} \frac{c_e^2}{c_t^2} c_m = \tilde{E} \quad \Big] \text{ always true.}$$

But $E = \tilde{E} \Rightarrow \dfrac{c_e^2}{c_t^2} c_m = 1$ (*)

Look at ① $(\tilde{\hbar} = 1)$

$$\underbrace{\hbar}_{\text{energy} \times \text{time}} \underbrace{\frac{c_e^2 c_m}{c_t^2}}_{=1 \text{ from } (*)} c_t = 1 \Rightarrow \boxed{c_t = \frac{1}{\hbar}} \quad (\ddagger)$$

$$\underbrace{\tilde{t}}_{1/\text{energy}} = t / \underbrace{\hbar}_{\text{energy} \cdot \text{time}}$$

③

Look at ② $(\tilde{c} = 1)$

$$c \frac{c_e}{c_t} = 1 \Rightarrow \frac{c_e}{c_t} = \frac{1}{c}$$

Using $(\ddagger)$ $\boxed{c_e = \dfrac{1}{\hbar c}}$ $\longrightarrow$ $\hbar c$ is a energy-length

$$\underbrace{\tilde{\ell}}_{\text{energy}^{-1}} = \frac{\ell}{\hbar c}$$

From (*) $c_m = \dfrac{c_t^2}{c_e^2}$

$$= \frac{\cancel{\hbar^2} c^2}{\cancel{\hbar^2}}$$

$$\boxed{c_m = c^2} \longrightarrow \tilde{m} = m c^2$$

masses are in term of energies

④

Suggestion for problem set:

Use ① $\tilde{\hbar}=1$ ② $\tilde{m}_p=1$ ③ $\underbrace{\tilde{e}=e}_{\text{not a unique choice}}$

$$\tilde{m}_p=1 \Rightarrow c_m=\frac{1}{m_p} \quad \text{in} \quad \tilde{m}=c_m m$$

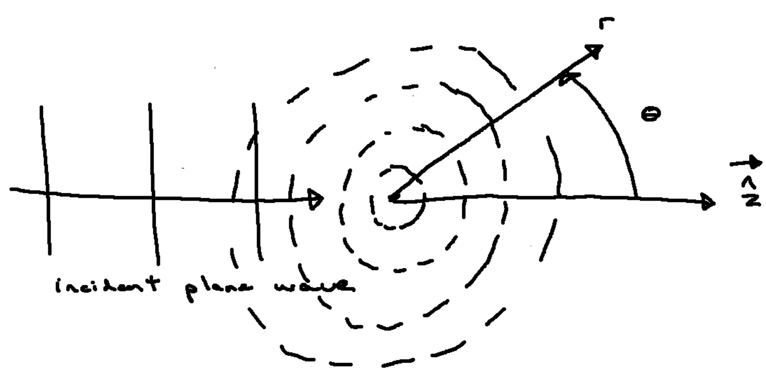
$\tilde{m}_p = 1$

$c_m m_p = 1$

$c_m = \frac{1}{m_p}$

⑤

Elastic scattering



(assume fixed target, but results are easily generalized)

for large r: $\psi(r,\theta) = A\left\{ e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \right\}$

$\frac{\hbar^2 k^2}{2m} = E$ (energy of incident particle)

note no ϕ dependence.

(6)

- recall probability conservation :

$$\oint \vec{j}\cdot d\vec{a} = -\frac{\partial}{\partial t}\left(\begin{array}{c}\text{probability of}\\ \text{being within}\\ \text{volume}\end{array}\right)$$

$$\Big\updownarrow \text{ divergence theorem.}$$

$$\nabla\cdot\vec{j} = -\frac{\partial}{\partial t}|\psi|^2$$

This all works if $\vec{j} := -\frac{i\hbar}{2m}\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right]$

Use $\psi_{incident} = A e^{ikz}$

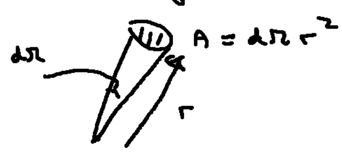
$$\vec{j}_{incident} = \underbrace{|A|^2}_{\text{probability / unit volume}} \underbrace{\frac{\hbar k}{m}}_{\text{speed}} \hat{z}$$

(7)

$$\psi_{scattered} = A\frac{e^{ikr}}{r} f(\theta)$$

$$\vec{j}_{scattered} = |A|^2 \frac{|f(\theta)|^2}{r^2}\frac{\hbar k}{m}\hat{r}$$

We are interested in the rate of scattering into a certain solid angle



$$R = d\Omega\, r^2 \left(\vec{j}_{scattered}\cdot\hat{r}\right)$$
$$= d\Omega\, |A|^2\, |f(\theta)|^2 \frac{\hbar k}{m}$$

⑧

$$d\sigma = \frac{R}{F} \leftarrow |\vec{j}_{\text{incident}}|$$

$$= \frac{d\Omega \cancel{|A|^2} |f(\theta)|^2 \cancel{\frac{\hbar k}{m}}}{\cancel{|A|^2} \cancel{\frac{\hbar k}{m}}}$$

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

We have to use the potential describing interaction between particles, and SOE to determine $f(\theta)$.

$$\underset{\uparrow}{\sigma} = \int d\Omega \frac{d\sigma}{d\Omega}$$

$$= \int d\Omega |f(\theta)|^2$$

2.18 2023-11-14 Lecture

Pre-lecture:

Scattering discussion follows D. J. Griffiths and D. F. Schroeter, *Introduction to quantum mechanics*, 3rd (Cambridge University Press, 2018).

What I (and Griffiths) call $a_\ell(k)$, Sakurai and Napolitano call $f_\ell(k)$.

①

We need to determine $f(\theta)$ by solving the Schrödinger equation.

If potential is spherically symmetric, then we know how to solve for wave-functions of well-defined orbital angular momenta.

$$e^{ikz} = \sum_{\ell=0}^{\infty} i^{\ell} (2\ell+1) \underbrace{j_{\ell}(kr)}_{\text{"spherical Bessel functions"}} \underbrace{P_{\ell}(\cos\theta)}_{\text{Legendre polynomials}}$$

Rayleigh's formula.

②

The spherical Bessel functions are the solutions to

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} \right] \underbrace{rR(r)}_{u(r)} = E \underbrace{rR(r)}_{u(r)}$$

which are "regular" at origin.

j_{ℓ}'s are known as "spherical Bessel functions of the first kind"
y_{ℓ}'s are known as "spherical Bessel functions of the second kind"

Asymptotic behaviour:

$$j_{\ell}(x) \simeq \frac{1}{x} \sin\left(x - \frac{1}{2}\ell\pi\right) \quad \text{at large } x.$$

$$y_{\ell}(x) \simeq -\frac{1}{x} \cos\left(x - \frac{1}{2}\ell\pi\right) \quad \text{"} .$$

③

$$\psi(\vec{r}) = A\left\{ e^{ikz} + \frac{f(\theta)\, e^{ikr}}{r} \right\}$$

suggests use of spherical Bessel functions of the third kind.

$$h_\ell^{(1)}(x) := j_\ell(x) + i y_\ell(x) \underset{\text{for large } x}{\approx} i^{-\ell-1} x^{-1} e^{ix}$$
$$h_\ell^{(2)}(x) := j_\ell(x) - i y_\ell(x) \approx i^{\ell+1} x^{-1} e^{-ix}$$

$$\frac{f(\theta) e^{ikr}}{r} = \sum_{\ell=0}^{\infty} i^{\ell+1} (2\ell+1) \underbrace{a_\ell(k)}_{\text{defined by this expression.}} \underbrace{h_\ell^{(1)}(kr)}_{i^{-\ell-1}\frac{1}{kr} e^{ikr} \quad (**)} k\, P_\ell(\cos\theta) \qquad (*)$$

④

$$\psi(\vec{r}) = A\left\{ \sum_{\ell=0}^{\infty} P_\ell(\cos\theta)(2\ell+1) \left[\underbrace{i^\ell j_\ell(kr)}_{\text{Rayleigh}} + \underbrace{i^{\ell+1} k\, a_\ell(k)\, h_\ell^{(1)}(kr)}_{\text{spherical waves}} \right] \right\}$$

$$= A\left\{ \sum_{\ell=0}^{\infty} P_\ell(\cos\theta)(2\ell+1) i^\ell \left[j_\ell(kr) + i k\, a_\ell(k)\, h_\ell^{(1)}(kr) \right] \right\} \qquad (\#)$$

Suppose I know the a_ℓ's, what is $\frac{d\sigma}{d\Omega}$ and σ?

From $(*)$ and $(**)$: $\boxed{f(\theta) = \sum_{\ell=0}^{\infty} (2\ell+1)\, a_\ell(k)\, P_\ell(\cos\theta)}$

$$\sigma = \int d\Omega\, |f(\theta)|^2$$

⑤

$$\sigma = \int d\Omega \; f(\theta) f^*(\theta)$$

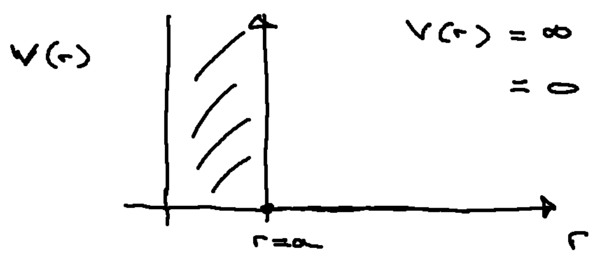
$$= \underbrace{\int_0^{2\pi} d\phi}_{2\pi} \int_0^{\pi} d\theta \, \sin\theta \sum_{l,l'} (2l+1)(2l'+1) \, a_l a_{l'}^* \, P_l(\cos\theta) P_{l'}(\cos\theta)$$

$$= 2\pi \sum_{l,l'} (2l+1)(2l'+1) \, a_l a_{l'}^* \underbrace{\int_0^{\pi} d\theta \, \sin\theta \, P_l(\cos\theta) P_{l'}(\cos\theta)}_{\delta_{l,l'} \frac{2}{2l+1}}$$

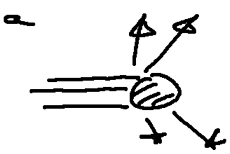
$$\boxed{\sigma = 4\pi \sum_{l=0}^{\infty} (2l+1) |a_l|^2}$$

⑥

- we will discuss the general procedure for determining a_l's next lecture, but we can do a simple example now.



$$V(r) = \infty \; , \; r < a$$
$$= 0 \; , \; r \geq a$$



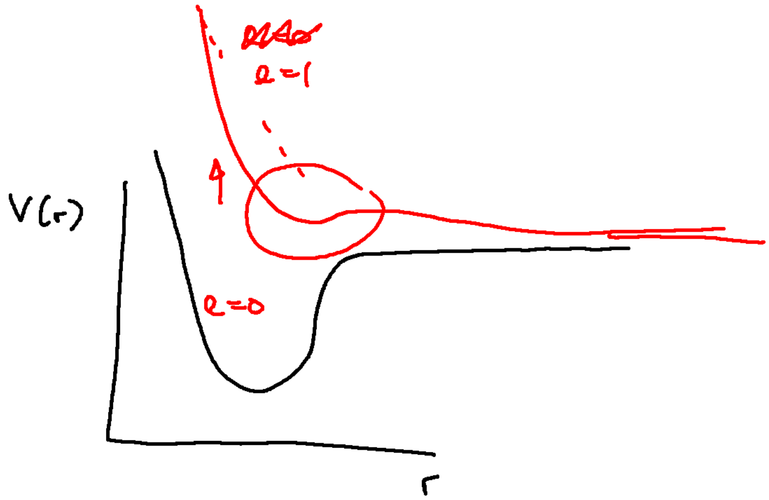
What are a_l's?

