1. Intro to the course & lightening recap of QM 1

SS 2024

AQM

[illegible]

[illegible]

IMPORTANT INFOS

2V + 2U ; No moodle - website with Lectures
Exercises

ph.nat.tum.de/ttpmath/teaching/ss-2024

Exercises MANDATORY for bonus

PARTICIPATION + ATTEMPT ALL SOLUTIONS
SOLVE ~ 50% correctly
DISCUSS 1 SOLUTION IN CLASS

START WEEK 3, ex out week 2

- 2 sessions, both obligatory !
  1] more info from tutors, start sol
  2] Discussion of solution
  $\Downarrow$
  Sign up on website during first two weeks

Written exam at the end

Oral if $\leq$ 15 people !

IMPORTANT

- Sign up for tutorials on DOODLES on website => INDICATE YOUR AVAILABILITY (both, in case)

Two ex classes fall on thursdays that are holidays, first on MAY 9th (Himmelfahrt)

⇓

it will be moved to MAY 8th

more details soon on website !

In this course we will deal with some more advanced topics in Quantum Mechanics, which have direct application to understand physically interesting phenomena

The main topics will be time-dependent phenomena:

1. Interaction of Atoms with EM. Field

   induced emission
   spontaneous emission } RADIATIVE DECAYS

2. Scattering / Collision theory

   Optical theorem, scattering Amplitudes
   Born approximation

To get there we need to develop our tools further - let's recap first what you all should know from your QM 1 courses

In Quantum Mechanics we describe a system using a formalism that is very different from Classical Physics

Concept of STATE OF SYSTEM in Quantum Mechanics is central and different from classical physics

- States are vectors in infinite dimensional vector space

$$|n\rangle , \; |p\rangle \; ; \; |a, b\rangle \qquad \text{kets}$$

Labels give value of "observables"

a, b two labels for two "compatible observables"

- A ket can be expressed as linear combination of other kets

$$|\psi\rangle = \sum_n c_n |n\rangle \qquad || \qquad |\psi\rangle = \int dx \; c(x) \, |x\rangle$$

$c_n \in \mathbb{C}$ 　　　　 Label can be continuous!

Vector space kets $\longrightarrow$ Dual vector space BRAS

$$|\psi\rangle \longrightarrow \langle\psi|$$

We can define a scalar product between bras & kets
BRA[c]KET

- $\langle\psi|\varphi\rangle \in \mathbb{C}$ complex number

- $\langle\varphi|\psi\rangle^* = \langle\psi|\varphi\rangle \Rightarrow \underline{\langle\psi|\psi\rangle = |\psi|^2 \in \mathbb{R}^+}$

- $\langle\varphi|\left(a\psi_1 + b\psi_2\right)\rangle = a\langle\varphi|\psi_1\rangle + b\langle\varphi|\psi_2\rangle$

- $|\psi\rangle \perp |\varphi\rangle$ if $\begin{cases} \langle\psi|\varphi\rangle = 0 \\ \langle\varphi|\psi\rangle = 0 \end{cases}$ (orthogonality)

- $\sqrt{\langle\psi|\psi\rangle} = \sqrt{|\psi|^2}$ length of vector

"Observables" are represented by OPERATORS

Operators represent dynamical variables

- $A|\psi\rangle = |\varphi\rangle$ operator on a state gives another state

- $(A|\psi\rangle)^* = \langle\psi| A^\dagger$

- $\langle\chi|A|\psi\rangle^* = \langle\psi| A^\dagger |\chi\rangle$

Adjoint operator

if $A^\dagger = A$ A is self-adjoint or Hermitian } REAL linear operator

if $|n\rangle$ set of eigenstates of A (complete & orthonormal)

$$A|n\rangle = n|n\rangle \qquad \langle n|m\rangle = \delta_{n,m}$$

$$|\psi\rangle = \sum_n c_n |n\rangle \Rightarrow c_n = \langle n|\psi\rangle$$

such that $|\psi\rangle = \underbrace{\sum_n |n\rangle\langle n|}\psi\rangle$

$\sum_n |n\rangle\langle n| = \mathbb{1}$ completeness relation

$|C_n|^2$ probability that a measurement of A on state $|\psi\rangle$ gives eigenvalue "n"

