QM2

Quantum Mechanics 2 notes by K. Sreeman Reddy.

Angular Momentum

$\mathbf{J} = \mathbf{L} + \mathbf{S}$
The following formulas are valid even if we replace $\mathbf{J}$ with $\mathbf{L}$ or $\mathbf{S}$.
$\mathbf{J} \times \mathbf{J} = i\hbar\mathbf{J}$
$[J_l, J_m] = i\hbar \sum_{n=1}^{3} \varepsilon_{lmn} J_n$
$J^2 \equiv J_x^2 + J_y^2 + J_z^2$
$\left[J^2, J_x\right] = \left[J^2, J_y\right] = \left[J^2, J_z\right] = 0$
$\sigma_{J_x}\sigma_{J_y} \geq \frac{\hbar}{2}\left|\langle J_z\rangle\right|$

Generator of rotations

$$R(\hat{n}, \Delta\theta) = \lim_{N\to\infty}\left(1 - \frac{i}{\hbar}\frac{\Delta\theta}{N}\hat{\mathbf{n}}\cdot\hat{\mathbf{J}}\right)^N = \exp\left(-\frac{i}{\hbar}\Delta\theta\hat{\mathbf{n}}\cdot\hat{\mathbf{J}}\right)$$

$$\begin{aligned} R(\hat{n}, \phi) &= \exp\left(-\frac{i\phi J_{\hat{n}}}{\hbar}\right) \\ &= R_{\text{internal}}(\hat{n}, \phi)\, R_{\text{spatial}}(\hat{n}, \phi) \end{aligned}$$

where $R_{\text{spatial}}(\hat{n}, \phi) = \exp\left(-\frac{i\phi L_{\hat{n}}}{\hbar}\right)$, and $R_{\text{internal}}(\hat{n}, \phi) = \exp\left(-\frac{i\phi S_{\hat{n}}}{\hbar}\right)$,

When the total angular momentum quantum number is a half-integer (1/2, 3/2, etc.), $R(\hat{n}, 360^\circ) = -1$, and when it is an integer, $R(\hat{n}, 360^\circ) = +1$. Mathematically, the structure of rotations in the universe is not SO(3), the group of three-dimensional rotations in classical mechanics. Instead, it is SU(2), which is identical to SO(3) for small rotations, but where a 360° rotation is mathematically distinguished from a rotation of 0°. A rotation of 720° is, however, the same as a rotation of 0°.

On the other hand, $R_{\text{spatial}}(\hat{n}, 360^\circ) = +1$ in all circumstances, because a 360° rotation of a spatial configuration is the same as no rotation at all. (This is different from a 360° rotation of the internal (spin) state of the particle, which might or might not be the same as no rotation at all.)

When rotation operators act on quantum states, it forms a representation of the Lie group $SU(2)$ (for R and R_{internal}), or $SO(3)$ (for R_{spatial}).

Conservation of angular momentum

In a spherically-symmetric situation, the Hamiltonian is invariant under rotations and angular momentum is conserved.

$$RHR^{-1} = H \Rightarrow [H, R] = 0 \Rightarrow [H, \mathbf{J}] = \mathbf{0}$$

Ladder operators

$J_+ = J_x + iJ_y,$
$J_- = J_x - iJ_y,$

$$[J_i, J_j] = i\hbar \sum_{k=1}^{3} \epsilon_{ijk} J_k,$$

where ϵ_{ijk} is the Levi-Civita symbol and each of i, j and k can take any of the values x, y and z.

From this, the commutation relations among the ladder operators and Jz are obtained,

$$[J_z, J_\pm] = \pm\hbar J_\pm$$

$$[J_+, J_-] = 2\hbar J_z$$

$$J_+|j,m\rangle = \hbar\sqrt{(j-m)(j+m+1)}|j\,(m+1)\rangle = \hbar\sqrt{j(j+1)-m(m+1)}|j\,(m+1)\rangle,$$

$$J_-|j,m\rangle = \hbar\sqrt{(j+m)(j-m+1)}|j\,(m-1)\rangle = \hbar\sqrt{j(j+1)-m(m-1)}|j\,(m-1)\rangle.$$