From (#) and $\psi(r=a, \theta) = 0$ for all θ, we have

$$0 = j_l(ka) + ik \, a_l(k) \, h^{(1)}(ka)$$

$$a_l(k) = \frac{-j_l(ka)}{ik \, h_l^{(1)}(ka)}$$

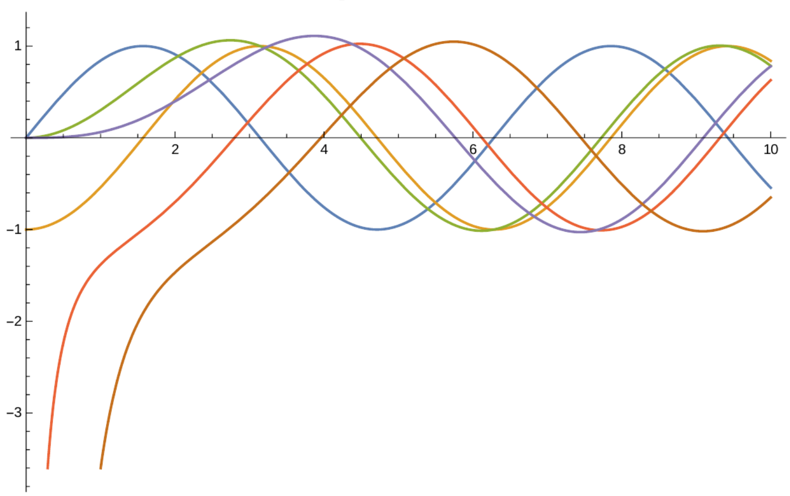
7



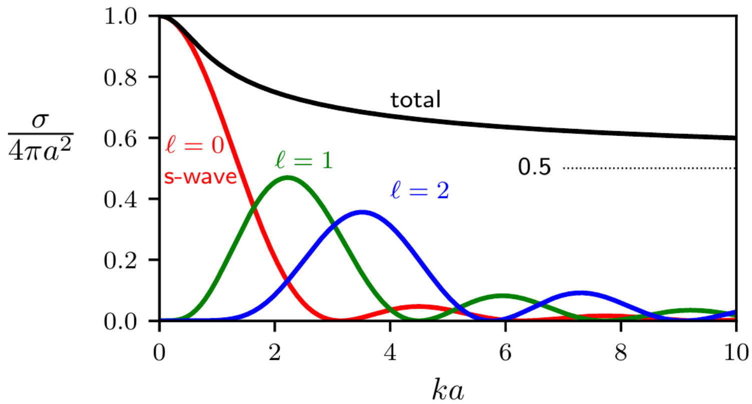
Spherical Bessel Functions

```
In[5]:= Plot[{x * SphericalBesselJ[0, x], x * SphericalBesselY[0, x],
      x * SphericalBesselJ[1, x], x * SphericalBesselY[1, x],
   x * SphericalBesselJ[2, x], x * SphericalBesselY[2, x]},
  {x, 0, 10}, ImageSize → 500]
```

Out[5]=



- hard-sphere elastic scattering cross-sections:



- note that only $\ell = 0$ contributes at low energies.

2.19 2023-11-16 Lecture

Ramsauer-Townsend effect is discussed in Sakurai and Napolitano [1], Section 6.6.

①

How do we get a_ℓ's for general $V(r)$?

Solve
$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} + \underbrace{V(r)}_{\substack{V(r)\to 0 \\ \text{as } r\to\infty}}\right]u(r) = \underbrace{\frac{\hbar^2 k^2}{2m}}\,u(r)$$

for $u(r)$ subject to BC $\lim_{r\to 0} u(r) = 0$

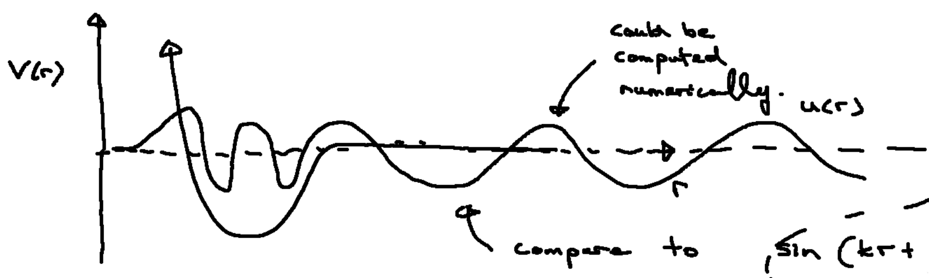
Then based on
$$\psi(r,\theta) = A\sum_{\ell=0}^{\infty} i^\ell(2\ell+1)\left[j_\ell(kr) + ik\,a_\ell(k)\,h_\ell^{(1)}(kr)\right] P_\ell(\cos\theta)$$

and $u(r) = rR(r)$, compare $u(r)$ to

$$r\left[j_\ell(kr) + ik\,a_\ell(k)\,h_\ell^{(1)}(kr)\right]$$

at large r.

②



compare to $\sin\left(kr + \underbrace{\delta_\ell(k)}_{\text{phase shift, determined by comparison with } u(r).} - \frac{\ell\pi}{2}\right)$

Introduce constant complex amplitude E, such that

$$\lim_{r\to\infty} u(r) = E\sin\left(kr + \delta_\ell(k) - \frac{\ell\pi}{2}\right)$$
$$= \frac{E}{2i}\left[e^{i[kr+\delta_\ell(k)-\ell\pi/2]} - e^{-i[kr+\delta_\ell(k)-\ell\pi/2]}\right]$$

③

Introduce C_+ and C_-

$$\lim_{r\to\infty} u(r) = C_+ e^{ikr} + C_- e^{-ikr}$$

We know $\left|\frac{C_+}{C_-}\right| = 1$

$$\frac{C_+}{C_-} = \frac{-e^{i[\delta_\ell(k)-\ell\pi/2]}}{e^{-i[\delta_\ell(k)-\ell\pi/2]}}$$

$$= -e^{2i\delta_\ell(k)} \underbrace{e^{-\ell\pi i}}_{(-1)^\ell} \qquad e^{-i\pi} = -1$$

$$\frac{C_+}{C_-} = e^{2i\delta_\ell(k)}(-1)^{\ell+1} \qquad (*)$$

④

Now look at asymptotic wavefunction in terms of a_ℓ: $r\,[\,j_\ell(kr) + ik\,a_\ell(k)\,h_\ell^{(1)}(kr)\,]$

$$j_\ell(kr) \to \frac{1}{2}\frac{1}{kr}\, i^{\ell+1}\left[(-1)^{\ell+1} e^{ikr} + e^{-ikr}\right] \qquad h_\ell^{(1)}(kr) \to \frac{1}{kr}(-i)^{\ell+1} e^{ikr}$$

$$\frac{C_+}{C_-} = \frac{\left[\frac{1}{2k}\, i^{\ell+1}(-1)^{\ell+1} + a_\ell\, i\,(-i)^{\ell+1}\right]}{\frac{1}{2k}\, i^{\ell+1}}$$

Multiply top and bottom by $2k / i^{\ell+1}$

$$\frac{C_+}{C_-} = (-1)^{\ell+1} + a_\ell(k)\, i(-1)^{\ell+1}\, 2k$$

Equate to $(*)$, giving:

5

$$e^{2i\delta_\ell(k)}\cancel{(-1)^{\ell+1}} = \cancel{(-1)^{\ell+1}}\left(1+2kia_\ell(k)\right)$$

$$\boxed{a_\ell(k) = \frac{e^{2i\delta_\ell(k)}-1}{2ki}}$$

$\delta_\ell(k)=0$ gives $a_\ell(k)=0$. No scattering.

e^- scattering off noble gases — historical

- as we go down periodic table, the effective potential becomes stronger, forming a RT minima near threshold:

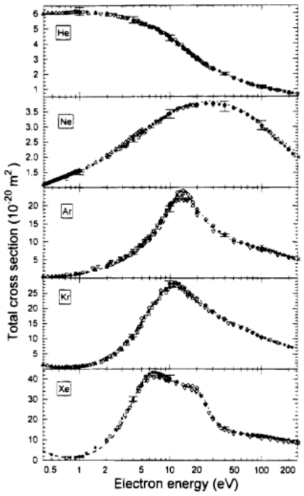


Fig. 1 from Szmytkowski *et al.*, `http://doi.org/fd55fj`

Kr at higher resolution:

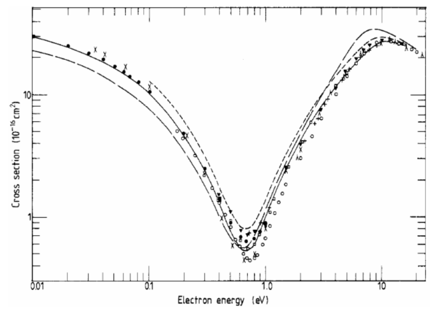
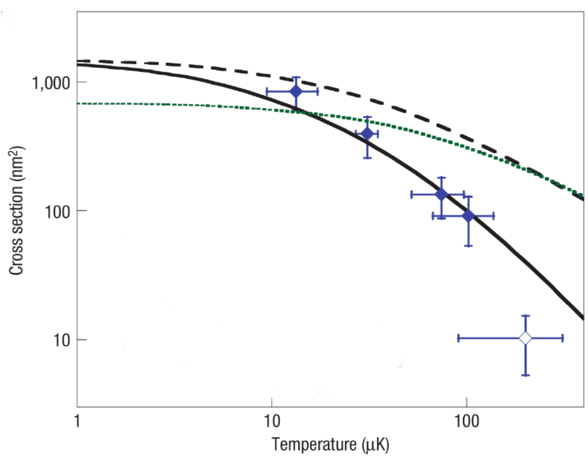


Fig. 4 from Bell *et al.*, `http://doi.org/fbj3wn`

"Sympathetic" cooling of one species by another relies on elastic scattering — modern

- some species can be directly cooled to lower temperatures than others.
- elastic scattering cross-section for ^{40}K, ^{87}Rb collisions:



RT minima

Fig. 4 from Aubin *et al.*, `http://doi.org/fsmgjd`

- sympathetic cooling ^{40}K using cold ^{87}Rb is hampered by low elastic cross-section due to RT minima.

