SPIN(½)

$S_x = \frac{\hbar}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix} = \frac{\hbar}{\sqrt2}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}$

$S_y = \frac{\hbar}{2}\begin{pmatrix}0&-i\\i&0\end{pmatrix} = \frac{\hbar}{\sqrt2}\begin{pmatrix}0&-i&0\\i&0&-i\\0&i&0\end{pmatrix}$

$S_z = \frac{\hbar}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix} = \frac{\hbar}{\sqrt2}\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}$

$\sigma_i\sigma_j = -\sigma_j\sigma_i$ $\quad \sigma_x^2=\sigma_y^2=\sigma_z^2 = I$

$\sigma_i\sigma_j = \delta_{ij} + i\epsilon_{ijk}\sigma_k$

$[\sigma_j, \sigma_k] = 2i\,\epsilon_{jkl}\sigma_l$ $\quad = -i\sigma_x\sigma_y\sigma_z$

eigenvects(σ) $\quad s^2 = \frac{3\hbar^2}{4}\begin{pmatrix}1&0\\0&1\end{pmatrix}$

	x	y	z
+1 :	$\frac{1}{\sqrt2}\begin{pmatrix}1\\1\end{pmatrix}$	$\frac{1}{\sqrt2}\begin{pmatrix}1\\i\end{pmatrix}$	$\begin{pmatrix}1\\0\end{pmatrix}$
−1 :	$\frac{1}{\sqrt2}\begin{pmatrix}1\\-1\end{pmatrix}$	$\frac{1}{\sqrt2}\begin{pmatrix}1\\-i\end{pmatrix}$	$\begin{pmatrix}0\\1\end{pmatrix}$

Bloch sphere

$\rho = \frac12[I + \vec{s}\cdot\vec{\sigma}]$, $\langle\vec\sigma\rangle = Tr[\rho\vec\sigma] = \vec s$

on the surface of sphere: pure. The origin is the maximally mixed state.

Applying any σ_i will rotate vector 180° about the axis i.

Angular Momentum

$L_i = \epsilon_{ijk} x_j p_k$

$[L^2, L_z] = 0$, $[L_i, L_j] = i\hbar\epsilon_{ijk}L_k$

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

$L_z|l,m\rangle = \hbar m|l,m\rangle$, $[L_z, L_\pm] = \pm\hbar L_\pm$

$L_x|l,m\rangle = \frac{\hbar}{2}\Big[\delta_{l'l}\delta_{m',m+1}\sqrt{(l-m)(l+m+1)} + \delta_{l'l}\delta_{m',m-1}\sqrt{(l+m)(l-m+1)}\Big]$

$L_y|l,m\rangle = \frac{\hbar}{2i}[\ldots]$, $L_\pm = L_x \pm iL_y$

$L_\pm|l,m\rangle = \hbar\sqrt{(l\mp m)(l\pm m+1)}\,|l,m\pm1\rangle$

$|l_1 - l_2| \le L \le l_1 + l_2$, $[L_+, L_z] = \hbar L_+$

Dimensionality of Spin Systems

i.e. three spin-1 particles

$1\otimes1\otimes1 = (1\otimes1)\otimes1$

$= (2\oplus1\oplus0)\otimes1 = (2\otimes1)\oplus(1\otimes1)\oplus(0\otimes1)$

$= (3\oplus2\oplus1)\oplus(2\oplus1\oplus0)\oplus(1)$

$= 3\oplus2\oplus1\oplus2\oplus1\oplus0\oplus1$

$7+5+3+5+3+1+3 = 27$

$3\cdot3\cdot3 = 27$ dimensionalities

generally:

$(M\otimes N) = (M+N)\oplus(M+N-1)\oplus\ldots\oplus(M-N)$

A space of spin-M has 2M+1 dimensions

General QM / MATH

$(\Delta A)(\Delta B) \ge \left|\frac{1}{2i}\langle[\hat A,\hat B]\rangle\right|$, $\Delta x\Delta p \ge \frac{\hbar}{2}$, $\Delta E\Delta t \ge \frac{\hbar}{2}$

$X_i|\psi\rangle \to x_i\psi$, $P_i|\psi\rangle \to -i\hbar\frac{\partial}{\partial x_i}\psi$

$e^{\hat A}Be^{-\hat A} = \hat B + [\hat A,\hat B] + \frac{1}{2!}[\hat A,[\hat A,\hat B]] + \ldots$

$\ln(\det(M)) = Tr(\ln(M))$

$[\hat A, \hat B\hat C] = [\hat A,\hat B]\hat C + \hat B[\hat A,\hat C]$

$[\hat A\hat B, \hat C] = \hat A[\hat B,\hat C] + [\hat A,\hat C]\hat B$

$\epsilon_{ijk}\epsilon_{mnk} = \delta_{im}\delta_{jn} - \delta_{in}\delta_{jm}$

$f(x) = \int_{-\infty}^{\infty} F(k)e^{2\pi ikx}dk$

$F(k) = \int_{-\infty}^{\infty} f(x)e^{-2\pi ikx}dx$

$\frac{d}{dt}\langle A\rangle = \frac{1}{i\hbar}\langle[A,H]\rangle + \langle\frac{\partial A}{\partial t}\rangle$ ehrenfest theorem.

POVM

$P(i) = Tr[B_i\rho B_i^\dagger] = Tr[B_i^\dagger B_i\rho]$

probability of outcome i

$P(t_i) = \sum_i B_i\rho B_i^\dagger$ measurement but not read out

$\rho(t) = \frac{B_i\rho(t_0)B_i^\dagger}{Tr[B_i^\dagger B_i\rho(t_0)]}$ state after measurement.

$(B_i^\dagger B_i)^\dagger = B_i^\dagger B_i$ effect operator herm. + pos def.

$\langle\phi|B_i^\dagger B_i|\phi\rangle = \|B_i|\phi\rangle\|^2 \ge 0$

$Tr[\sum B_i^\dagger B_i\rho] = 1$

PVM

$\hat A = \sum\lambda_i P_i$, $P(\lambda_i) = Tr[\rho P_i]$

$\rho' = \frac{P_i\rho P_i^\dagger}{Tr[P_i\rho]}$ $\quad P_iP_j = \delta_{ij}P_i$

state after mst. $\quad \sum_i P_i = I$

Reduced Density / Partial Trace

let F be an operator s.t.