Since $-j \le m \le j$
$J_+|j\,j\rangle = 0$
$J_-|j\,(-j)\rangle = 0$

The Variational Method

$$E[\psi] \equiv \frac{\langle\psi|H|\psi\rangle}{\langle\psi \mid \psi\rangle} \ge E_0$$

If ψ is a function of $\alpha, \beta, \ldots$ then $E[\psi]$ reduces to a function, $E(\alpha, \beta, \ldots)$. We then find the values $(\alpha_0, \beta_0, \ldots)$ which minimize E. This minimum $E\left(\alpha_0, \beta_0, \ldots\right)$ provides an upper bound on E_0.

Higher energy states

For example to get the energy of the 1st excited state we can find all states which are perpendicular to $\psi\left(\alpha_0, \beta_0, \ldots\right)$ and then minimize the energy. That will given an upper bound to the 1st excited state.

If H is rotationally invariant, the energy eigenstates have definite angular momentum. The ground state will have $l = 0$. By varying spherically symmetric trial functions we can estimate the ground-state energy. If we next choose $l = 1$ trial functions $\left[\psi = R(r) Y_1^m\right], E[\psi]$ wil obey

$$E[\psi] \ge E_{l=1}$$

where $E_{l=1}$ is the lowest energy level with $l = 1$. We can clearly keep going up in l.

The WKB Method

The energy eigenfunctions with eigenvalue E are

$$\psi(x) = \psi(0) e^{\pm ipx/\hbar}, \quad p = [2m(E-V)]^{1/2}$$

Suppose that V varies very slowly. We then expect that over a small region ψ will still behave like a plane wave, with the local value of the wavelength

$$\lambda(x) = \frac{2\pi\hbar}{p(x)} = \frac{2\pi\hbar}{\{2m[E-V(x)]\}^{1/2}}$$

then

$$\psi(x) = \psi\left(x_0\right) \exp\left[\pm(i/\hbar) \int_{x_0}^{x} p\left(x'\right) dx'\right]$$

Validity

$$\left|\frac{\delta\lambda}{\lambda}\right|=\left|\frac{(d\lambda/dx)\cdot\lambda}{\lambda}\right|=\left|\frac{d\lambda}{dx}\right|\ll 1$$

1st order

Without loss of generality we let $\psi(x)=\exp[i\phi(x)/\hbar]$

$$\Rightarrow -\left(\frac{\phi'}{\hbar}\right)^2+\frac{i\phi''}{\hbar}+\frac{p^2(x)}{\hbar^2}=0$$

let

$$\phi=\phi_0+\hbar\phi_1+\hbar^2\phi_2+\cdots$$

if we neglect all $\hbar$ terms we get the previous result. But if we include $\hbar\phi_1$ we get

$$\psi(x)=\psi\left(x_0\right)\left[\frac{p\left(x_0\right)}{p(x)}\right]^{1/2}\exp\left[\pm\frac{i}{\hbar}\int_{x_0}^{x}p\left(x'\right)dx'\right]$$

Time-Independent Perturbation Theory

Developed by Erwin Schrödinger.

$$\begin{aligned}H&=H^0+H'\\|n\rangle&=\left|n^0\right\rangle+|n'\rangle+\left|n^2\right\rangle+\cdots\\E_n&=E_n^0+E_n'+E_n^2+\cdots\end{aligned}$$

Equating each order we get

$$\begin{aligned}H^0\left|n^0\right\rangle&=E_n^0\left|n^0\right\rangle\\H^0\left|n'\right\rangle+H'\left|n^0\right\rangle&=E_n^0\left|n'\right\rangle+E_n'\left|n^0\right\rangle\\H^0\left|n^2\right\rangle+H'\left|n'\right\rangle&=E_n^0\left|n^2\right\rangle+E_n'\left|n'\right\rangle+E_n^2\left|n^0\right\rangle\end{aligned}$$