"n" need not be descrete eigenvalues

X, P position & momentum operators

$X|x\rangle = x|x\rangle$ $\qquad \langle x|x'\rangle = \delta(x-x')$

$$\Rightarrow |\psi\rangle = \int_{-\infty}^{+\infty} dx'\, c(x')\, |x'\rangle$$

$$c(x) = \langle x|\psi\rangle \equiv \psi(x)$$ wave function

similarly $P|p\rangle = p|p\rangle$ & $\langle p|p'\rangle = \delta(p-p')$

$\Rightarrow$ $\phi(p) = \langle p|\psi\rangle$ wave function in momentum representation

and

$$\psi(x) = \langle x|\psi\rangle = \int_{-\infty}^{+\infty} dp\, \langle x|p\rangle\langle p|\psi\rangle$$

$$= \int_{-\infty}^{+\infty} dp\, \langle x|p\rangle\, \phi(p)$$

$$\overset{!}{=} \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dp\, \phi(p)\, e^{ipx/\hbar}$$

Fourier Transform

$$\Rightarrow \langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{ipx/\hbar}$$

Note that if $A|n\rangle = n|n\rangle$ then we can build operator $P_n = |n\rangle\langle n|$

$$\left.\begin{array}{l} P_m P_n = \delta_{mn} P_n \\ \sum_n P_n = 1 \end{array}\right\} \text{Projector on } |n\rangle \text{ !}$$

$P_n|\psi\rangle = |n\rangle\langle n|\psi\rangle$ projects ψ onto $|n\rangle$

so we can write $A = \sum_n n\, |n\rangle\langle n|$

$$\langle\psi|A|\psi\rangle = \sum_n n\, |\langle\psi|n\rangle|^2$$

average of eigen values with $\langle\psi|n\rangle$ as "weights" !

State vectors and operators can be neatly represented as VECTORS and MATRICES once we fix a "basis" $|n\rangle$

Kets $\Rightarrow$ column vectors

Bras $\Rightarrow$ row vectors

Operators $\Rightarrow$ matrices

$$|\psi\rangle = A|\phi\rangle$$

$$\underbrace{\langle m|\psi\rangle}_{} = \sum_n \langle m|A|n\rangle\langle n|\phi\rangle$$

$$\begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \vdots \end{pmatrix} = \begin{bmatrix} & & \\ & A_{mn} & \\ & & \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \vdots \end{bmatrix}$$

$$\langle\phi|n\rangle \Rightarrow (\alpha_1^*, \alpha_2^*, \dots\ )$$

$$\langle\phi|\psi\rangle = \sum_n \alpha_n^* \beta_n$$ scalar product

ANGULAR MOMENTUM (& SPIN)

$\vec{L} = \vec{r} \times \vec{p}$ $\Rightarrow$ QM operator such that

$$[L_i, L_j] = i \varepsilon_{ijk} \hbar L_k$$

$$[L_i, L^2] = 0 \qquad L^2 = L_x^2 + L_y^2 + L_z^2$$

if H rotation invariant $[H, L_i] = 0$

$\Rightarrow$ Set of commuting operators for centrally symmetric problem $\{H, L^2, L_i\}$

one of the components

$|l, m\rangle$ such that

$$L^2 |l, m\rangle = \hbar^2 l(l+1) |l, m\rangle$$

$$L_z |l, m\rangle = \hbar m \; |l, m\rangle$$

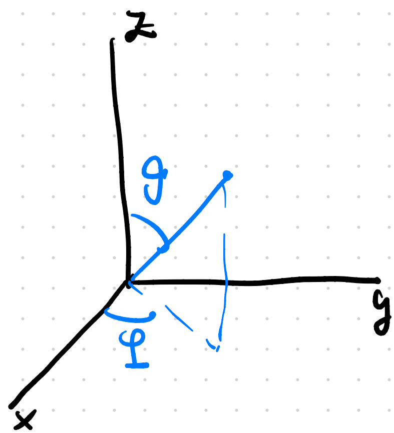
by consistency one finds $\ell \geq 0$

$$\begin{cases} \ell(\ell+1) \geq m(m+1) \\ \ell(\ell+1) \geq m(m-1) \end{cases} \Rightarrow \underline{-\ell \leq m \leq +\ell}$$

m takes $2\ell+1$ values $\quad \ell = \begin{cases} \text{integer} \\ \text{half-integer [SPIN]} \end{cases}$