$F: U\otimes V \to U\otimes V$

$Tr_V F = \sum_{j=1}^{n}\sum_{i=1}^{m}\Big[\sum_k \langle u_i|\langle v_k|F|v_k\rangle|u_j\rangle\Big]|u_i\rangle\langle u_j|$

yields an operator in U

$Tr_V[A_U\otimes B_V] = A_U\,Tr[B_V]$

$Tr_U[Tr_V[F]] = Tr_V[Tr_U[F]] = Tr[F]$

$Tr[A_U\otimes B_V] = Tr_U[A_U]\,Tr_V[B_V]$

$Tr_V[F] = \sum_{i=1}^{n}\langle v_i|F|v_i\rangle$

if $\rho_U = Tr_V\rho$, $\rho_V = Tr_U\rho$, $\rho_U\otimes\rho_V \ne \rho$

let ρ describe an N-particle system. to "filter-out" particles after some n, we reduce ρ with partial trace

$\rho_n = Tr_{n+1}\ldots Tr_{N-1}Tr_N\,\rho$

now ρ_n describes particles 1, …, n

– the reduced density operator can be pure, even if the original is mixed

Integrals / Series

$\int_{-\infty}^{\infty} f(x)\frac{d}{dx}\delta(x-x')dx = -f'(x')$

$\int_{-\infty}^{\infty} dk\,e^{ik(x-x')} = 2\pi\delta(x-x')$

$\int\frac{dx}{\sqrt{x^2+a^2}} = \ln(x+\sqrt{x^2+a^2})$

$\int\frac{d}{(x^2+a^2)^{3/2}} = \frac{x}{a^2\sqrt{x^2+a^2}}$

$\int_0^\infty x^{2n}e^{-ax^2}dx = \frac{(2n-1)!!}{a^n2^{n+1}}\sqrt{\frac{\pi}{a}}$

$\int_0^\infty x^{2n+1}e^{-ax^2}dx = \frac{n!}{2a^{n+1}}$

$\int x\sin x\,dx = -x\cos x + \sin x$

$\int x\cos x\,dx = x\sin x - \cos x$

$\int\sin^2 x\,dx = \frac{x}{2} - \frac14\sin(2x)$

$\int\cos^2 x\,dx = \frac{x}{2} + \frac14\sin(2x)$

$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \ldots + \frac{x^n}{n!}$

$\sin x = \sum_{n=0}(-1)^n\frac{x^{2n+1}}{(2n+1)!}$

$\cos x = \sum_{n=0}(-1)^n\frac{x^{2n}}{(2n)!}$

$\ln(1+x) = \sum_{n=1}(-1)^{n+1}\frac{x^n}{n}$

$\tan^{-1}(x) = \sum_{n=0}(-1)^n\frac{x^{2n+1}}{2n+1}$

$\int_{-\infty}^{\infty} e^{-x^2}dx = \sqrt\pi$, $\int_{-\infty}^{\infty} xe^{-x^2}dx = \frac12$

$\int_{-\infty}^{\infty} e^{-a(x+b)^2}dx = \sqrt{\frac{\pi}{a}}$

Density operators (ρ)

$\rho = \sum P_i|\phi_i\rangle\langle\phi_i|$, $\quad \rho^\dagger = \rho$, $Tr(\rho) = 1$, $\rho \ge 0$

$Tr[\rho^2] \le Tr[\rho] = 1$

if $Tr(\rho^2) = Tr(\rho)$, then $\rho^2 = \rho$ and ρ must be a pure state.

Pure states: $S[\rho] = 0$, $Rank[\rho] = 1$

$\rho(t) = U(t,t_0)\rho(t_0)U^\dagger(t,t_0)$

$\frac{\partial\rho}{\partial t} = \frac{1}{i\hbar}[H(t), \rho(t)]$

$\langle A\rangle = Tr[A\rho]$

for eigenvalues λ_i of ρ,

$\sum\lambda_i = 1$, $\lambda_i \ge 0$, $\lambda_i \in \mathbb{R}$

Von Neumann entropy

$S = -Tr[\rho\log\rho] = -\sum\lambda_i\log\lambda_i$

$S = 0$ iff ρ is pure.

Ehrenfest Theorem

$\langle A(t)\rangle = Tr[A(t)\rho(t)]$

$\frac{d}{dt}\langle A(t)\rangle = \langle\frac{\partial A}{\partial t}\rangle + \frac{1}{i\hbar}\langle[A(t), H(t)]\rangle$

useful misc.

in spin-½: $\sigma_z|+\rangle = |+\rangle$, $\sigma_z|-\rangle = -|-\rangle$

$\sigma_x|+\rangle = |-\rangle$, $\sigma_y|+\rangle = i|-\rangle$

$\sigma_x|-\rangle = |+\rangle$, $\sigma_y|-\rangle = -i|+\rangle$

if all operators in a set commute, they will have a common eigenbasis if they are diagonalizable.

Pauli spin matrices form a basis for the set of all spin-½ operators

If an operator commutes with each operator in a CSCO, it must be a function of those operators.

If a hamiltonian is rotationally invariant about some axis n, it will commute w/ S_n.

$\hat A|\psi\rangle = \alpha|\psi\rangle + \beta|\psi_\perp\rangle$

$\sigma_A = 0$ iff $|\psi\rangle$ is an eigenstate of $\hat A$

The maximally mixed state, which is minimal knowledge of the state vector, is $\rho = \frac12\mathbb{1}$

if $|\psi\rangle = |a\rangle\otimes|b\rangle$, $\rho = |\psi\rangle\langle\psi|$

$Tr_V[\rho] = |a\rangle\langle a|$ and $Tr_U[\rho] = |b\rangle\langle b|$

$S_U = -Tr[\rho_U\log\rho_U] = S_V = -Tr[\rho_V\log\rho_V]$

in QM, maximal knowledge ≠ complete knowledge

Quantum Logic

$A\wedge B$, A and B, $Span(Im(A)\cup Im(B))$

$A\vee B$, A or B, $Im(A)\cap Im(B)$

$\neg A$ not A

$A\le B$ if A is T, B must be T.

$(A^\perp)^\perp = A$, $A\wedge A^\perp = 0$, $A\vee A^\perp = 1$

$(A\wedge B)^\perp = A^\perp\vee B^\perp$, $(A\vee B)^\perp = A^\perp\wedge B^\perp$

if $A\le B$, $B^\perp \le A^\perp$

the distributive law does NOT hold under quantum logic!

$A\wedge(B\vee C) = (A\wedge B)\vee(A\wedge C)$

$A\vee(B\wedge C) = (A\vee B)\wedge(A\vee C)$

if $A\le C$, then $A\vee(A^\perp\wedge C) = C$

Interpretations / Paradoxes

Hidden-Variable (KS, EPR, etc.) assumes operators have some pre-existing assigned value.

This is contradicted by using different combinations of observables that multiply to values expected to be the same, but are not.

$(ABC)(DEF)(GHK) = (+1)^3 = +1$

$(ADG)(BEH)(CFK) = (+1)^2(-1) = -1$

Hardy Paradox

A "locally realistic" theory dictates that a system must specify the result of all possible measurements

example of violation:

Alice measures A or A′ (±1)

Bob measures B or B′ (±1)

local realism states the following are impossible, but QM says it is:

i) if A and B measured, A = +1, B = +1 sometimes occurs

ii) if A′ and B or A and B′, A′ = B = +1 or A = B′ = 1 never occurs.

iii) if A′ and B′ measured, A′ = B′ = −1 never occurs.

using $\hat n = \cos(2\theta)\hat z + \sin(2\theta)\hat x$ and $A = \sigma_{1z}$, $A' = \hat n\cdot\sigma_1$, $B = \sigma_{2z}$, $B' = \hat n\cdot\sigma_2$

this can be proven to happen in QM.

"Many worlds" – the wavefunction never collapses, it splits and people are only aware of one aspect of reality.