Using $\left\langle n^0 \mid n^r\right\rangle=0$ for $r\geq 1$ we get

$$\begin{aligned}E_n^1&=\left\langle n^0\left|H'\right|n^0\right\rangle\\\left|n^1\right\rangle&=\sum_{m\neq n}\frac{\left|m^0\right\rangle\left\langle m^0\left|H^1\right|n^0\right\rangle}{E_n^0-E_m^0}\\E_n^2&=\left\langle n^0\left|H'\right|n'\right\rangle=\sum_{m\neq n}\frac{\left|\left\langle n^0\left|H'\right|m^0\right\rangle\right|^2}{E_n^0-E_m^0}\end{aligned}$$

Validity

A necessary condition for $\left|n^1\right\rangle$ to be small compared to $\left|n^0\right\rangle$ is that

$$\left|\frac{\left\langle m^0\left|H^1\right|n^0\right\rangle}{E_n^0-E_m^0}\right|\ll 1$$

Selection rules

Degenerate Perturbation Theory

We need to find the basis that diagonalizes H^1 only within the degenerate space and not the full Hilbert space.

Time-Dependent Perturbation Theory

Method of variation of constants

Developed by Paul Dirac. Let $H(t) = H^0 + H^1(t)$ and assume that we know the eigenstates $|n^0\rangle$ of H^0 which form a **complete basis** then

$$\begin{aligned}|\psi(t)\rangle &= \sum_n c_n(t)|n^0\rangle \\ &= \sum_n d_n(t)e^{-iE_nt/\hbar}|n^0\rangle \\ \Rightarrow i\hbar\frac{d}{dt}|\psi(t)\rangle = (H^0 + H^1(t))|\psi(t)\rangle &= \sum_n (i\hbar\dot{d}_n + E_n)e^{-iE_nt/\hbar}|n^0\rangle\end{aligned}$$

$$\boxed{\frac{\mathrm{d}d_f}{\mathrm{d}t} = \frac{-i}{\hbar}\sum_n \langle f^0|H^1(t)|n^0\rangle\, d_n(t)\, e^{-i(E_n-E_f)t/\hbar}\,.}$$

in the above eqn we need to substitute i th order solution to get $i+1$ th order. Let at $|\psi(0)\rangle = |i^0\rangle$ then d_i to the zeroth order is $\delta_{fi} \Rightarrow$

$$\boxed{d_f^{(0)}(t) + d_f^{(1)}(t) = \delta_{fi} - \frac{i}{\hbar}\int_0^t dt'\ \langle f^0|H^1(t')|i^0\rangle\, e^{\frac{i(E_f^0-E_i^0)t'}{\hbar}}}$$

$|d_f|^2$ is the probability that the state will go from $|i^0\rangle$\$ to $|f^0\rangle$ if we apply $H^1(t)$ from $0 \to t$. $d_f =$ **transition amplitude**. Often we define $\omega_{fi} = \dfrac{E_f^0 - E_i^0}{\hbar}$.

Sudden Perturbation

$$\lim_{\epsilon\to 0} i\hbar(|\Psi(\epsilon/2)\rangle - |\Psi(-\epsilon/2)\rangle) = \int_{-\epsilon/2}^{\epsilon/2} \hat{H}|\Psi(t)\rangle dt = 0$$

unless $\hat{H}$ is a multiple of $\delta(t)$. If the transition probability is calculated perturbatively, it must vanish **to any given order**.

Adiabatic Perturbation

Let $H(t)|n(t)\rangle = E_n(t)|n(t)\rangle$ and $|\psi(t)\rangle = \sum_n c_n(t)|n(t)\rangle$ (**complete basis**) then

$$\begin{aligned}i\hbar|\dot{\psi}(t)\rangle &= H(t)|\psi(t)\rangle \\ \Rightarrow i\hbar(\sum_n \dot{c}_n(t)|n(t)\rangle + \sum_n c_n(t)|\dot{n}(t)\rangle) &= \sum_n c_n(t)E_n(t)|n(t)\rangle \\ \Rightarrow i\hbar\dot{c}_m(t) + i\hbar\sum_n c_n(t)\langle m(t)|\dot{n}(t)\rangle &= c_m(t)E_m(t) \\ \dot{H}(t)|n(t)\rangle + H(t)|\dot{n}(t)\rangle &= \dot{E}_n(t)|n(t)\rangle + E_n(t)|\dot{n}(t)\rangle \\ \Rightarrow \langle m(t)|\dot{n}(t)\rangle &= -\frac{\langle m(t)|\dot{H}(t)|n(t)\rangle}{E_m(t) - E_n(t)} \qquad (m \neq n) \\ \Rightarrow \dot{c}_m(t) + \left(\frac{i}{\hbar}E_m(t) + \langle m(t)|\dot{m}(t)\rangle\right)c_m(t) &= \sum_{n\neq m}\frac{\langle m(t)|\dot{H}|n(t)\rangle}{E_m(t) - E_n(t)}c_n(t)\end{aligned}$$