For $\underbrace{\ell \text{ integer}}_{\text{ORBITAL ANGULAR MOMENTUM}}$, eigenfunctions or Spherical Harmonics

$$Y_{\ell m}(\vartheta,\varphi) = \langle \vartheta,\varphi | \ell,m \rangle$$



$$\langle \vartheta'\varphi' | \vartheta,\varphi \rangle = \frac{1}{\sin\vartheta} \delta(\vartheta-\vartheta')\,\delta(\varphi-\varphi')$$

due to spherical coord.

normalization

$$Y_{\ell m}(\vartheta,\varphi) = C(\ell,m)\, P_\ell^m(\cos\vartheta)\, e^{im\varphi}$$

Legendre Polynomials

PARITY $\quad P\, Y_{\ell m} \to (-1)^\ell\, Y_{\ell m} \quad$ IMPORTANT !

SCHRÖDINGER EVOLUTION EQUATION

By solving eigenvalue eqs. for some operators we get information about system at a given time

$$\begin{cases} L^2 |\psi_{\ell,m}\rangle = \hbar^2 \ell(\ell+1) |\psi_{\ell,m}\rangle \\ L_z |\psi_{\ell,m}\rangle = \hbar m |\ell, m\rangle \\ H |\psi_n\rangle = E_n |\psi_n\rangle \quad \text{etc} \end{cases}$$

How do we get dynamical Evolution with time?

$$|\psi(t)\rangle = f\,|\psi(t_0)\rangle \quad \text{with } t_0 < t \quad ?$$

In QM, each state evolves through some linear operator T

$$|\psi(t)\rangle = T(t, t_0)\,|\psi(t_0)\rangle$$

Conservation of probability during evolution $\Rightarrow$ "conservation of length"

$$TT^\dagger = T^\dagger T = \mathbb{1}$$

unitary evolution !

Now infinitesimally, if $t = t_0 + \delta t$

$$\lim_{t\to t_0} \frac{|\psi(t)\rangle - |\psi(t_0)\rangle}{t-t_0} = \frac{d}{dt_0}|\psi(t_0)\rangle$$

$$\equiv \lim_{\delta t\to 0} \underbrace{\left[\frac{T(t,t_0) - \mathbb{1}}{\delta t}\right]}\,|\psi(t_0)\rangle$$

one can prove that:

it must be a purely imaginary linear

operator $= \dfrac{H(t_0)}{i\hbar}$ with $H(t_0)$ REAL such that

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle \quad \left(\begin{array}{c}\text{renamed} \\ t_0 \to t\end{array}\right)$$

Schrödinger Evolution Equation if

we identify $\underline{H(t_0) \equiv \text{HAMILTONIAN}}$

Cannot be "proven", it is a postulate!

now using $|\psi(t)\rangle = T(t, t_0) |\psi(t_0)\rangle$

$$i\hbar \frac{d T(t, t_0)}{dt} |\psi(t_0)\rangle = H(t) T(t, t_0) |\psi(t_0)\rangle$$

$$\Rightarrow i\hbar \frac{dT}{dt} = H(t) T$$

Schrödinger eq for evolution operator!

if $\mathcal{H}(t)$ is CONSTANT in t $\equiv \mathcal{H}$ then

we can write formal solution

$$\begin{cases} T(t, t_0) = e^{-iH(t-t_0)/\hbar} \\ \text{which assumes } T(t_0, t_0) \equiv \mathbb{1} \end{cases}$$

$$\Rightarrow |\psi(t)\rangle = e^{-iH(t-t_0)/\hbar} |\psi(t_0)\rangle$$

if $|\psi(t_0)\rangle = |n\rangle$ s.t. $H|n\rangle = E_n|n\rangle$

then

$$|\psi(t)\rangle = e^{-iE_n(t-t_0)/\hbar} |n\rangle$$

$|\psi(t)\rangle$ differs from $|n\rangle$ only by a phase !