The Ramsauer-Towsend minima has applications!

- notice the RT "dip" at 24 keV:

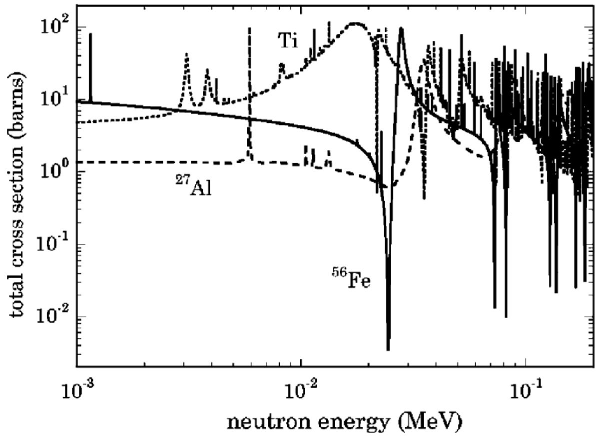


Fig. 1 from Barbeau *et al.*, `http://doi.org/b66cgh`

- by putting Al in series, transmission due to higher energy windows can be blocked.

Use to create a monoenergetic neutron source at 24 keV

- neutrons emerging from nuclear reactor cover a range of energies.
- using ^{56}Fe and ^{27}Al we can filter out all but a specific energy range:

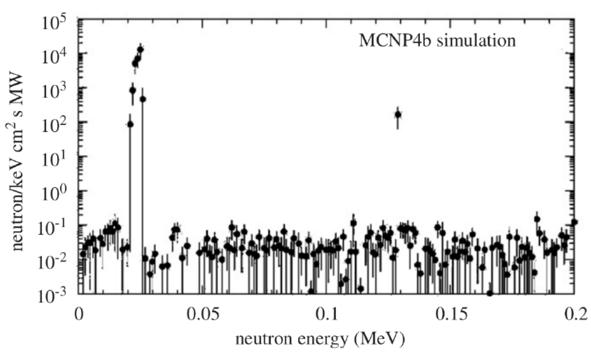


Fig. 3 from Barbeau *et al.*, `http://doi.org/b66cgh`

- this is a test source for detectors looking at elastic nuclear recoils (neutrino scattering etc...).

2.20 2023-11-21 Lecture

Lecture cancelled.

2.21 2023-11-23 Lecture

Born approximation material adapted from: D. J. Griffiths and D. F. Schroeter, *Introduction to quantum mechanics*, 3rd (Cambridge University Press, 2018).

①

Relationship between scattering length and the low-energy s-wave phase shift

- at zero energy, $k=0$, at large r, the wavefunction becomes a straight line: $u(r) = C(r-a)$ $\quad (*)$
  (a: scattering length.)

- at non-zero +ve energies, the wavefunction has the form at large-r:

$$u(r) = D \sin(kr + \delta_0(k)). \qquad (\pm)$$

As $k \to 0$, Eq. $(\pm)$ should be consistent with $(*)$.

Let's consider logarithmic derivatives: $u'(r)/u(r)$

(takes out normalization factors).

②

For $k=0$, $\dfrac{u'(r)}{u(r)} = \dfrac{1}{r-a}$

For $k>0$, $\dfrac{u'(r)}{u(r)} = \underbrace{\dfrac{k\cos(kr+\delta_0(k))}{\sin(kr+\delta_0(k))}}$

For consistency we require

$$\frac{1}{r-a} = \lim_{k\to 0} \frac{k\cos(kr+\delta_0(k))}{\sin(kr+\delta_0(k))}$$

If $\lim_{k\to 0} \delta_0(k) \neq 0$, then RHS will be zero, and it will be impossible to satisfy this equation.

3

Consider $\delta_0 = c_1 k + c_2 k^2 + \cdots\cdots$

Then

$$\frac{1}{r-a} = \lim_{k \to 0} \frac{k \cos(kr + c_1 k + c_2 k^2 + \cdots)}{\sin(kr + c_1 k + c_2 k^2 + \cdots)}$$

$\downarrow$ L'Hopital

$$\frac{\underbrace{\cos(\cdots)}_{=1} + \underbrace{k \sin(kr \cdots)}_{\to 0}}{\underbrace{\cos(\cdots)}_{=1}\,(r + c_1 + c_2 k \cdots)}$$

$$= \frac{1}{r + c_1}$$

$$\boxed{\delta_0(k) = -ak + O(k^2)}$$

scattering length

4

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2(\delta_l)$$

For $k \to 0$, s-wave $(l=0)$:

$$\sigma = \frac{4\pi}{k^2} (-ak)^2$$

$$\boxed{\sigma = 4\pi a^2}$$

(5)

Born approximation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

$$\leftarrow \frac{\hbar^2 k^2}{2m}$$

$$Q := \frac{2m}{\hbar^2} V\psi$$

$$-\nabla^2\psi + Q = k^2\psi$$

$$(\nabla^2 + k^2)\psi = Q \qquad (*)$$

If we "forget" that ψ is contained in Q, this the Helmholtz equation

(6)

The "standard approach" to these type of problems is that of Green's functions.

i.e. solve $(\nabla^2 + k^2)\, G(\vec{r}) = \underbrace{\delta^3(\vec{r})}_{\text{point source at origin}}$

and use superposition. i.e.

$$\psi(\vec{r}) = \int d^3\vec{r}_0 \; G(\vec{r}-\vec{r}_0)\, Q(\vec{r}_0)$$

2.22 2023-11-28 Lecture

Born approximation material adapted from: D. J. Griffiths and D. F. Schroeter, *Introduction to quantum mechanics*, 3rd (Cambridge University Press, 2018).

The proton scattering example [11] is shown in Sakurai and Napolitano [1].

1

Does this solution satisfy $\underbrace{(\nabla^2 + k^2)\psi}_{\text{LHS}} = \underbrace{Q}_{\text{RHS}}$?

$$\text{LHS} = (\nabla^2 + k^2) \int d^3\vec{r}_0 \; G(\vec{r} - \vec{r}_0)\, Q(\vec{r}_0)$$

$$= \int d^3\vec{r}_0 \; \delta^3(\vec{r} - \vec{r}_0)\, Q(\vec{r}_0)$$

$$= Q(\vec{r})$$

$$\left(\text{Reminder: } Q := \frac{2m}{\hbar^2} V\psi\right)$$

Same as RHS ✓

In this case, a suitable Greens function is:

$$G(\vec{r}) = \frac{-e^{ikr}}{4\pi r}$$

satisfies $(\nabla^2 + k^2) G(\vec{r}) = \delta^3(\vec{r})$

②

$$\psi(\vec{r}) = \left[\int d^3\vec{r}_0 \; G(\vec{r}-\vec{r}_0)\, Q(\vec{r}_0) \right] + \underbrace{\psi_0(\vec{r})}_{\substack{\text{satisfies} \\ \text{free particle} \\ \text{TISE.}}}$$

$$\psi(\vec{r}) = \psi_0(\vec{r}) - \frac{m}{2\pi\hbar^2} \int d^3\vec{r}_0 \; \frac{e^{ik|\vec{r}-\vec{r}_0|}}{|\vec{r}-\vec{r}_0|} V(\vec{r}_0)\, \psi(\vec{r}_0) \qquad (*)$$

This is an integral equation for $\psi(\vec{r})$.

Let's imagine there is a region outside of which $V(\vec{r}) = 0$. And we are far away from this region ($\simeq$ origin of our coordinate system), so $\frac{r}{r_0} \gg 1$

How does integral simplify?

③

$$\begin{aligned} |\vec{r}-\vec{r}_0|^2 &= r^2 + r_0^2 - 2\vec{r}\cdot\vec{r}_0 \\ &= r^2\left(1 + \frac{r_0^2}{r^2} - 2\hat{r}\cdot\frac{\vec{r}_0}{r}\right) \\ &\simeq r^2\left(1 - 2\hat{r}\cdot\frac{\vec{r}_0}{r}\right) \end{aligned}$$

Using $\sqrt{1+x} \simeq 1 + \frac{x}{2} + \cdots$

$$|\vec{r}-\vec{r}_0| \simeq r - \hat{r}\cdot\vec{r}_0$$

Define $\vec{k} = k\hat{r}$, so that:

$$\frac{e^{ik|\vec{r}-\vec{r}_0|}}{|\vec{r}-\vec{r}_0|} \simeq \frac{e^{ikr}\, e^{-i\vec{k}\cdot\vec{r}_0}}{r}$$

contributes to irrelevant order for scattering

④

For scattering we take $\psi_0(\vec{r}) = A e^{ikz}$, so that the integral equation (*) on pg 2 becomes:

$$\psi(\vec{r}) = \underbrace{A e^{ikz}} - \frac{m}{2\pi\hbar^2}\,\frac{e^{ikr}}{r}\int d^3\vec{r}_0\; e^{-i\vec{k}\cdot\vec{r}_0}\, V(\vec{r}_0)\,\psi(\vec{r}_0)$$

Compare to: $\psi(r,\theta) = A\left\{ e^{ikz} + f(\theta)\,\frac{e^{ikr}}{r} \right\}$

to determine that

$$f(\theta) = \frac{-m}{2\pi\hbar^2}\,\frac{1}{A}\int d^3\vec{r}_0\; e^{-i\vec{k}\cdot\vec{r}_0}\, V(\vec{r}_0)\,\psi(\vec{r}_0)$$

Remember (!), we still don't know

⑤

Now we make the first Born approximation. We assume that the wavefunction that appears in integrand can be taken as the free particle wavefunction: $\psi_0(\vec{r}_0) = A e^{ik'z_0}$

$$f(\theta) = -\frac{m}{2\pi\hbar^2}\int d^3\vec{r}_0\; V(\vec{r}_0)\, e^{i\vec{k}'\cdot\vec{r}_0 - i\vec{k}\cdot\vec{r}_0}$$

points in θ direction.

before scattering (points in $\hat{z}$ direction) $\vec{k}' = k\hat{z}$

Introduce $\vec{q} := \vec{k}' - \vec{k}$, so that

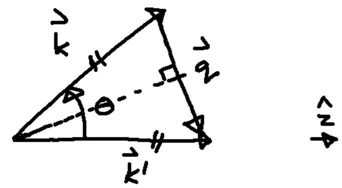
$$\boxed{f(\theta) = -\frac{m}{2\pi\hbar^2}\int d^3\vec{r}_0\; V(\vec{r}_0)\, e^{i\vec{q}\cdot\vec{r}_0}}$$

— implicit dependence on θ.