Isospin

$I_3 \in \{-I, -I+1, \ldots, I\}$

eigenstates $|I\,I_3\rangle$, $I \in \{0, \frac12, 1, \ldots\}$

proton $|p\rangle \propto |\frac12\,\frac12\rangle$, $= |uud\rangle$

neutron $|n\rangle \propto |\frac12\,-\frac12\rangle$, $= |udd\rangle$

Pions $|\pi^+\rangle \propto |1\,1\rangle$, $= |u\bar d\rangle$

$|\pi^0\rangle \propto |1\,0\rangle$, $= \frac{1}{\sqrt2}(|u\bar u\rangle - |d\bar d\rangle)$

$|\pi^-\rangle \propto |1\,-1\rangle$, $= |d\bar u\rangle$

quarks and antiquarks

$|u\rangle \propto |\frac12\,\frac12\rangle$ $\quad |\bar u\rangle \propto |\frac12\,-\frac12\rangle$

$|d\rangle \propto |\frac12\,-\frac12\rangle$ $\quad |\bar d\rangle \propto -|\frac12\,\frac12\rangle$

deuteron

$|d\rangle = \frac{1}{\sqrt2}(|pn\rangle - |np\rangle) = |00\rangle$

other (triplet) of nucleons: $|1\,1\rangle = |pp\rangle$

$|1\,0\rangle = \frac{1}{\sqrt2}(|pn\rangle + |np\rangle)$

(NONEXISTENT) $|1\,-1\rangle = |nn\rangle$

Changes in energy of coupled particles

$\Delta H \propto \vec I_1\cdot\vec I_2 = \frac12\big[|I_1+I_2|^2 - |I_1|^2 - |I_2|^2\big]$

for nucleon triplets

$\Delta H \propto \frac12\big[(1)(2) - \frac12\frac32 - \frac12\frac32\big] = +\frac14$

for nucleon singlet:

$\Delta H \propto \frac12\big[(0)(1) - \frac12\frac32 - \frac12\frac32\big] = -\frac34$

In decay, we assume $[H, \vec I] = 0$ (so the same for time evol. U.)

Fine Structure

when $p = \frac{mv}{\sqrt{1-v^2/c^2}}$

$K = \frac{mc^2}{\sqrt{1-\frac{v^2}{c^2}}} - mc^2 = \sqrt{p^2c^2 + m^2c^4} - mc^2$

$= mc^2\Big(1 + \frac12\big(\frac{p}{mc}\big)^2 - \frac18\big(\frac{p}{mc}\big)^4 + \ldots\Big) = \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} \ldots$

$E_r^{(1)} = -\frac{1}{8m^3c^2}\langle p^2\psi|p^2\psi\rangle$, $p^2\psi = 2m(E-V)\psi$

$= -\frac{1}{2mc^2}\Big[E_n^2 + 2E_n\frac{e^2}{4\pi\epsilon_0}\langle\frac1r\rangle + \big(\frac{e^2}{4\pi\epsilon_0}\big)^2\langle\frac{1}{r^2}\rangle\Big]$

$\langle\frac1r\rangle = \frac{1}{n^2a}$ $\quad \langle\frac{1}{r^2}\rangle = \frac{1}{(l+\frac12)n^3a^2}$ $\quad \langle\frac{1}{r^3}\rangle = \frac{1}{l(l+\frac12)(l+1)n^3a^3}$

$E_r^{(1)} = -\frac{E_n^2}{2mc^2}\Big(\frac{4n}{l+\frac12} - 3\Big)$ for hydrogen, $\langle V\rangle = 2E_n$

Since $V = -\frac{e^2}{4\pi\epsilon_0}\frac1r$, $-\frac{e^2}{4\pi\epsilon_0}\langle\frac1r\rangle = -2\Big[\frac{m}{2\hbar^2}\big(\frac{e^2}{4\pi\epsilon_0}\big)^2\Big]\frac{1}{n^2}$

Spin-orbit coupling

$H = -\vec\mu\cdot\vec B$, $\vec B = \frac{1}{4\pi\epsilon_0}\frac{e}{mc^2r^3}\vec L$, $\mu_e = -\frac{e}{m}\vec S$

$H_{so} = \frac{e^2}{8\pi\epsilon_0}\frac{1}{m^2c^2r^3}\vec S\cdot\vec L$, $E_{so}^{(1)} = \frac{E_n^2}{mc^2}\frac{n[j(j+1) - l(l+1) - \frac34]}{l(l+\frac12)(l+1)}$

Zeeman

$H = -(\vec\mu_l + \vec\mu_s)\cdot\vec B_{ext}$ $\quad \vec\mu_s = -\frac{e}{m}\vec S$, $\vec\mu_l = -\frac{e}{2m}\vec L$

$H_z = \frac{e}{2m}(\vec L + 2\vec S)\cdot\vec B_{ext}$

WEAK-FIELD: fine struct dominates H_z is perturb.

$E_z^{(1)} = \frac{e}{2m}B_{ext}\hat z\cdot\langle\vec L + 2\vec S\rangle = \mu_B g_J B_{ext} m_j$

$\langle\vec L + 2\vec S\rangle = \Big[1 + \frac{j(j+1) - l(l+1) + s(s+1)}{2j(j+1)}\Big]\langle\vec J\rangle = g_J\langle\vec J\rangle$

STRONG-FIELD: opposite.

$E_{n,m_l,m_s} = -\frac{13.6\,eV}{n^2} + \mu_B B_{ext}(m_l + 2m_s)$

$E_{fs}^{(1)} = \frac{13.6\,eV}{n^3}\alpha^2\Big[\frac{3}{4n} - \frac{l(l+1) - m_lm_s}{l(l+\frac12)(l+1)}\Big]$

Stark Effect

$H_1 = eEz$ const in z-direction

$\Delta E = \langle nlm|-ezE|n'l'm'\rangle$

Selection rules: $\Delta l = \pm1$, $\Delta m = 0$

$\Delta E^{(2)} = -\frac12\alpha E^2$, $\alpha = 2\sum_{k\ne0}\frac{|\langle k|ez|0\rangle|^2}{E_k - E_0}$

Hyperfine

$\vec F = \vec I + \vec J$

$\Delta E_{hf} = A\Big(\frac{F(F+1) - I(I+1) - J(J+1)}{2}\Big)$

Perturbation Theory (Time-Independent)

$H = H_0 + H_1\lambda$ $\quad E_n = E_n^{(0)} + \lambda E_n^{(1)} + \ldots$

$|\psi_n\rangle = |\psi_n^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle + \ldots$

matching λ^1 terms,

$H_0|\psi_n^{(1)}\rangle + H_1|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(1)}\rangle + E_n^{(1)}|\psi_n^{(0)}\rangle$

$\langle\psi_n^{(0)}|H_1|\psi_n^{(0)}\rangle = E_n^{(1)}$

$E_n^{(2)} = \langle\psi_n^{(0)}|H_1|\psi_n^{(1)}\rangle = \sum_{k\ne n}\frac{|\langle\psi_k^{(0)}|H_1|\psi_n^{(0)}\rangle|^2}{E_n^{(0)} - E_k^{(0)}}$

returning to the expansion,

$E_k^{(0)}\langle\psi_k^{(0)}|\psi_n^{(1)}\rangle + \langle\psi_k^{(0)}|H_1|\psi_n^{(0)}\rangle = E_n^{(0)}\langle\psi_k^{(0)}|\psi_n^{(1)}\rangle$

$\langle\psi_k^{(0)}|\psi_n^{(1)}\rangle = \frac{\langle\psi_k^{(0)}|H_1|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}}$