STATIONARY STATE !

TIME-INDEPENDENT PERTURBATION THEORY

When energy is conserved [Potential is time independent]

it is still extremely difficult to solve Schrödinger Equation exactly $\Rightarrow$ perturbation theory allows us to get approximate results starting from a problem that we can solve.

$$H = \underbrace{H_0}_{\text{problem that we can solve (f.e. Hydrogen Atom)}} + \lambda H_1$$

λH_1: perturbation, parametrized by SMALL PARAMETER λ

Assume $H_0 |\phi_n\rangle = E_n^{(0)} |\phi_n\rangle$ known

We would like to solve

$$(H_0 + \lambda H_1) |\psi_n\rangle = E_n |\psi_n\rangle$$

where we assume $E_n(\lambda) \xrightarrow[\lambda \to 0]{} E_n^{(0)}$

the $|\phi_n\rangle$ form a complete set, so we can write

$$|\psi_n\rangle = N(\lambda) \left\{ |\phi_n\rangle + \sum_{k \neq n} \underbrace{c_{nk}(\lambda)}_{O(\lambda)} |\phi_k\rangle \right\}$$

COEFFICIENT = 1 !

we guarantee this by picking appropriate phase for $|\psi_n\rangle$ so that first order perturbation is ORTHOGONAL to unperturbed state

$N(\lambda) \in \mathbb{R}$ to fix "NORMALIZATION"

$$|\psi_n^{(1)}\rangle = \sum_{k\neq n} C_{n,k}(\lambda)\,|\phi_k\rangle \quad \underset{\Longrightarrow}{\text{with}} \quad N(0) = 1$$

$$\& \quad C_{nk}(0) = 0$$

$$C_{nk}(\lambda) = \lambda\, C_{nk}^{(1)} + \lambda^2\, C_{nk}^{(2)} + O(\lambda^3)$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + O(\lambda^3)$$

plugging them in schrödinger Eq & collecting λ^n

$\lambda^{(0)} \Rightarrow \quad H_0|\phi_n\rangle = E_n|\phi_n\rangle$ trivially satisfied

$$\lambda^{(1)} \Rightarrow \quad H_0 \sum_{k\neq n} C_{nk}^{(1)}\,|\phi_k\rangle + H_1|\phi_n\rangle$$

$$= E_n^{(0)} \sum_{k\neq n} C_{nk}^{(1)}\,|\phi_k\rangle + E_n^{(1)}\,|\phi_n\rangle$$

such that:

$$E_n^{(1)}\,|\phi_n\rangle = H_1|\phi_n\rangle + \sum_{k\neq n}\left[E_k^{(0)} - E_n^{(0)}\right] C_{nk}^{(1)}\,|\phi_k\rangle \quad (*)$$

and contracting with $\langle\phi_n|$:

$$\boxed{\lambda E_n^{(1)} = \langle \phi_n | \lambda H_1 | \phi_n \rangle}$$

First order energy shift $\propto$ Expectation value of perturbing Hamiltonian on unperturbed state!

Contracting $(*)$ with $\langle \phi_m |$ with $m \neq n$

$$\lambda C_{nm}^{(1)} = \frac{\langle \phi_m | \lambda H_1 | \phi_n \rangle}{E_n^{(0)} - E_m^{(0)}}$$

which provides coefficients of the eigenstate!

Using this on $O(\lambda^2)$ terms we get

$$E_n^{(2)} = \sum_{k \neq n} \frac{|\langle \phi_n | H_1 | \phi_k \rangle|^2}{\underbrace{E_n^{(0)} - E_k^{(0)}}_{\text{nearby levels tend to have bigger effect!}}}$$

these formulas of course assume that energy levels are NON-DEGENERATE

If H_0 is degenerate, one has to first diagonalize the perturbation on the degenerate entries in order to REMOVE DEGENERATION and then proceed in the same way as before