Shows scattering amplitude is related to Fourier transform of potential.

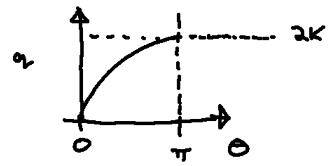
⑥

What is relationship between q and θ?



$$\frac{q}{2} = k \sin\left(\frac{\theta}{2}\right)$$

or $$q^2 = 4k^2 \sin^2(\theta/2)$$
$$q^2 = 2k^2(1-\cos\theta)$$



- now lets look at the spherically symmetric potential case. $\quad V(\vec{r}_0) = V(r_0)$

⑦

Introduce θ_0, as the angle between $\vec{q}$ and $\vec{r}_0$.

$$f(\theta) = -\frac{m}{2\pi\hbar^2} \int_0^{2\pi} d\phi_0 \int_0^{\pi} d\theta \sin\theta_0 \int_0^{\infty} dr_0\, r_0^2\, V(r_0)\, e^{iqr_0\cos\theta_0}$$

$$= -\frac{m}{\hbar^2} \int_0^{\infty} dr_0\, r_0^2\, V(r_0) \underbrace{\int_0^{\pi} d\theta_0 \sin\theta_0\, e^{iqr_0\cos\theta}}_{\frac{2\sin(qr_0)}{qr_0}}$$

$$\boxed{f(\theta) = -\frac{2m}{\hbar^2}\frac{1}{q}\int_0^{\infty} dr\, r\, V(r) \sin(qr)}$$

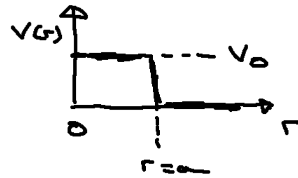
Sakurai Eq. 6.3.5

for a spherically symmetric potential.

8

Example: finite square well

$$V(r) = \begin{cases} V_0\,, & r \le a \\ 0\,, & r > a \end{cases}$$



$$f(\theta) = -\frac{2m}{\hbar^2}\frac{V_0 a^3}{(qa)^2}\left[\frac{\sin(qa)}{qa} - \cos(qa)\right]$$

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

Determining "Size" of Nucleus from proton scattering

What is k for 800 MeV protons? [L. Ray et al. PRC, v.23, pg 828 (1980).]

$$E = \frac{\hbar^2 k^2}{2m}$$

$$k = \frac{1}{\hbar}\sqrt{2mE}$$

$$= \frac{1}{1.054 * 10^{-34}} \frac{s}{kg \cdot m^2} \sqrt{2 * 1.673 * 10^{-27} kg * 800 * 1.6 * 10^{-13} kg \cdot \frac{m^2}{s^2}}$$

$$= 6.2 * 10^{15} m^{-1}$$

With first zero @ $7°$, in Fig 1 of Ray et al.

$$q = 2k \sin\left(\frac{\theta}{2}\right) \qquad (S6.3.4)$$

$$= 2 * 6.2 * 10^{15} m^{-1} \sin\left(7° * \frac{\pi}{180°} * \frac{1}{2}\right)$$

$$= 7.6 * 10^{14} m^{-1}$$

Using $qa = 4.49$

$$a = \frac{4.49}{7.6 * 10^{14} m^{-1}}$$

$$\simeq 5.9 * 10^{-15} m$$ "radius of nucleus"?

Compare to $R \simeq r_0 A^{1/3}$ with $r_0 = 1.25 * 10^{-15} m$ [Wikipedia, "Atomic Nucleus"]

For ^{48}Ca : $R \simeq 4.5 * 10^{-15} m$

Reasonable agreement.

2.23 2023-11-30 Lecture

Breit-Wigner formula treatment follows Sakurai and Napolitano.

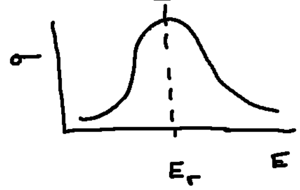
The idea of the H-Kr example is from J. M. Thijssen, *Computational physics*, 2nd ed (Cambridge University Press, Cambridge, UK ; New York, 2007).

1

Resonance scattering and the Breit-Wigner Formula

From $\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l$

we expect resonances



to correspond to $\delta_l \simeq \pi/2 \mod \pi$ at E_r, for a specific l.

Simplest model for how δ_l varies around E_r:

$$\cot \delta_l \approx -c(E - E_r) \qquad (\ddagger)$$

(2)

$$\cot \delta_\ell = \frac{\cos \delta_\ell}{\sin \delta_\ell}$$

rearrange to give:

$$\sin \delta_\ell = \frac{\cos \delta_\ell}{\cot \delta_\ell}$$

$$\sin^2 \delta_\ell = \frac{\cos^2 \delta_\ell}{\cot^2 \delta_\ell}$$

$$= \frac{1 - \sin^2 \delta_\ell}{\cot^2 \delta_\ell}$$

Solve for $\sin^2 \delta_\ell$

$$\sin^2 \delta_\ell \left(1 + \frac{1}{\cot^2 \delta_\ell} \right) = \frac{1}{\cot^2 \delta_\ell}$$

$$\sin^2 \delta_\ell = \frac{1}{\cot^2 \delta_\ell \left(1 + \frac{1}{\cot^2 \delta_\ell} \right)}$$

$$\sin^2 \delta_\ell = \frac{1}{\cot^2 \delta_\ell + 1}$$

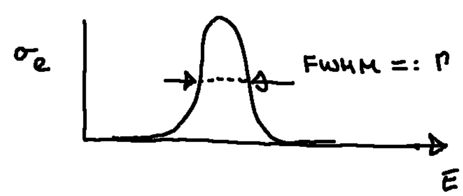
(3)

Define $\sigma_\ell := \frac{4\pi}{k^2} (2\ell+1) \sin^2 \delta_\ell$

so that $\sigma = \sum \sigma_\ell$.

Using (*) :

$$\sigma_\ell \approx \frac{4\pi}{k^2} \frac{(2\ell+1)}{\left(c\,(E-E_r)\right)^2 + 1}$$



What is relationship between Γ and c?

(4)

$$\frac{2\ell+1}{2} = \frac{2\ell+1}{\left(c\,\frac{\Gamma}{2}\right)^2 + 1}$$

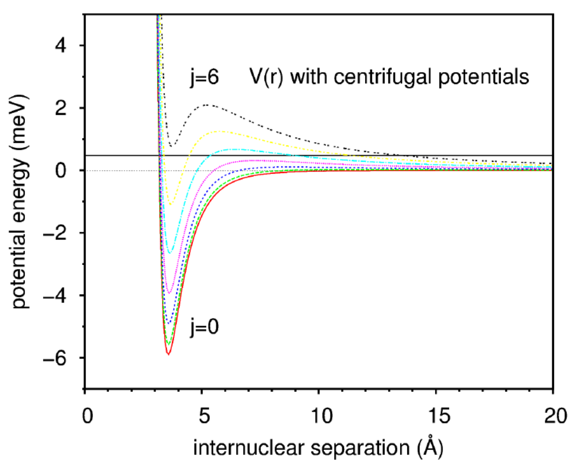
gives $c = \frac{2}{\Gamma}$

$$\boxed{\sigma_\ell = \frac{4\pi}{k^2}\left[\frac{(2\ell+1)}{\left[\frac{2}{\Gamma}(E-E_r)\right]^2+1}\right]}$$

Breit-Wigner Formula

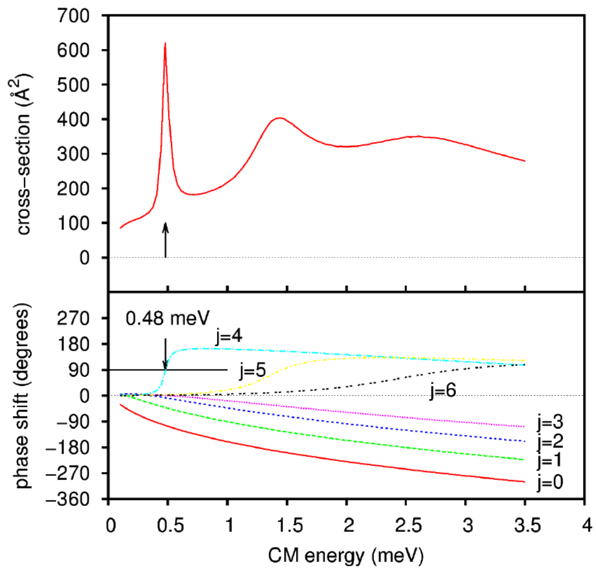
Lennard-Jones potential for H-Kr interaction

$$V(r) = \epsilon\left[\left(\frac{r_m}{r}\right)^{12} - 2\left(\frac{r_m}{r}\right)^{6}\right] \qquad \begin{aligned}\epsilon &= 5.9\,\mathrm{meV}\\ r_m &= 3.57\,\text{Å}\end{aligned}$$