$|\psi_n^{(1)}\rangle = |\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\psi_n^{(1)}\rangle = |\psi_n^{(0)}\rangle + \sum_{k\ne n}\lambda\frac{\langle\psi_k^{(0)}|H_1|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}} + O(\lambda^2)$

degenerate: $|\psi_n^{(0)}\rangle = \sum_i^N c_i|\psi_{n_i}^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle + \ldots$

using same as above,

$\langle\psi_{n_j}^{(0)}|H_1|\psi_{n_i}^{(0)}\rangle c_i = E_n^{(1)}c_i$ $\qquad \begin{pmatrix}(H_1)_{11} & (H_1)_{12}\\(H_1)_{21} & (H_1)_{22}\end{pmatrix}\begin{pmatrix}v_1\\v_2\end{pmatrix} = E_n^{(1)}\begin{pmatrix}v_1\\v_2\end{pmatrix}$

$(H_1)_{ij} = \langle\psi_{n_i}^{(0)}|H_1|\psi_{n_j}^{(0)}\rangle$

WKB

For particle in energy E, potential V $(E>V)$

$\psi(x) = Ae^{\pm ikx}$, $k = \sqrt{2m(E-V)}/\hbar$

if V varies (relatively) slowly, WKB. Turning points at $E \approx V$. $p(x) = \sqrt{2m(E-V(x))}$

$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi \rightarrow \frac{d^2\psi}{dx^2} = -\frac{p^2}{\hbar^2}\psi$

guessing $\psi(x) = A(x)e^{i\phi(x)}$,

$\frac{d^2\psi}{dx^2} = (A'' + 2iA'\phi' + iA\phi'' + A\phi'^2)e^{i\phi}$

Plugging back in and separating to real/imag.

$A'' - A\phi'^2 = -\frac{p^2}{\hbar^2}A \rightarrow A'' = A(\phi'^2 - \frac{p^2}{\hbar^2})$

$2A'\phi' + A\phi'' = 0 \rightarrow (A^2\phi')' = 0$

evaluating + solving:

$A = \frac{C}{\sqrt{|\phi'|}}$ $\quad \phi = \pm\frac{1}{\hbar}\int p(x)\,dx$

$\psi(x) \simeq \frac{C}{\sqrt{p(x)}} e^{\pm\frac{i}{\hbar}\int p(x)dx}$ $\quad |\psi|^2 \simeq \frac{|C|^2}{p(x)}$

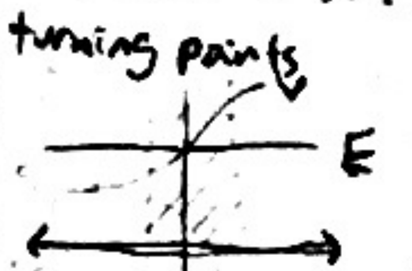
nonclassical $(E<V)$

$\psi(x) = \frac{C}{\sqrt{|p(x)|}} e^{\pm\frac{1}{\hbar}\int |p(x)|\,dx}$ — exactly the same except p is imaginary

$T \simeq e^{-2\gamma}$, $\gamma = \frac{1}{\hbar}\int_0^a |p(x)|\,dx$

$A \rightarrow$ ⊓ $\rightarrow F$, $B \leftarrow$ $\quad T = \frac{|F|^2}{|A|^2}$ transmission probability.

turning points — patching region correction



$\psi(x) = \begin{cases} \frac{1}{\sqrt{p(x)}}\left[Be^{\frac{i}{\hbar}\int_x^0 p(x')dx'} + Ce^{-\frac{i}{\hbar}\int_x^0 p(x')dx'}\right], & x<0 \\ \frac{1}{\sqrt{|p(x)|}}De^{-\frac{1}{\hbar}\int_0^x |p(x')|dx'}, & x>0 \end{cases}$

Approx $V = E + V'(0)x$, solve Schrodinger

$\frac{d^2\psi}{dx^2} = \alpha^3 x\psi$; $\alpha = \left(\frac{2m}{\hbar^2}V'(0)\right)^{\frac{1}{3}}$

use substitution $z = \alpha x$

$\frac{d^2\psi}{dz^2} = z\psi$, $\psi = aAi(\alpha x) + bBi(\alpha x)$

$Ai(z) \simeq \frac{1}{2\sqrt{\pi}z^{1/4}}e^{-\frac{2}{3}z^{\frac{3}{2}}}$ $\quad Bi(z) \simeq \frac{1}{\sqrt{\pi}z^{1/4}}e^{\frac{2}{3}z^{\frac{3}{2}}}$, $z \gg 0$

$Ai(z) \simeq \frac{1}{\sqrt{\pi}(-z)^{1/4}}\sin\left(\frac{2}{3}(-z)^{\frac{3}{2}} + \frac{\pi}{4}\right)$ $\quad Bi(z)$ = same but w/ cos $\quad z \ll 0$

Rayleigh-Ritz Variational

$E_{gs} \leq \langle\psi|H|\psi\rangle$ — when known H, but unable to find $|\psi\rangle$

pf: express ψ through eigenfunctions of H

$\psi = \sum c_n\psi_n$, $\quad 1 = \sum|c_n|^2$

$\langle H\rangle = \sum E_n|c_n|^2$, since E_{gs} is the smallest E_n,

$E_{gs}\sum|c_n|^2 \leq \langle H\rangle$

Atomic orbitals

1s 2s 2p 3s 3p 4s 3d 4p 5s 4d 5p 6s 4f 5d

Madelung rule: orbitals filled with incr. $n+l$; if value same, lower n filled

Hund's rule(s): 1. state with highest S has lowest E. 2. For given spin, highest L lower E. 3. if subshell < half filled, then lowest E-level has $J = |L-S|$; if > half filled, lowest E-level has $J = L+S$.

if $l = 0$, spherically sym.

n – energy level $= 0, 1, 2, \ldots$

l – orbital ang. momentum $= 0, 1, 2, \ldots, n-1$

m_l – magnetic qn. $= -l, \ldots, 0, \ldots, l$

m_s – spin qn. $= -s, \ldots, s$

multiplicity $\rightarrow {}^{2S+1}_{n}L_J$ $\quad L = 0, \ldots, l_1 + l_2 + \ldots$; S = total spin. if paired, cancel

$[Se] = 1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^4$

$S=0, L=0 \rightarrow J=0$

$S=0, L=2 \rightarrow J=2$ $\quad {}^3P_2 < {}^3P_1 < {}^3P_0 < {}^1D_2 < {}^1S_0$

$S=1, L=1 \rightarrow J = 0, 1, 2$

$\vec{J} = \vec{L} + \vec{S}$, $\vec{L}\cdot\vec{S} = \frac{1}{2}(J^2 - L^2 - S^2)$

eigen vals $= \frac{1}{2}[j(j+1) - l(l+1) - s(s+1)]$

for given spin S, single-particle dim $= 2S+1$

for indistinguishable, view as N particles with state dividers. for example, to sort N with $2S+1$ possible, $\binom{N + (2S+1) - 1}{N} = \frac{(2S+N)!}{N!(2S)!}$

For 2 spin-$\frac{1}{2}$ particles: $S^2 = \frac{3}{4}\hbar^2$

$|S=1, m=1\rangle = |++\rangle$ $\quad |S=1, m=-1\rangle = |--\rangle$

$|S=1, m=0\rangle = (|+-\rangle + |-+\rangle)\frac{1}{\sqrt{2}}$ $\quad |S=0, m=0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle)$

w/o hybridization: $\sigma(2s) < \sigma^*(2s) < \pi(2p) < \sigma(2p) < \pi^*(2p) < \sigma^*(2p)$

with hybridization:

$\sigma(2s) < \sigma^*(2s) < \sigma(2p) < \pi(2p) < \pi^*(2p) < \sigma^*(2p)$

bond order 0: unstable, unpaired e^-: paramag.