neglect the right hand side if $\dot{H}(t)$ is small and there is a **finite** gap $E_m(t) - E_n(t) \neq 0$ between the energies.

$$\boxed{\Rightarrow c_n(t) = c_n(0)e^{i\theta_n(t)}e^{i\gamma_n(t)} \Rightarrow |c_n(t)|^2 = |c_n(0)|^2}$$

with the dynamical phase $\theta_m(t) = \frac{-1}{\hbar}\int_0^t E_m(t')dt'$ and geometric phase $\gamma_m(t) = i\int_0^t \langle m(t')|\dot{m}(t')\rangle dt'$

Periodic Perturbation

Let $H^1(t) = H^1 e^{-i\omega t}$ be started at $t = 0$ then

$$
\begin{aligned}
d_f(t) &= -\frac{i}{\hbar}\int_0^t dt' \ \langle f^0|H^1|i^0\rangle \, e^{i(\omega_{fi}-\omega)t'} \\
&= -\frac{i}{\hbar}\langle f^0|H^1|i^0\rangle \int_0^t dt' \ e^{i(\omega_{fi}-\omega)t'} \\
\Rightarrow P_{i\to f} = |d_f(t)|^2 &= \frac{\langle f^0|H^1|i^0\rangle^2}{\hbar^2}\left(\frac{sin((\omega_{fi}-\omega)t/2)}{(\omega_{fi}-\omega)t/2}\right)^2 t^2
\end{aligned}
$$

For small t, the system shows no particular preference for the level with $E_f^0 = E_i^0 + h\omega$. Only when $\omega t >> 2\pi$ does it begin to favor $E_f^0 = E_i^0 + h\omega$. Now we know that $\delta(x) = \frac{1}{2\pi}\lim_{\epsilon\to 0}\int_{-\frac{1}{\epsilon}}^{\frac{1}{\epsilon}} e^{ikx}dx = \lim_{\epsilon\to 0}\frac{\sin(x/\epsilon)}{\pi x}$

$$
\lim_{t\to\infty} P_{i\to f} = \frac{\langle f^0|H^1|i^0\rangle^2}{\hbar^2}(\delta((\omega_{fi}-\omega)/2)\pi)^2 = 4\frac{\langle f^0|H^1|i^0\rangle^2}{\hbar^2}(\delta(\omega_{fi}-\omega)\pi)^2
$$

since $\delta(\alpha x) = \frac{\delta(x)}{|\alpha|}$ and

$$
\lim_{t\to\infty}\frac{sin^2(yt)}{\pi y^2 t} = \lim_{t\to\infty}\frac{\pi^2\delta(y)^2}{\pi t} = \delta(y) \Rightarrow \delta(y)^2 = \lim_{t\to\infty}\delta(y)\frac{t}{\pi}
$$

Fermi's golden rule

Derived by Dirac.

$$
R_{i\to f} = \frac{P_{i\to f}}{T} = \frac{2\pi}{\hbar}|\langle f^0|H^1|i^0\rangle|^2\delta(E_f^0 - E_i^0 - \hbar\omega)
$$

The transition probability per unit of time from the initial state $|i\rangle$ to a set of final states $|f\rangle$ is essentially constant.