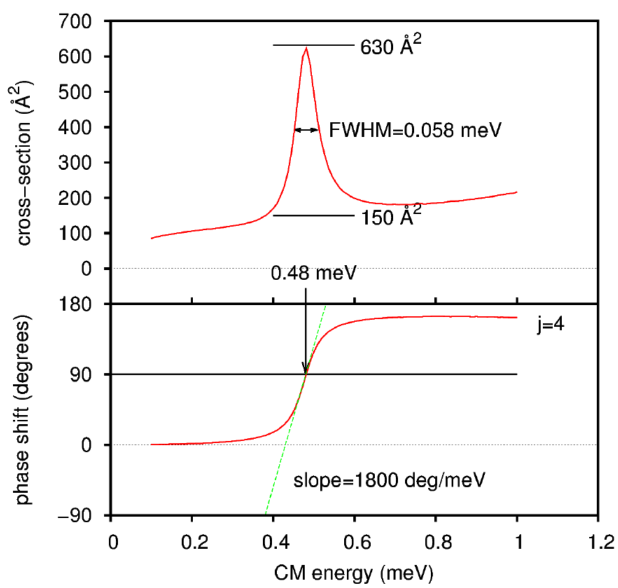


Calculations based on example in Thijssen, *Computational Physics*

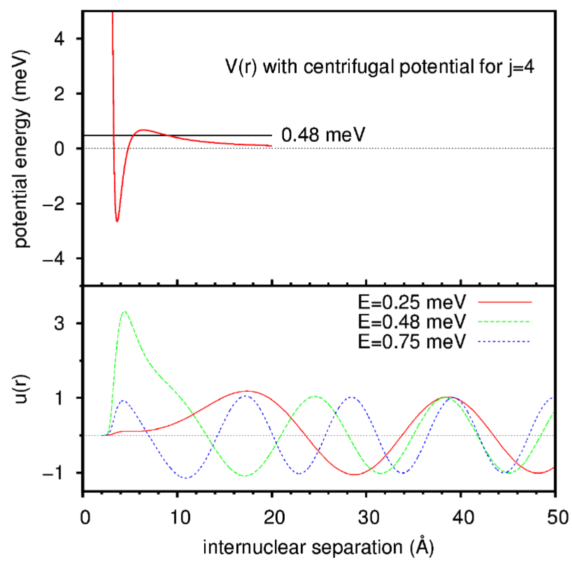
H-Kr elastic scattering cross-section



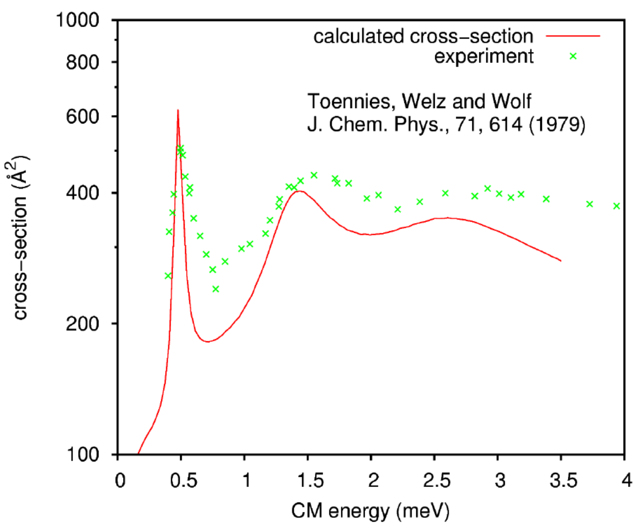
A closer look at first resonance



H-Kr quasi-bound states



H-Kr scattering; comparison between experiment and theory



experimental cross-sections have been rescaled for comparison.

2.24 2023-12-05 Lecture

In this lecture I go through some formulae in Cooley's paper [13] for numerically solving the Schrödinger equation in one-dimension. I should have done this at the start of the course.

I change the notation from his paper so as to be more consistent with the notation used in this course.

Cooley [13] discusses two approaches:

(1) determining the wavefunction $u(r)$ directly (which he calls $P(r)$), and

(2) determining

$$Y(r) = [1 - \frac{h^2}{12}(V(r) - E)]u(r) \tag{1}$$

using the Numerov method (see Eq. 2.7 of Cooley).

The second approach, working with $Y(r)$, or more precisely, its discretization, Y_i, is expected to be more accurate than the first approach using u_i (for the same r_i grid). But since the first approach is a bit simpler, I go through it in this lecture, despite the fact the formulae for the second approach are what should be used in practice; i.e., as described in Cashion [14]. However, the derivations for the relevant formulae for both approaches are quite similar; so if you understand the derivations here, you will also understand the more accurate but slightly more complicated determination of Y_i.

1

Deriving the formulae 1-d used in Cooley for solving the Schrödinger equation numerically

$u''(r) = (V(r) - E)\,u(r)$ (SDE) $\left(\frac{\hbar^2}{2m} = 1 \text{ unit system}\right)$

BC's $u(0) = 0$, $u(r)$ is bounded.

step size.

Discretize: $r_i = ih$, $i = 0, 1, \ldots, n+1$

$u_i = u(r_i)$

$V_i = V(r_i)$

② $$u_{i+1} + u_{i-1} = \sum_{k=0}^{\infty} \frac{2h^{2k}}{(2k)!} u_i^{(2k)}$$

the $2k^{th}$ derivative

use Taylor series expansion about u_i

Keep only $k=0$ and $k=1$ terms to get:

$$u_{i+1} + u_{i-1} = 2u_i + \frac{2h^2}{2!} u_i''$$

replace using SDE

$$u_{i+1} + u_{i-1} - 2u_i = h^2 (V(r) - E) u_i$$

If we have u_{i-1} and u_i we can get u_{i+1}. i.e. outwards integration.

③ With $u_0 = u_{n+1} = 0$ we have a system of simultaneous linear equations that the u_i ($i=1$ to n) must satisfy.

$$(2/h^2 + V_1 - E) u_1 - \frac{1}{h^2} u_2 = 0$$

$$-h^2 u_{i-1} + (2/h^2 + V_i - E) u_i - \frac{1}{h^2} u_{i+1} = 0 \quad \Big\} \text{ n-2 of these.}$$

$$-h^2 u_{n-1} + (2/h^2 + V_n - E) u_n = 0$$

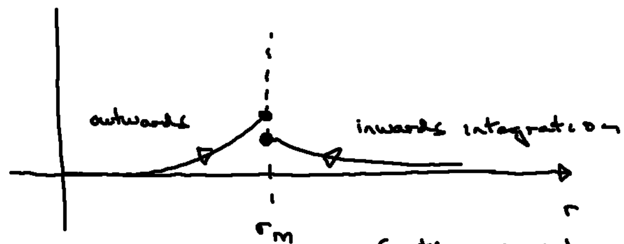
Condense into a matrix eqn:

(*) $$\underset{n \times n}{M} \vec{u} = \vec{0}$$

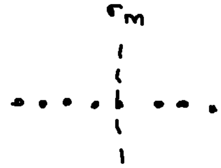
$\vec{0}$: n×1 column vector $\begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}$

$\vec{u}$: n×1 column vector $\begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix}$

(4)



Continuous picture: $u_i'(r_m) \neq u_o'(r_m)$



discrete: update formula not consistent with $\underbrace{u_{m-1} , u_m , u_{m+1}}$

Set $u_m = 1$ (rescaling). Partition (*) :

Put mismatched eqn on first row.

$$\underset{1\times 1 \text{ matrix}}{} \begin{pmatrix} M_{11} & \overset{1\times(n-1)}{M_{a1}^{+}} \\ \underset{(n-1)\times 1}{M_{a1}} & \underset{(n-1)\times(n-1)}{M_{aa}} \end{pmatrix} \begin{pmatrix} 1 \\ \vec{u}_a \end{pmatrix} = \begin{pmatrix} F(E) \\ 0 \end{pmatrix}$$

Win this game by making $F(E)=0$

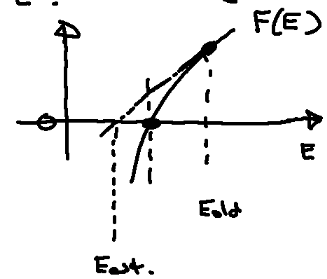
(5)

$$M_{11} + M_{1a}^{+} \vec{u}_a = F(E) \qquad *$$

$$M_{a1} + M_{aa} \vec{u}_a = \vec{0} \qquad (‡)$$

Differentiate wrt E. (denote by ' s)

[Why?



Newton's method:

$$E_{estimated} = E_{old} - \frac{F(E)}{\underbrace{F'(E)}}$$

$$M_{11}' + M_{a1}^{+\prime} \vec{u}_a + M_{a1}^{+} \vec{u}_a' = F'(E) \qquad (*)$$

$$(n-1)\times 1 \rightarrow M_{a1}' + M_{aa}' \vec{u}_a + M_{aa} \vec{u}_a' = \vec{0}$$

$\leftarrow$ multiply from left by $\vec{u}_a^{+}$

(6)

$$\vec{u}_a^{+} M_{a1}' + \vec{u}_a^{+} M_{aa}' \vec{u}_a + \vec{u}_a^{+} M_{aa} \vec{u}_a' = 0$$

add to (*) to give :

$$M_{11}' + M_{a1}^{+\prime} \vec{u}_a + \cancel{M_{a1}^{+} \vec{u}_a'} + \vec{u}_a^{+} M_{a1}' + \vec{u}_a^{+} M_{aa}' \vec{u}_a + \cancel{\vec{u}_a^{+} M_{aa} \vec{u}_a'}$$

$$= F'(E)$$

Based on (*) cancel

$$(M_{a1} + M_{aa} \vec{u}_a = \vec{0})$$

$$\vec{u}_a^{+\prime} M_{a1} + \vec{u}_a^{+\prime} M_{aa} \vec{u}_a = \vec{0}$$

$$M_{a1}^{+} \vec{u}_a' + \vec{u}_a^{+} M_{aa}^{+} \vec{u}_a' = \vec{0}^{t}$$

M_{aa} is $= M_{aa}^{+}$.

Conclude $\quad F'(E) = \vec{u}^{+} M' \vec{u}$

$$D(E) := E_{new} - E_{old} \quad ; \quad E_{new} = E_{old} + D(E)$$

(7)

by Newton's method

$$D(E) = - \frac{F(E)}{F'(E)}$$

$$\boxed{D(E) = [\,(-u_{m-1} + 2u_m - u_{m+1})/h^2 + (V_m - E)\, u_m]\,) \,/\, \sum u_i^2}$$

3 Supplemental notes

3.1 Magnetic fields in classical mechanics

Reference: R. Shankar, *Principles of quantum mechanics*, 2nd ed (Plenum Press, New York, 1994).

- Maxwell's field equations (rationalized MKSA):

$$\nabla \cdot \mathbf{E} = \rho/\epsilon_0 \tag{2}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{3}$$

$$\nabla \cdot \mathbf{B} = 0 \tag{4}$$

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \epsilon_0 \mu_0 \frac{\partial \mathbf{E}}{\partial t} \tag{5}$$

- in quantum mechanics we introduce electromagnetic fields using *potentials* rather than fields.
- the introduction of potentials allows 2 of Maxwell's equations to automatically be satisfied. i.e. writing

$$\mathbf{B} = \nabla \times \mathbf{A} \tag{6}$$

  automatically satisfies

$$\nabla \cdot \mathbf{B} = 0 \tag{7}$$

  Likewise:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{8}$$

$$= -\frac{\partial}{\partial t} \nabla \times \mathbf{A} \tag{9}$$

$$\nabla \times \left(\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} \right) = \mathbf{0}. \tag{10}$$

  If we introduce a scalar potential ϕ, such that

$$\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} = -\nabla \phi \tag{11}$$

  then Eq. 10 is automatically satisfied.

- our plan will be to write out a classical Lagrangian that reproduces the Lorentz force law, then get classical Hamiltonian using normal recipe. We will then consider the quantities in this expression to be quantum mechanical operators (i.e. replace c#'s by q#'s).
- let's show that the Lagrangian

$$\mathcal{L} = \frac{1}{2} m \, \mathbf{v} \cdot \mathbf{v} - e \, \phi + e \, \mathbf{v} \cdot \mathbf{A} \tag{12}$$

  reproduces the Lorentz force law for a particle of charge e.

- there are 3 Euler-Lagrange equations (see earlier review of Lagrangian and Hamiltonian dynamics):

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_i}\right) = \frac{\partial \mathcal{L}}{\partial q_i} \tag{13}$$

for each of the 3 dimensions (i corresponding to x, y, and z).