Quantum pictures

$\hat{U} = e^{-\frac{i}{\hbar}Ht}$ – evol. operator

Heisenberg picture

$\hat{A}_H(t) = \hat{U}^\dagger A\hat{U}$

equivalency:

$\langle\psi(t)|A|\psi(t)\rangle = \langle\psi(0)|U^\dagger AU|\psi(0)\rangle$

Schrodinger picture

$\hat{H}\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)$

$|\psi_S(t)\rangle = e^{iH_0t/\hbar}|\psi_S(t)\rangle$

when

$|\psi_S(t)\rangle = e^{-iH_0t/\hbar}|\psi(0)\rangle$

Interaction picture

$H_S = H_{0,S} + H_1(t)$, $\hat{A}_I(t) = e^{iH_0t/\hbar}A_S(t)e^{-iH_0t/\hbar}$

$H_{1,I}(t) = e^{iH_0t/\hbar}H_{1,S}e^{-iH_0t/\hbar}$

$i\hbar\frac{d}{dt}A_I(t) = [A_I(t), H_{0,I}]$

Heisenberg pict.

$\frac{dA(t)}{dt} = \frac{i}{\hbar}[H, A(t)] + \left(\frac{\partial A}{\partial t}\right)_H$

Dyson Expansion

$V_I = e^{iH_0(t-t_0)/\hbar}V_S e^{-iH_0(t-t_0)/\hbar}$

evol/dyson operator

$\psi(t) = U(t,t_0)\psi(t_0)$

$U(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t}V(t_1)U(t_1,t_0)dt_1$

$T(\psi^n) = \left(-\frac{i}{\hbar}\right)^n n!\int dt_1\int dt_2 \ldots H(t)$

$\psi(t) = T\left(e^{-\frac{i}{\hbar}\int H(t')dt'}\right)\psi(0)$

Fermi's Golden Rule

$\Gamma = \frac{2\pi}{\hbar}|\langle f|V|i\rangle|^2\rho\,d\Omega$

$\rho(E) = \frac{dN(E)}{dE}$ — the derivative of number of states by E

Adiabatic Theorem

$\psi_n(t) = e^{i\theta_n(t)}e^{i\gamma_n(t)}\psi_n(t)$ — when $\psi_n(t)$ is an eigenstate of inst. $H(t)$

$\theta_n(t) = -\frac{1}{\hbar}\int E_n(t')dt'$

$\gamma_n = \gamma(T) - \gamma(0)$

$\gamma = i\int_0^t\langle\psi_n(t)|\frac{\partial}{\partial t}|\psi_n(t)\rangle dt$

Indistinguishable particles

$\Pi_{12}|a,b\rangle = |b,a\rangle$ — adds a phase

$\Pi_{12}|\psi\rangle = e^{i\phi}|\psi\rangle$, $\Pi_{12}^2|\psi\rangle = |\psi\rangle$

$= \lambda|\psi\rangle$, allowed states are eigenst. w/ eigenval λ

antisymmetrizer $\mathcal{A} \equiv \frac{1}{N!}\sum_{j=1}^{N!}(-1)^{\Pi_j}\Pi_j$

$|\psi_S\rangle = \frac{1}{\sqrt{2}}|a,b\rangle + \frac{1}{\sqrt{2}}|b,a\rangle$ $\quad \lambda = 1$ $\quad \Pi_{12} = \begin{pmatrix}0&1\\1&0\end{pmatrix}$

$|\psi_A\rangle = \frac{1}{\sqrt{2}}|a,b\rangle - \frac{1}{\sqrt{2}}|b,a\rangle$ $\quad \lambda = -1$

Sudden approx

$\tau \ll \frac{\hbar}{\Delta E}$

$H_i\psi_n^{(i)} = E_n^{(i)}\psi_n^{(i)}$, $H_f\psi_m^{(f)} = E_m^{(f)}\psi_m^{(f)}$ $\rightarrow \psi_n^{(i)} = \sum c_m\psi_m^{(f)}$

$P_{n\rightarrow m} = |c_m|^2 = |\langle\psi_m^{(f)}|\psi_n^{(i)}\rangle|^2$

Helium

$H = \left[-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{1}{4\pi\epsilon_0}\frac{2e^2}{r_1}\right] + \left[-\frac{\hbar^2}{2m}\nabla_2^2 - \frac{1}{4\pi\epsilon_0}\frac{2e^2}{r_2}\right] + \frac{1}{4\pi\epsilon_0}\frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$

spin singlet – parahelium, anti. spin triplet – orthohelium, sym.

ignoring interaction term,

$\psi(r_1, r_2) = \psi_{nlm}(\vec{r}_1)\psi_{nlm}(\vec{r}_2)$

$E = 4(E_n + E_{n'})$

Time-Dep Perturb

$\dot{c}_n e^{-\frac{iE_n^{(0)}t}{\hbar}}H_1|E_n^{(0)}\rangle = i\hbar\frac{dc_n}{dt}e^{-\frac{iE_n^{(0)}t}{\hbar}}|E_n^{(0)}\rangle$

$c_f^{(1)} = -\frac{i}{\hbar}\int_{t_0}^{t}dt'\langle f|V(t')|i\rangle e^{\frac{i(E_f^{(0)} - E_i^{(0)})t}{\hbar}}$

$P_{i\rightarrow f} = |c_f(t)|^2$

Scattering

$\psi_{sc} = A\left[e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right]$ for large r.

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

BORN APPROX: $f(\vec{k}, \vec{k}') = -\frac{m}{2\pi\hbar^2}\int e^{i(\vec{k}-\vec{k}')\cdot\vec{r}_0}V(r_0)d^3r_0$

PARTIAL WAVE EXP

$\psi(r,\theta) = A\left[e^{ikz} + k\sum_{l=0}^{\infty}i^{l+1}(2l+1)a_l h_l^{(1)}(kr)P_l(\cos\theta)\right]$

for r→∞, $f(\theta) = \sum_{l=0}^{\infty}(2l+1)a_lP_l(\cos\theta)$

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

Bohr-Sommerfeld Quantization

$\int p\,dq = 2\pi\hbar(n+\alpha)$, $\int p_i\,dq_i = n_i\hbar$

$p = \frac{\partial L}{\partial \dot{q}}$

$p = \pm\sqrt{2m(E-V)} = k\hbar$, quantization cond.

hard: potential wall, wavefunct must vanish. soft: smooth, V is finite + diff.