- substitution of our $\mathcal{L}$ into the Euler-Lagrange equations gives:

$$\frac{d}{dt}(m\dot{x}_i + eA_i) = -e\frac{\partial \phi}{\partial x_i} + e\frac{\partial(\mathbf{v}\cdot\mathbf{A})}{\partial x_i} \tag{14}$$

- all 3 equations can be written together using vector notation:

$$\frac{d}{dt}(m\mathbf{v} + e\mathbf{A}) = -e\nabla\phi + e\nabla(\mathbf{v}\cdot\mathbf{A}) \tag{15}$$

- rearranging gives:

$$\frac{m}{e}\frac{d\mathbf{v}}{dt} = -\nabla\phi - \frac{d\mathbf{A}}{dt} + \nabla(\mathbf{v}\cdot\mathbf{A}) \tag{16}$$

- the evaluation of the derivative A is a *total* derivative i.e. evaluated along the path of the particle. We can replace this, using the chain rule of differentiation:

$$\frac{d\mathbf{A}}{dt} = \frac{\partial \mathbf{A}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{A} \tag{17}$$

- substitution into Eq. 16 gives:

$$\frac{m}{e}\frac{d\mathbf{v}}{dt} = -\nabla\phi - \frac{\partial\mathbf{A}}{\partial t} - (\mathbf{v}\cdot\nabla)\mathbf{A} + \nabla(\mathbf{v}\cdot\mathbf{A}) \tag{18}$$

- the last two terms can be simplified with the identity, for a constant vector $\mathbf{c}$ and the arbitrary vector field $\mathbf{y}$:

$$\mathbf{c}\times(\nabla\times\mathbf{y}) = \nabla\cdot(\mathbf{c}\cdot\mathbf{y}) - (\mathbf{c}\cdot\boldsymbol{\nabla})\mathbf{y} \tag{19}$$

with $\mathbf{c}=\mathbf{v}$ and $\mathbf{y}=\mathbf{A}$. Usage in Eq. 18 gives:

$$\frac{m}{e}\frac{d\mathbf{v}}{dt} = -\nabla\phi - \frac{\partial\mathbf{A}}{\partial t} + \mathbf{v}\times(\nabla\times\mathbf{A}) \tag{20}$$

- recognizing the expressions for $\mathbf{E}$ and $\mathbf{B}$ in this expression (i.e. Eq.'s 11 and 6), allows us to write:

$$m\frac{d\mathbf{v}}{dt} = e\left(\mathbf{E} + \mathbf{v}\times\mathbf{B}\right), \tag{21}$$

which is the Lorentz force law.

- knowing that the Lagrangian of Eq. 12 reproduces the Lorentz force law, we are now free to use it to define canonical momenta and the corresponding Hamiltonian (the conventional recipe of classical mechanics).

- The definition of canonical momenta is:

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \tag{22}$$

which for our $\mathcal{L}$ (Eq. 12) gives:

$$p_i = mv_i + e\,A_i. \tag{23}$$

- by definition, the Hamiltonian is:

$$H = \sum_i \dot{q}_i p_i - \mathcal{L} \tag{24}$$

which in this case is (rearranging Eq. 23 to substitute for v_i):

$$\begin{aligned} H &= \frac{(\mathbf{p} - e\mathbf{A})}{m} \cdot \mathbf{p} - \frac{1}{2} m \frac{(\mathbf{p} - e\mathbf{A})^2}{m^2} + e\phi - e\frac{(\mathbf{p} - e\mathbf{A})}{m} \cdot \mathbf{A} \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (25) \\ &= \frac{p^2}{m} - \frac{e}{m}\mathbf{A} \cdot \mathbf{p} - \frac{1}{2}\frac{p^2}{m} - \frac{e^2 A^2}{2m} + \frac{e}{m}\mathbf{p} \cdot \mathbf{A} + e\phi - \frac{e}{m}\mathbf{p} \cdot \mathbf{A} + \frac{e^2 A^2}{m} \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (26) \\ &= \frac{p^2}{2m} + \frac{1}{2}\frac{e^2 A^2}{m} - \frac{e}{m}\mathbf{p} \cdot \mathbf{A} + e\phi \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (27) \\ H &= \frac{1}{2m}(\mathbf{p} - e\mathbf{A})^2 + e\phi \qquad\qquad\qquad\qquad\qquad\qquad\qquad (28) \end{aligned}$$

— an important result!

- in quantum mechanics we consider $\mathbf{p}$ as an operator and use $\mathbf{p}$ with $-i\hbar\nabla$ in position space, which ensures that the canonical commutation relationship is preserved. Note that we can no longer consider $\mathbf{p} = m\mathbf{v}$ in the presence of a vector potential.
- ultimately the validity of this form of the Hamiltonian must be confirmed by experiment (e.g. Aharanov-Bohm effect — to be discussed)

3.2 The path integral approach to the Aharonov-Bohm effect

Reference: Section 2.7 of J. J. Sakurai and J. Napolitano, *Modern quantum mechanics*, 2nd ed (Addison-Wesley, Boston, 2011).

- there have been no "clean" observations of the bound-state Aharonov-Bohm effect (AB) (e.g. spectroscopic experiments resolving the $\pm n$ splitting of the "ring-around-a-solenoid" example of the previous section)
- however the AB effect *has* been clearly observed in double-slit type interference experiments.[1]

[1]For a high-level review of the AB effect see H. Batelaan and A. Tonomura, "The Aharonov–Bohm effects: Variations on a subtle theme", Physics Today **62**, 38–43 (2009) .

- analysis of the double slit interference AB experiments is a bit awkward in the conventional formulation of quantum mechanics (which was entirely adequate for the "ring-around-a-solenoid" example).

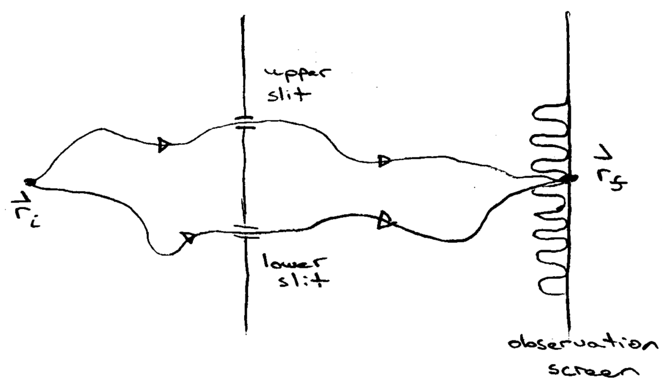
- instead, Feynman's path integral approach to quantum mechanics gives a concise explanation of the AB effect in double slit experiments.[2]

- path integrals provide an expression for the **propagator**, which tells us the probability *amplitude* that a particle at location $\mathbf{r}_i$ at time t_i will be found at $\mathbf{r}_f$ at time t_f:

$$\langle \mathbf{r}_f | U(t_f, t_i) | \mathbf{r}_i \rangle = \int_{\mathbf{r_i},\, t_i}^{\mathbf{r_f},\, t_f} \mathcal{D}[\mathbf{r}(t)] \; \exp\left(i \frac{S[\mathbf{r}(t)]}{\hbar} \right). \tag{29}$$

  Here the integration is "over different trajectories" i.e. varying $\mathbf{r}(t)$. The quantity $S[\mathbf{r}(t)]$ is the classical action for each of these trajectories, computed while leaving the initial and final conditions ($\mathbf{r}_i$, t_i and $\mathbf{r}_f$, t_f) fixed. In general this infinite-dimensional integral is not straightforward to evaluate. Luckily, we shall avoid direct evaluation in what follows — instead using the path integral to compare the contributions of different trajectories to the propagator.

- consider the infamous double slit experiment, performed with electrons:



- the interference pattern observed on the screen is determined by the propagator from the source to screen. It is reasonable to assume that trajectories for which the electron travels through the slits multiple times do not contribute much to the propagator to the screen and thus can be ignored. With this approximation the path integral (Eq. 29) can be split into two parts, corresponding to whether the trajectory passes through the upper or lower slit:

$$\langle \mathbf{r}_f | U(t_f, t_i) | \mathbf{r}_i \rangle = \underbrace{\int_{\mathbf{r_i},\, t_i}^{\mathbf{r_f},\, t_f} \mathcal{D}[\mathbf{r}_{\text{upper}}(t)] \; \exp\left(i \frac{S[\mathbf{r}_{\text{upper}}(t)]}{\hbar} \right)}_{\equiv A_{\text{upper}}} . + \underbrace{\int_{\mathbf{r_i},\, t_i}^{\mathbf{r_f},\, t_f} \mathcal{D}[\mathbf{r}_{\text{lower}}(t)] \; \exp\left(i \frac{S[\mathbf{r}_{\text{lower}}(t)]}{\hbar} \right)}_{\equiv A_{\text{lower}}} . \tag{30}$$

[2] The path integral approach to the AB effect seems (to me) to be an exception to the general rule that little is to be gained from the path integral approach in single particle quantum mechanics. The primary reason to study the path integral approach to single particles seems to be in preparation for the generalization to quantum field theory and statistical physics where path integrals are useful.

- for complete *destructive* interference between the top and bottom paths, we require:

$$\frac{A_{\text{upper}}}{A_{\text{lower}}} = \exp\left(i(\pi + 2\pi n)\right), \text{ where } n = -\infty, \ldots -1, 0, 1, 2 \ldots \infty. \tag{31}$$

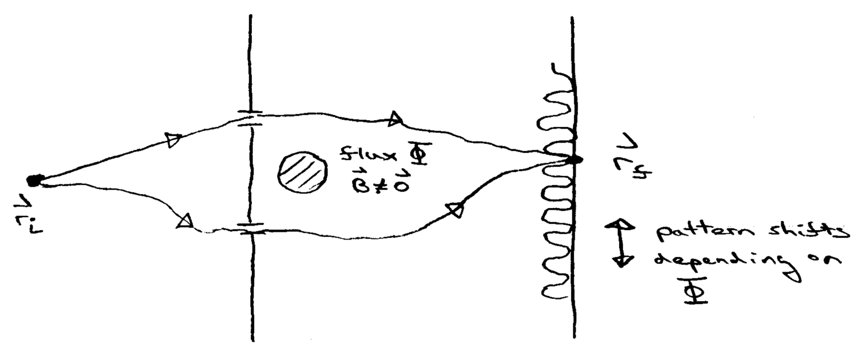
  Likewise, for complete *constructive* interference between the top and bottom paths, we require:

$$\frac{A_{\text{upper}}}{A_{\text{lower}}} = \exp\left(i2\pi n\right), \text{ where } n = -\infty, \ldots -1, 0, 1, 2 \ldots \infty. \tag{32}$$

  Let us assume that the magnitude of $A_{\text{upper}}/A_{\text{lower}}$ is always one, and define the phase difference between the amplitudes as $\Delta\phi_{\text{upper,lower}} \equiv \phi_{\text{upper}} - \phi_{\text{lower}}$, so that

$$\frac{A_{\text{upper}}}{A_{\text{lower}}} = \exp(i\Delta\phi_{\text{upper,lower}}). \tag{33}$$

- consider a source of magnetic flux placed in between the two paths. In principle this can be done in such a way that none of the trajectories to the screen contributing to either A_{upper} or A_{lower} pass through this flux region:



- now we will consider how the phase difference between upper and lower slit paths changes due to the enclosed flux. Quantities corresponding to non-zero flux will be given a "prime", i.e. $\phi'_{\text{upper,lower}}$. Remember that the action S that appears in the path integral propagator (Eq. 29) is the time integral of the Lagrangian, which now contains a non-zero vector potential $\mathbf{A}$:

$$\mathcal{L} = \frac{1}{2}m\,\mathbf{v}\cdot\mathbf{v} - e\,\varphi + e\,\mathbf{v}\cdot\mathbf{A}. \tag{34}$$

  Recall from the "ring-around-a-solenoid" example that the vector potential can be non-zero even in regions of zero magnetic field.