$\oint p(x)\,dx = \left(n + \frac{1}{2}\alpha + \frac{1}{4}\beta\right)\hbar\pi$

(α: # of hard turning; β: # of soft turning points)

transition prob. $T = \exp\left[-\frac{2}{\hbar}\int_a^b|p(x)|\,dx\right]$

Bloch Theorem (q = crystal momentum)

1. $V(x) = V(x+a)$, $\psi(x+a) = e^{iqa}\psi(x)$

2. $\psi(x) = A\sin(kx) + B\cos(kx)$ for $0<x<a$

$\psi(x) = e^{-iqa}[A\sin(k(x+a)) + B\cos(k(x+a))]$ for $-a<x<0$

at $x=a$: (for imaginary periodic potentials w/ delta)

$B = e^{-iqa}[A\sin(ka) + B\cos(ka)]$

$kA - ke^{-iqa}[A\cos(ka) - B\sin(ka)] = \frac{2m\alpha}{\hbar^2}B$

$\cos(qa) = \cos(ka) + \frac{m\alpha}{\hbar^2k}\sin(ka)$

$f(z) = \cos(z) + \beta\frac{\sin(z)}{z}$ $\quad z = ka$, $\beta = \frac{m\alpha a}{\hbar^2}$

[illegible]

Common quantum systems

infinite sq. well: $\psi(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$, $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$

free particle: $\psi(x) = \frac{1}{\sqrt{2\pi}}\int dk\,f(k)e^{i(kx-\omega t)}$, $E_n = \frac{\hbar^2k^2}{2m}$

$f(k) = \frac{1}{\sqrt{2\pi}}\int dx\,e^{-ikx}\psi(x,0)$

Harmonic oscillator: $\psi(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\frac{1}{\sqrt{2^nn!}}H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{-\frac{m\omega x^2}{2\hbar}}$

$E_n = (n+\frac{1}{2})\hbar\omega$, $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\frac{\hat{p}}{\sqrt{2m\hbar\omega}}$

Hydrogen atom: $Y_l^m = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}e^{im\phi}P_l^m(\cos\theta)$

$\psi_{100} = \frac{1}{\sqrt{\pi a_0^3}}e^{-r/a_0}$

$2s$: $\psi_{200} = \frac{1}{4\sqrt{2\pi}a_0^{3/2}}\left(2 - \frac{r}{a_0}\right)e^{-r/2a_0}$

$2p$: $\psi_{210} = \frac{1}{4\sqrt{2\pi}a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}\cos\theta$

$\psi_{21\pm1} = \mp\frac{1}{8\sqrt{\pi}a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}\sin\theta\, e^{\pm i\phi}$

Particle in a ring: $\psi(x) = \frac{1}{\sqrt{2\pi R}}e^{\frac{inx}{R}}$, $E_n = \frac{n^2\hbar^2}{2mR^2}$

Attractive Delta funct: $\psi_0 = \sqrt{\kappa}e^{-\kappa|x|}$, $E = -\frac{\hbar^2\kappa^2}{2m}$

$\kappa = \frac{m\beta}{\hbar^2}$, $V = -\beta\delta(x)$

More misc.

H-atom

$H_0 = \frac{p^2}{2\mu} - \frac{e^2}{r}$

$R_{nl} = \sqrt{\left(\frac{2}{na}\right)^3\frac{(n-l-1)!}{2n[(n+l)!]^3}}e^{-\frac{r}{na}}\left(\frac{2r}{na}\right)^l\left[L_{n-l-1}^{2l+1}\left(\frac{2r}{na}\right)\right]$

$\psi_{nlm} = R_{nl}(r)Y_{lm}(\theta,\phi)$ $\quad R_{10} = 2a^{-\frac{3}{2}}e^{-\frac{r}{a}}$ $\quad R_{20} = \frac{1}{\sqrt{2}}a^{-\frac{3}{2}}\left(1 - \frac{r}{2a}\right)e^{-\frac{r}{2a}}$

$E_{nlm} = -\frac{\mu e^4}{8h^2\epsilon_0^2}\frac{1}{n^2}$ $\quad R_{21} = \frac{1}{\sqrt{24}}a^{-\frac{3}{2}}\left(\frac{r}{a}\right)e^{-\frac{r}{2a}}$

Hermite poly.

$H_0(x) = 1$

$H_1 = 2x$

$H_2 = 4x^2 - 2$

$H_3 = 8x^3 - 12x$

$H_4 = 16x^4 - 48x^2 + 12$

$H_5 = 32x^5 - 160x^3 + 120x$

Laguerre poly

$L_0 = 1$

$L_1 = -x + 1$

$L_2 = \frac{1}{2}(x^2 - 4x + 2)$

$L_3 = \frac{1}{6}(-x^3 + 9x^2 - 18x + 6)$

$L_4 = \frac{1}{24}(x^4 - 16x^3 + 72x^2 - 96x + 24)$

Legendre: $P_n = \frac{1}{2^nn!}\frac{d^n}{dx^n}(x^2-1)^n$

$P_0 = 1$

$P_1 = x$

$P_2 = \frac{1}{2}(3x^2 - 1)$

$P_3 = \frac{1}{2}(5x^3 - 3x)$

$P_4 = \frac{1}{8}(35x^4 - 30x^2 + 3)$

Spherical Harm

$Y_0^0 = \sqrt{\frac{1}{4\pi}}$

$Y_1^{-1} = \sqrt{\frac{3}{8\pi}}\sin\theta\, e^{-i\phi}$

$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$

$Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}$

Hankel funct

$h_0^{(1)} = -i\frac{e^{ix}}{x}$

$h_1^{(1)} = \left(-\frac{i}{x^2} - \frac{1}{x}\right)e^{ix}$

$h_2^{(1)} = \left(-\frac{3i}{x^3} - \frac{3}{x^2} + \frac{i}{x}\right)e^{ix}$

$h_l^{(1)} \rightarrow \frac{1}{x}(-i)^{l+1}e^{ix}$

$h_l^{(2)} \rightarrow \frac{1}{x}(i)^{l+1}e^{-ix}$

for $x \gg 1$

$h_l^{(1)}(kr) = j_l(kr) + in_l(kr)$

$h_l^{(2)}(kr) = j_l(kr) - in_l(kr)$

Neumann (n_l)

$n_0(kr) = -\frac{\cos(kr)}{kr}$

$n_1(kr) = -\frac{\cos(kr)}{(kr)^2} - \frac{\sin(kr)}{kr}$

Spherical Bessel funct

$j_0(kr) = \frac{\sin(kr)}{kr}$,

$j_1(kr) = \frac{\sin(kr)}{(kr)^2} - \frac{\cos(kr)}{kr}$

$j_2(kr) = \left(\frac{3}{(kr)^3} - \frac{1}{kr}\right)\sin(kr) - \frac{3\cos(kr)}{(kr)^2}$

Density of states $\rho(E)$ calculation samples

for free particle $E = \frac{\hbar^2 k^2}{2m}$, $k = \frac{2\pi}{L} n$

each state takes up $\Delta k = \frac{2\pi}{L}$, so $N(k) = \frac{L}{\pi} k$ the number of states less than k.

$k = \frac{\sqrt{2mE}}{\hbar}$, $N(E) = \frac{L}{\pi}\frac{\sqrt{2mE}}{\hbar}$

$\rho(E) = \frac{dN}{dE} = \frac{L}{\pi\hbar}\frac{1}{\sqrt{2mE}}$

Multipole Expansion

$A(\vec{r}) = A_{mono} + A_{dip} + A_{quadrupole} + \dots$

Dipoles:

$E_1 = \vec{r}$, $M_1 = \vec{L} + 2\vec{S}$

Quad:

$E_2 = r^2 Y_{2m}(\theta, \phi)$

each atomic orb. has parity $\pi_\ell = (-1)^\ell$

E: even → odd

M: even → even, odd → odd

selection rules:

$E_1: \Delta \ell = \pm 1$, $\Delta m = 0, \pm 1$, $\pi_i \neq \pi_f$

$M_1: \Delta \ell = 0, \pm 2$, $\Delta m = 0, \pm 1$, $\pi_i = \pi_f$

$E_2: \Delta \ell = 0, \pm 2$, $\Delta m = 0, \pm 1, \pm 2$, $\pi_i = \pi_f$

total ang. momentum $\vec{J}$ can't go $0 \to 0$.

for dipole (E/M):

$H_{int} = -\vec{d}\cdot\vec{E} - \vec{\mu}\cdot\vec{B} + \dots$, $\vec{d} = e\vec{r}$, $\vec{\mu} \sim \vec{L} + 2\vec{S}$

transitions happen if: $E_f - E_i = \hbar\omega = \frac{\hbar c(2\pi)}{\lambda}$

$\omega = \frac{2\pi c}{\lambda}$

Roto-vibr / Morse

for diatomic molecule, $H = T_{vib} + T_{rot} + V(r)$

$T_{vib} = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}$ vibrational kinetic

$T_{rot} = \frac{L^2}{2\mu r^2}$ rotational kinetic ($L^2 = \hbar^2 J(J+1)$)

$V(r) = D_e\left(1 - e^{-a(r-r_e)}\right)^2$ Morse potential. D_e - dissociation E. r_e - equil. bond length. a - width param.