- all paths now contain additional phases due to the vector potential. For a given trajectory $x(t)$ the change in the action gives a change in phase $S[x(t)]/\hbar$:

$$\theta' - \theta = \frac{1}{\hbar}\int_{\mathbf{r_i},\,t_i}^{\mathbf{r_f},\,t_f} e\,\mathbf{v}\cdot\mathbf{A}\,dt. \tag{35}$$

The appearance of velocity $\mathbf{v} = d\mathbf{r}/dt$ allows us to change the variable of integration from time to an integral over space, assuming $\mathbf{A}$ is time-independent:

$$\theta' - \theta = \frac{1}{\hbar}\int_{\mathbf{r_i}}^{\mathbf{r_f}} e\,\mathbf{A}\cdot d\mathbf{r}. \tag{36}$$

Therefore, for any pair of trajectories, one passing through the upper slit and one passing through the lower slit, the change in the difference of the phase of their trajectories is now:

$$\begin{aligned}
(\theta'_{\text{upper}} - \theta_{\text{upper}}) - (\theta'_{\text{lower}} - \theta_{\text{lower}}) &= \frac{e}{\hbar}\Bigg(\underbrace{\int_{\mathbf{r_i}}^{\mathbf{r_f}} \mathbf{A}\cdot d\mathbf{r}}_{\text{upper}} - \underbrace{\int_{\mathbf{r_i}}^{\mathbf{r_f}} \mathbf{A}\cdot d\mathbf{r}}_{\text{lower}}\Bigg) & (37)\\
&= \frac{e}{\hbar}\Bigg(\underbrace{\int_{\mathbf{r_i}}^{\mathbf{r_f}} \mathbf{A}\cdot d\mathbf{r}}_{\text{upper}} + \underbrace{\int_{\mathbf{r_f}}^{\mathbf{r_i}} \mathbf{A}\cdot d\mathbf{r}}_{\text{lower}}\Bigg) & (38)\\
&= \frac{e}{\hbar}\underbrace{\oint \mathbf{A}\cdot d\mathbf{r}}_{\text{around flux region}}. & (39)
\end{aligned}$$

The change in the difference between the phase of upper and lower trajectories has been converted to a *closed* loop line integral of $\mathbf{A}$.

- a closed loop line integral suggests the use of Stoke's theorem. For all vector fields $\mathbf{w}$:

$$\oint \mathbf{w}\cdot d\mathbf{r} = \int_S (\boldsymbol{\nabla}\times\mathbf{w})\cdot d\mathbf{a}, \tag{40}$$

and thus since $\mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A}$, Eq. 39 can be rewritten using Stokes theorem as:

$$(\theta'_{\text{upper}} - \theta_{\text{upper}}) - (\theta'_{\text{lower}} - \theta_{\text{lower}}) = \frac{e}{\hbar}\int_S \mathbf{B}\cdot d\mathbf{a}. \tag{41}$$

The surface integral that appears here is the total enclosed magnetic flux Φ between the upper and lower trajectories. This phase difference induced by the flux is identical for any pair of trajectories that enclose the flux. For this reason, we conclude that in the presence of the flux, Eq. 33 will be modified to:

$$\frac{A'_{\text{upper}}}{A'_{\text{lower}}} = \exp\left\{i\,\left(\Delta\phi_{\text{upper,lower}} + \frac{e}{\hbar}\Phi\right)\right\}. \tag{42}$$

Or equivalently:

$$\Delta\phi'_{\text{upper,lower}} = \Delta\phi_{\text{upper,lower}} + \frac{e}{\hbar}\Phi. \tag{43}$$

By tuning the enclosed flux Φ, we can readily shift the interference pattern on the screen. For example, $\Phi = \pi\hbar/e$ reverses the locations of constructive and destructive interference.

- the first experimental demonstration of the AB effect is due to Chambers. In his experiment a tapered magnetic whisker caused the enclosed flux for the interfering trajectories to vary as one moved along the length of the whisker (into/out of the page in the schematic diagrams that we have been using). One can clearly observe the interference pattern "moving" as the enclosed flux varied:

Experimental observation by Chambers

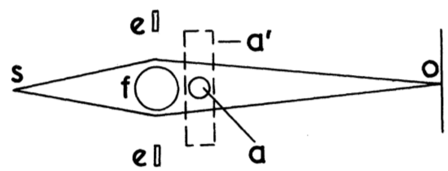
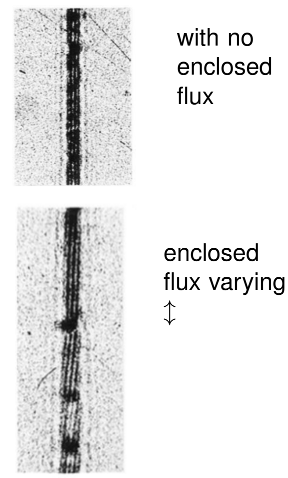


FIG. 1. Schematic diagram of interferometer, with source s, observing plane o, biprism e, f, and confined and extended field regions a and a'.



from Chambers, Phys. Rev. Lett., 5, 3 (1960)

- Chambers' experiment is not as clean a demonstration of the AB effect as we might wish, since the magnetic field is still non-zero along the electron trajectories. This criticism was addressed by a series of experiments performed by Tonomura and co-workers, which used superconductors to enclose the magnetic flux so that the magnetic field is zero along the interfering trajectories:

With magnetic field confined using superconductor

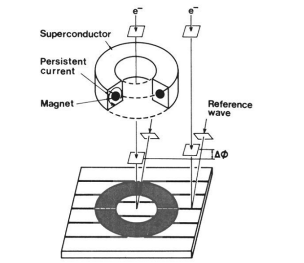
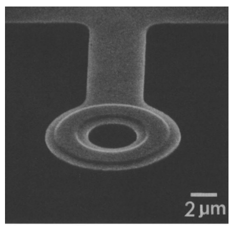


FIG. 1. Conceptual diagram of the experiment. A Cu layer for shielding from an electron wave is not shown.



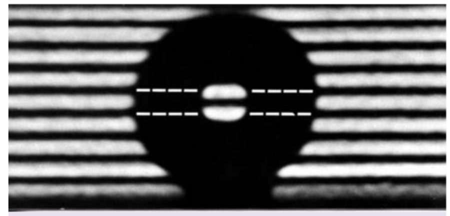


Figure 3. Electron interference pattern demonstrating the magnetic Aharonov–Bohm effect in an experiment that strictly excludes all stray fields.[4] A coherent electron beam traveling normal to the page is made to pass around a toroidal magnet (seen as a shadow) or through its 4-µm-diameter hole. The magnet's superconducting cladding prevents all stray fields. Having threaded or passed around the magnet, the beam is made to interfere with a reference plane wave. The resulting pattern, with the interference fringe inside the hole offset by half a cycle from those outside whenever the magnet flux is an odd multiple of $h/2e$, indicates an AB phase shift of π (modulo 2π) between the threading and bypassing electrons.

from Osakabe *et al.* , *Phys. Rev. A, 34, 815 (1986)*, and Batelaan and Tonomura, *Physics Today, Sept. 2009*

- it is an interesting quirk of superconductivity that the magnetic flux enclosed by a superconductor can only be integer multiples of $\hbar/(2e)$, where e is the elementary charge. The factor of two arises from the Cooper pairing of electrons. Comparison of this "flux quantization" condition with Eq. 43 is why in the experiments of Tonomura and co-workers the phase difference due to enclosed flux can only be varied by integer multiples of π i.e. the electron interference pattern shown above corresponds to a phase difference of π.
- although the Aharonov-Bohm effect is quite surprising, there is a wonderful picture which provides some physical insight:

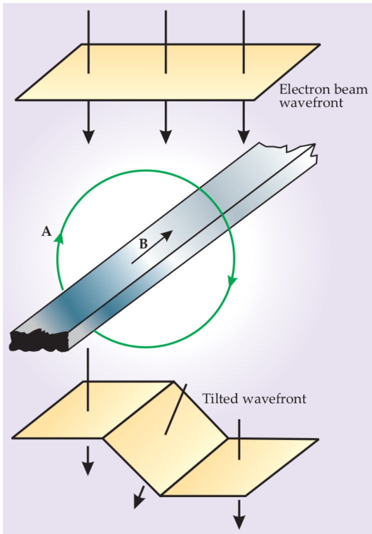


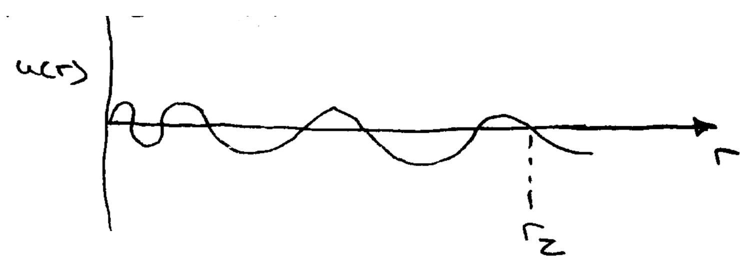
Figure 2. Semiclassical argument for the magnetic Aharonov–Bohm effect. Consider the plane wavefront of a coherent electron beam passing through and around a uniformly magnetized bar. Electrons going through the bar are deflected by the Lorentz force, tilting their sector of the wavefront. Electrons passing outside the bar see no magnetic field, so their sectors remain untilted. But because continuity requires the three sectors of the constant-phase front to remain contiguous, the two untilted sectors are now displaced along the beam direction, which implies a corresponding phase shift across a cross section of the beam. The phase shift thus calculated in terms of the Lorentz force is the same as that predicted by the AB effect in terms of the vector potential **A** circling the bar.

from Batelaan and Tonomura, Physics Today, Sept. 2009

3.3 Determining scattering phase shifts from wavefunctions

- scattering phase shifts $\delta_\ell(k)$'s are determined by comparing the $u(r)$ wavefunctions at large r to:
$$u(r) \propto \sin\left(kr + \delta_\ell(k) - \frac{\ell\pi}{2}\right) \tag{44}$$
In many cases the $u(r)$ wavefunctions will be obtained from numerical integration of the Schrödinger equation.