Anharmonic E-level spacing

$E_V = \hbar\omega_e(v + \frac{1}{2}) - \hbar\omega_e x_e(v + \frac{1}{2})^2$ vibrational E. $v = 0, 1, 2, \dots$ ω_e = harmonic freq. x_e = anharm const.

$E_J = B_v J(J+1)$, $B_v \approx B_e - \alpha_e(v + \frac{1}{2})$ rotational E. B_v = rot. const. α_e = vibration-rot

selection rules: $\Delta V = \pm 1$, $\Delta J = \pm 1$

Bonding / Antibonding

$\psi_b = \psi_a + \psi_b$

Bond Order $= \frac{b-a}{2}$ $\psi_a = \psi_a - \psi_b$

order: $\pi, \sigma, \pi^*, \sigma^*$

σ bonding orbitals - end-to-end overlap of s or p. Along bond axis

$\psi_\sigma = \frac{1}{\sqrt{2}}\left(\psi_{1s}^{(A)} + \psi_{1s}^{(B)}\right)$, $\psi_{\sigma^*} = \frac{1}{\sqrt{2}}\left(\psi_{1s}^{(A)} - \psi_{1s}^{(B)}\right)$

π-bonding orbitals perp. to bond axis, i.e. if along x, it would be y or z.

$\psi_\pi = \frac{1}{\sqrt{2}}\left(\psi_{2p_z}^{(A)} + \psi_{2p_z}^{(B)}\right)$, $\psi_{\pi^*} = \frac{1}{\sqrt{2}}\left(\psi_{2p_z}^{(A)} - \psi_{2p_z}^{(B)}\right)$

Hybrid:

sp^2: $\psi_1 = \frac{1}{\sqrt{3}}\psi_{2s} + \frac{1}{\sqrt{2}}\psi_{2p_x} + \frac{1}{\sqrt{6}}\psi_{2p_y}$ 120° apart orthonorm.

$\psi_2 = \frac{1}{\sqrt{3}}\psi_{2s} - \frac{1}{\sqrt{2}}\psi_{2p_x} + \frac{1}{\sqrt{6}}\psi_{2p_y}$

$\psi_3 = \frac{1}{\sqrt{3}}\psi_{2s} - \frac{2}{\sqrt{6}}\psi_{2p_y}$

Dirac-delta integrations / Deriv.

$\nabla\cdot\left(\frac{\hat{r}}{r^2}\right) = 4\pi\delta^3(\vec{r})$

$\nabla^2\left(\frac{1}{|\vec{r}|}\right) = -4\pi\delta^3(\vec{r})$

$\int \delta^3(\vec{r})\,\partial_i f(\vec{r})\,d^3r = -\int \partial_i\delta^3(\vec{r}) f(\vec{r})\,d^3r$

Eikonal Approx.

High Energy: $\psi(\vec{r}) = e^{ikz} e^{i\chi(\vec{b}, z)}$

$\chi(\vec{b}) = -\frac{1}{\hbar v}\int_{-\infty}^{\infty} V(\vec{b}, z')\,dz'$

$f(k, k') = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int_0^\infty b\,db\int_0^{2\pi} d\phi\, e^{-i q b \cos\phi}\int_{-\infty}^{\infty} dz\, V(\sqrt{b^2+z^2})\, e^{-\frac{i}{\hbar v}\int_{-\infty}^{z} V\,dz'}$

RWA

Terms such as $e^{i(\omega_0 - \omega)t}$, $e^{i(\omega_0 - \omega)t}$

drop them "non-resonant" terms when $\omega \approx \omega_0$

"forbidden" transitions by parity or spin-flip

Electric dipole (E1)

$T_{i\to f} \propto |\langle f|\vec{d}\cdot\vec{E}|i\rangle|^2\,\delta(E_f - E_i - \hbar\omega)$

Parity must change; spin will not.

$\Delta \ell = \pm 1$, $\Delta J = 0, \pm 1$, $\Delta m = 0, \pm 1$

Mag dipole (M1)

$\Delta \ell = 0$, $\Delta J = 0, \pm 1$, $\Delta m = 0, \pm 1$

Parity stays same, spin can flip.

$L_\pm|\ell, m\rangle = \sqrt{\ell(\ell+1) - m(m\pm 1)}\,|\ell, m\pm 1\rangle$

Two-Body Scattering

two masses, m_1 and m_2, $V = V(\vec{r}_1 - \vec{r}_2)$

$\vec{r} = \vec{r}_1 - \vec{r}_2$, $\vec{R} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1 + m_2}$ center of mass pos.

$H = -\frac{\hbar^2}{2M}\nabla_R^2 - \frac{\hbar^2}{2\mu}\nabla_r^2 + V(\vec{r})$

$M = m_1 + m_2$, $\mu = \frac{m_1 m_2}{m_1 + m_2}$

$\Psi(R, r) = \psi_{com}(\vec{R})\,\psi_{rel}(\vec{r})$

$-\frac{\hbar^2}{2M}\nabla_R^2\psi_{com} = E_{com}\psi_{com}$ free particle

$\left[-\frac{\hbar^2}{2\mu}\nabla_r^2 + V(\vec{r})\right]\psi_{rel} = E_{rel}\psi_{rel}$ particle in potential V

Simplification of Born

$V(\vec{r}) = V(r)$ spherically sym.

$f(\theta) = -\frac{2\mu}{\hbar^2 q}\int_0^\infty r V(r)\sin(qr)\,dr$

short range:

$f(0) = -\frac{2\mu}{\hbar^2}\int_0^R r^2 V(r)\,dr$

Delta funct scattering

$V(\vec{r}) = \delta^3(\vec{r})\,V_0$

$f(\theta) = -\frac{2\mu}{4\pi\hbar^2}V_0$

Rutherford scattering

for Yuk $\beta = \frac{q_1 q_2}{4\pi\epsilon_0}$, $\mu = 0$,

$f(\theta) = -\frac{2m q_1 q_2}{4\pi\epsilon_0\hbar^2 k^2} \approx \frac{q_1 q_2}{16\pi\epsilon_0 \sin^2(\frac{\theta}{2})}$

Yukawa scattering

$V(r) = \beta e^{-\mu r}\frac{1}{r}$

$f(\theta) = -\frac{2m\beta}{\hbar^2 K}\int_0^\infty e^{-\mu r}\sin(kr)\,dr = \frac{-2m\beta}{\hbar^2(\mu^2 + k^2)}$

Adiabatic thm

Condition: $\left|\frac{\langle\psi_m(t)|\dot{H}(t)|\psi_n(t)\rangle}{(E_m(t) - E_n(t))^2}\right| \ll 1$

rate of Hamiltonian change is small compared to minimum E gap.

OR System passes through crossing where $\Delta E \to 0$ so transitions occur b/w eigenstates

Sudden Approx.

Condition: $\delta t \ll \frac{\hbar}{\Delta E}$ change occurs much faster than relevant energy differences

For Harmonic oscillator, $\langle T\rangle = \langle V\rangle = \frac{1}{2}E$

Differential cross-section: $d\Omega = \sin\theta\,d\theta\,d\phi$

Kinetic Energy operator is $-\frac{\hbar^2}{2m}\nabla^2$ to apply to pos-space

for incident momentum k and outgoing k' at angle θ,

$|k - k'| = \sqrt{2}\,k\sqrt{1 - \cos\theta} = 2k\sin\frac{\theta}{2}$

s-wave means $\ell = 0$.

WKB (very brief)

$p(x) = \sqrt{2m(E - V(x))}$ classical momentum

classically allowed $(E > V)$: $\psi(x) \approx \frac{C}{\sqrt{p(x)}}\exp\left(\pm\frac{i}{\hbar}\int^x p(x')\,dx'\right)$

classically forbidden $(E < V)$: $\psi(x) \approx \frac{C}{\sqrt{|p(x)|}}\exp\left(\pm\frac{1}{\hbar}\int^x |p(x')|\,dx'\right)$

for barrier b/w x_1, x_2: $T = \exp\left(-\frac{2}{\hbar}\int_{x_1}^{x_2}|p(x)|\,dx\right)$

in classically allowed regions: $|\psi(x)|^2 \propto \frac{1}{p(x)}$

for some soln $\psi(x) = \frac{1}{\sqrt{p(x)}}e^{\pm\frac{i}{\hbar}\int p(x')\,dx'}$, $\vec{J} = \frac{\hbar}{2mi}\left(\psi^*\frac{d\psi}{dx} - \psi\frac{d\psi^*}{dx}\right)$, $J = \pm\frac{1}{m}$

Patching functions:

Common Boundary Conditions

for infinite potentials: $\psi(x = a) = 0$

for finite (but mostly inescapable potential walls): $\left.\frac{d\psi}{dx}\right|_{x=a} = 0$

for piecewise potentials (like $V = V_0$ in region, 0 else): $\psi(x^-) = \psi(x^+)$

$\psi'(x^-) = \psi'(x^+)$ if potential finite.

delta funct at $x = a$: $V = -\alpha\delta(x-a)$ → $\psi'(a^+) - \psi'(a^-) = -\frac{2m\alpha}{\hbar^2}\psi(a)$

Born Approx. Validity:

scattering wave much smaller than incident wave.

1. $|V(r)| \ll E$ potential energy much smaller than particle E.
2. $ka \gg 1$, k = incident wavenumber, a = potential range
3. Short range potentials ($V(r) \to 0$ fast as $r \to \infty$).

Cross section small ($\frac{d\sigma}{d\Omega}$) compared to cross section of eff. potential range

$V_{eff} = V(r) + \frac{\hbar^2\ell(\ell+1)}{2\mu r^2}$ → this is why we consider s-waves!

Born

$\frac{\mu V_0 a^2}{\hbar^2} \ll 1$ low energy

$\frac{2m|V_0|a}{\hbar^2 k}\ln ka \ll 1$ high energy

Partial wave expansion (cont'd)

$f(\theta) = \sum_{\ell=0}^{\infty}(2\ell+1)\,a_\ell(k)\,P_\ell(\cos\theta)$, $\sigma_0 = 4\pi|a_0(k)|^2 = \frac{4\pi}{k^2}\sin^2\delta_0$

$a_\ell(k) = \frac{1}{k}e^{i\delta_\ell}\sin\delta_\ell \to a_0(k) = \frac{1}{k}e^{i\delta_0}\sin\delta_0$

Phase shifts

$\psi(x) = A\left(e^{ikx} - e^{i(2\delta - kx)}\right)$

$\psi^{(\ell)} \approx A\frac{(2\ell+1)}{2ikr}\left[e^{i(kr + 2\delta_\ell)} - (-1)^\ell e^{-ikr}\right]P_\ell(\cos\theta)$

$f(\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\,e^{i\delta_\ell}\sin(\delta_\ell)\,P_\ell(\cos\theta)$

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

for first born Approx:

$\sin(\delta_0) = -\frac{2m}{\hbar^2}\frac{1}{k}\int_0^\infty V(r)\sin^2(kr)\,dr$

Hydrogen Atom (combined things)

$E_n = -\frac{13.6\,eV}{n^2} = -\frac{1}{2}\alpha^2 mc^2\frac{1}{n^2} = -\frac{1}{2}\frac{e^4 m_e}{(4\pi\epsilon_0)^2\hbar^2 n^2} = -\frac{\hbar^2}{2m_e a_0^2 n^2}$

$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}$

For time

$$V = \begin{cases} \frac{1}{2}kx^2 & x > 0 \\ +\infty & x < 0 \end{cases}$$

half HO, so we use solution but require only odd parity eigenstates.

$E_n = (n+\frac{1}{2})\hbar\omega, \quad n = 1, 3, 5, \ldots$

$E_n = (2n+\frac{3}{2})\hbar\omega, \quad n \in \mathbb{Z}^+$

Spin - Combination three

$$H = \frac{3\varepsilon}{\hbar^2}(\vec{S}_1 + \vec{S}_3)\cdot\vec{S}_2 + \frac{2\varepsilon}{\hbar^2}\left|(\vec{S}_1 + \vec{S}_3) + \vec{S}_2\right|^2$$

$$= \frac{3\varepsilon}{\hbar^2}\vec{S}_{13}\cdot\vec{S}_2 + \frac{2\varepsilon}{\hbar^2}\left|\vec{S}_{13} + \vec{S}_2\right|^2$$

$$\vec{S}_{13}\cdot\vec{S}_2 = \frac{1}{2}\left(|\vec{S}_{13} + \vec{S}_2|^2 - |\vec{S}_{13}|^2 - |\vec{S}_2|^2\right)$$

Dirac - Delta

$V = -\alpha\delta(x-a)$

define $\kappa = \frac{\sqrt{-2mE}}{\hbar}$, $E = -\frac{\hbar^2\kappa^2}{2m}$

$\frac{d^2\psi}{dx^2} = \kappa^2\psi$, $\psi = \begin{cases} Ae^{\kappa x} & x < a \\ Be^{-\kappa x} & x > a \end{cases}$

$-\kappa Be^{-\kappa a} - \kappa Ae^{\kappa a} = -\frac{2m\alpha}{\hbar^2}Ae^{\kappa a}$

$\kappa = \frac{m\alpha}{\hbar^2}$, $E = -\frac{m\alpha^2}{2\hbar^2}$

$\psi(x) = \sqrt{\kappa}\, e^{-\kappa|x-a|}$

$= \sqrt{\frac{m\alpha}{\hbar^2}}\, e^{-\frac{m\alpha}{\hbar^2}|x-a|}$

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positive potential $V = \alpha\delta(x-a)$

$\psi(x) = \begin{cases} e^{ikx} + Re^{-ikx} & x < a \\ Te^{ikx} & x > a \end{cases}$

$\beta = \frac{m\alpha}{\hbar^2}$, $T = \frac{ik}{ik-\beta}$, $R = \frac{\beta}{ik-\beta}$