- an easy way to make the comparison is by looking for a "zero-crossing" (node) of $u(r)$ at the largest r possible:



Note that r_z is a function of k.

- Equation 44 tells us that zero-crossings will appear when
$$kr + \delta_\ell(k) - \frac{\ell\pi}{2} = n\pi \tag{45}$$

where n is any integer. Substituting r_z and rearranging gives:

$$\delta_\ell(k) = -kr_z + \frac{\ell\pi}{2} + n\pi \tag{46}$$

Note that $\delta_\ell(k)$ is only determined "modulo π". i.e. we can add or subtract any integer multiple of π to δ_ℓ and still obtain the same $f(\theta)$, and thus $d\sigma/d\Omega$ and σ.

- however, from a practical point of view it is nice to adopt a "phase" convention that resolves this ambiguity in the δ_ℓ's. Two possible (and easy to apply) conventions are:

$$0 \leq \delta_\ell < \pi \tag{47}$$

and

$$-\frac{\pi}{2} < \delta_\ell \leq \frac{\pi}{2}. \tag{48}$$

In both of these cases δ_ℓ can show "jumps" if it is plotted as a function of k (or energy). For this reason it is sometimes desirable to adopt the convention that δ_ℓ varies *continuously* with k. In this case, we use the integer multiple of π flexibility to set δ_ℓ such that:

$$\lim_{k\to 0} \delta_\ell(k) = 0 \tag{49}$$

or alternately:

$$\lim_{k\to \infty} \delta_\ell(k) = 0. \tag{50}$$

The second convention is particularly nice when considered in the context of **Levinson's theorem**:

> The number of bound states (of a given orbital angular momentum ℓ) that a potential supports is given by
>
> $$N_\ell = \frac{1}{\pi}(\delta_\ell(0) - \delta_\ell(\infty)). \tag{51}$$

(Weinberg[3] gives a "physicist's proof" and Taylor[4] gives a more complete proof of Levinson's theorem. The theorem does not hold if there is a bound state right at "threshold", $k = 0$ — but this is a pathological case of almost no practical importance.[5]) Obviously for Levinson's theorem to make sense, we must be considering δ_ℓ to be varying continuously as we vary k from 0 to ∞.

If we adopt the convention that $\lim_{k\to\infty} \delta_\ell(k) = 0$, then the phase shift at zero energy tells us the number of bound states that a potential supports:

$$N_\ell = \frac{\delta_\ell(0)}{\pi}. \tag{52}$$

That is neat!

[3] S. Weinberg, *Lectures on quantum mechanics*, Second edition (Cambridge University Press, Cambridge, United Kingdom ; New York, NY, 2015).

[4] J. R. Taylor, *Scattering theory: the quantum theory on nonrelativistic collisions* (Wiley, New York, 1972).

[5] Since Levinson's theorem is specific to the *non-relativistic* Schrödinger equation, it is essential that the potential be sufficiently weak, for $\delta_\ell(k)$'s to go to zero at high k, before relativistic corrections become important. See Ref. [18].

4 Notes on sources

4.1 General references

There are many interesting textbooks on quantum mechanics. The challenge is to make a list of reasonably small length. Here are some books, listed either because they are good and widely available, or something about them appeals to me.

(1) J. J. Sakurai and J. Napolitano, *Modern Quantum Mechanics*, 3rd (Cambridge University Press, Cambridge, 2021) A "default" standard. Some material is excellent (angular momentum chapter).

(2) D. J. Griffiths and D. F. Schroeter, *Introduction to quantum mechanics*, 3rd (Cambridge University Press, 2018) Good for basic scattering material.

(3) R. Shankar, *Principles of quantum mechanics*, 2nd ed (Plenum Press, New York, 1994) Errata can be found at: http://www.erratapage.com/pages/Shankar.pdf Good for all of the basics. You can download a copy from UW's library.

(4) M. Le Bellac, *Quantum physics* (Cambridge University Press, Cambridge, UK ; New York, 2006) This book has well-thought out problems.

(5) S. Weinberg, *Lectures on quantum mechanics*, Second edition (Cambridge University Press, Cambridge, United Kingdom ; New York, NY, 2015) What does one of the inventors of the "standard model" think that you should know about basic quantum mechanics? Read this book to find out.

(6) K. Gottfried and T.-M. Yan, *Quantum mechanics: fundamentals*, 2nd ed, Graduate Texts in Contemporary Physics (Springer, New York, 2003) Errata can be found at: https://www.classe.cornell.edu/books/QM-I/ Gottfried and Yan provide a unique perspective on all aspects of this course (basic QM, scattering, relativistic wave equations, quantization of electromagnetic field). I really like this book.

(7) F. Schwabl, *Quantum mechanics*, 4th ed (Springer, Berlin, Germany, 2010)
F. Schwabl, *Advanced quantum mechanics*, 4th ed (Springer, Berlin, 2008)
Both of these are good for the number of details worked out and reasonable thoroughness.

(8) R. Golub and S. K. Lamoreaux, *The historical and physical foundations of quantum mechanics* (Oxford University Press, Oxford, 2023)
A unique book that discusses the historical development of quantum mechanics without skimping on the details — which are presented in modern notation.

(9) B. C. Hall, *Quantum Theory for Mathematicians*, Vol. 267, Graduate Texts in Mathematics (Springer New York, New York, NY, 2013) Errata can be found at https://www3.nd.edu/~bhall/book/Qcorrections.pdf
If the physics approach to mathematics makes you queasy ...

4.2 One-particle relativistic wave equations

(10) J. D. Bjorken and S. D. Drell, *Relativistic quantum mechanics* (McGraw-Hill, New York, 1964) The standard reference.

(11) W. Greiner, *Relativistic quantum mechanics: wave equations*, 3rd ed (Springer, Berlin ; New York, 2000) More details ...

4.3 Scattering

(12) J. R. Taylor, *Scattering theory: the quantum theory on nonrelativistic collisions* (Wiley, New York, 1972) Thorough and well-written, but lacking experimental examples of principles discussed.

(13) J. R. Taylor, *Classical mechanics* (University Science Books, Sausalito, Calif, 2005) A fairly complete discussion of classical scattering (e.g. Rutherford cross-section etc...).

4.4 Quantization of the electromagnetic field

(14) R. Loudon, *The quantum theory of light*, 3rd ed, Oxford Science Publications (Oxford University Press, Oxford ; New York, 2000) A standard.

(15) C. Cohen-Tannoudji et al., *Photons and atoms: introduction to quantum electrodynamics* (Wiley, New York, 1989) More complete — fills an interesting gap. For the curious.

4.5 Mathematics

(16) The canonical reference for the functions of mathematical physics is:
"NIST Digital Library of Mathematical Functions",
https://dlmf.nist.gov/
I *try* to stick to its conventions, except when common usage in physics deviates.

References

[1] J. J. Sakurai and J. Napolitano, *Modern Quantum Mechanics*, 3rd (Cambridge University Press, Cambridge, 2021).

[2] M. Le Bellac, *Quantum physics* (Cambridge University Press, Cambridge, UK ; New York, 2006).

[3] B. C. Hall, *Quantum Theory for Mathematicians*, Vol. 267, Graduate Texts in Mathematics (Springer New York, New York, NY, 2013).

[4] C. Cohen-Tannoudji, B. Diu, and F. Laloë, *Quantum Mechanics Volume I: Basic Concepts, Tools, and Application* (2020).

[5] R. Shankar, *Principles of quantum mechanics*, 2nd ed (Plenum Press, New York, 1994).

[6] D. J. Griffiths and D. F. Schroeter, *Introduction to quantum mechanics*, 3rd (Cambridge University Press, 2018).

[7] S. Weinberg, *Lectures on quantum mechanics*, Second edition (Cambridge University Press, Cambridge, United Kingdom ; New York, NY, 2015).

[8] F. Schwabl, *Advanced quantum mechanics*, 4th ed (Springer, Berlin, 2008).

[9] F. Schwabl, *Quantum mechanics*, 4th ed (Springer, Berlin, Germany, 2010).

[10] C. J. Foot, *Atomic physics*, Oxford Master Series in Physics 7. Atomic, Optical, and laser physics (Oxford University Press, Oxford ; New York, 2005).

[11] L. Ray et al., "Proton elastic scattering from ^{40,42,44,48}Ca at 800 MeV", Physical Review C **23**, 828–837 (1981).

[12] J. M. Thijssen, *Computational physics*, 2nd ed (Cambridge University Press, Cambridge, UK ; New York, 2007).

[13] J. W. Cooley, "An Improved Eigenvalue Corrector Formula for Solving the Schrodinger Equation for Central Fields", Mathematics of Computation **15**, 363 (1961).

[14] J. K. Cashion, "Testing of Diatomic Potential-Energy Functions by Numerical Methods", The Journal of Chemical Physics **39**, 1872–1877 (1963).

[15] J. J. Sakurai and J. Napolitano, *Modern quantum mechanics*, 2nd ed (Addison-Wesley, Boston, 2011).

[16] H. Batelaan and A. Tonomura, "The Aharonov–Bohm effects: Variations on a subtle theme", Physics Today **62**, 38–43 (2009).

[17] J. R. Taylor, *Scattering theory: the quantum theory on nonrelativistic collisions* (Wiley, New York, 1972).

[18] S. Weinberg, "What is an elementary particle?", SLAC Beam Line **27N1**, 17–21 (1999).

[19] K. Gottfried and T.-M. Yan, *Quantum mechanics: fundamentals*, 2nd ed, Graduate Texts in Contemporary Physics (Springer, New York, 2003).

[20] R. Golub and S. K. Lamoreaux, *The historical and physical foundations of quantum mechanics* (Oxford University Press, Oxford, 2023).

[21] J. D. Bjorken and S. D. Drell, *Relativistic quantum mechanics* (McGraw-Hill, New York, 1964).

[22] W. Greiner, *Relativistic quantum mechanics: wave equations*, 3rd ed (Springer, Berlin ; New York, 2000).

[23] J. R. Taylor, *Classical mechanics* (University Science Books, Sausalito, Calif, 2005).

[24] R. Loudon, *The quantum theory of light*, 3rd ed, Oxford Science Publications (Oxford University Press, Oxford ; New York, 2000).

[25] C. Cohen-Tannoudji, J. Dupont-Roc, and G. Grynberg, *Photons and atoms: introduction to quantum electrodynamics* (Wiley, New York, 1989).

[26] "NIST Digital Library of Mathematical Functions",