Harmonic Perturbation

$H^1(t) = V\exp(\mathrm{i}\omega t) + V^\dagger\exp(-\mathrm{i}\omega t)$ (emission+absorption)
$c_f(t) = -\frac{\mathrm{i}}{\hbar}\int_0^t [V_{fi}\exp(......i\omega t')]\exp(\mathrm{i}\omega_{fi}t')dt'$
$c_f(t) = -\frac{\mathrm{i}t}{\hbar}\left(V_{fi}\exp\left[\mathrm{i}(\omega_{fi})t/2\right]\mathrm{sinc}\left[(\omega+\omega_{fi})t/2\right] \ + V_{fi}^\dagger\exp\left[-\mathrm{i}(\omega-\omega_{fi})t/2\right]\mathrm{sinc}\left[(\omega-\omega_{fi})t/2\right]\right),$
$P_{i\to f}(t) = \frac{t^2}{\hbar^2}\left\{|V_{fi}|^2\mathrm{sinc}^2\left[(\omega+\omega_{fi})t/2\right] + |V_{fi}^\dagger|^2\mathrm{sinc}^2\left[(\omega-\omega_{fi})t/2\right]\right\}$
$V_{fi} = \langle f|V|i\rangle,$
Detailed balancing:
emission rate for i -> [n] /density of final states for [n] =
absorption rate for n -> [i]/density of final states for [i]

For constant perturbation, we obtain appreciable transition probability for $|i^0\rangle \to |n^0\rangle$ only if $E_n \approx E_i$. In contrast, for harmonic perturbation, we have appreciable transition probability only if $E_n \approx E - i\hbar\omega$ (stimulated emission) or $E_n \approx i\hbar\omega$ (absorption).

Interaction of Atoms with Radiation

$$
\left[\frac{1}{2m}(\boldsymbol{\sigma}\cdot(\mathbf{p}-q\mathbf{A}))^2 + q\phi\right]|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle
$$

Pictures

	Heisenberg	Interaction	Schrödinger
Ket state	constant	$\mid\psi_{\rm I}(t)\rangle = e^{iH_{0,\rm S}\,t/\hbar}\mid\psi_{\rm S}(t)\rangle$	$\mid\psi_{\rm S}(t)\rangle = e^{-iH_{\rm S}\,t/\hbar}\mid\psi_{\rm S}(0)\rangle$
Observable	$A_{\rm H}(t) = e^{iH_{\rm S}\,t/\hbar}A_{\rm S}e^{-iH_{\rm S}\,t/\hbar}$	$A_{\rm I}(t) = e^{iH_{0,\rm S}\,t/\hbar}A_{\rm S}e^{-iH_{0,\rm S}\,t/\hbar}$	constant
Density matrix	constant	$\rho_{\rm I}(t) = e^{iH_{0,\rm S}\,t/\hbar}\rho_{\rm S}(t)e^{-iH_{0,\rm S}\,t/\hbar}$	$\rho_{\rm S}(t) = e^{-iH_{\rm S}\,t/\hbar}\rho_{\rm S}(0)e^{iH_{\rm S}\,t/\hbar}$

Heisenberg Picture

$$\frac{d}{dt}A_{\rm H}(t) = \frac{i}{\hbar}[H_{\rm H}, A_{\rm H}(t)] + \left(\frac{\partial A_{\rm S}}{\partial t}\right)_{\rm H}$$

Interaction Picture

If $H_{\rm S} = H_{0,\rm S} + H_{1,\rm S}$,

$$\begin{aligned} i\hbar\frac{d}{dt}|\psi_{\rm I}(t)\rangle &= H_{1,\rm I}(t)|\psi_{\rm I}(t)\rangle, \\ i\hbar\frac{d}{dt}A_{\rm I}(t) &= [A_{\rm I}(t), H_{0,\rm S}]. \\ i\hbar\frac{d}{dt}\rho_{\rm I}(t) &= [H_{1,\rm I}(t), \rho_{\rm I}(t)], \end{aligned}$$

Method of Dyson series

Scattering Theory

Lippmann–Schwinger equation

Let $H = H_0 + V$, where the eigenstates of H_0 are known exactly, and the potential V gives corrections that are **small** in some sense

$$H_0|\phi\rangle = E|\phi\rangle$$

If the energies E are continuous, we should be able to find an eigenstate $|\psi\rangle$ of the full Hamiltonian with the same eigenvalue:

$$H|\psi\rangle = E|\psi\rangle$$

we can see that if

$$\begin{aligned} |\psi\rangle = |\phi\rangle + \frac{1}{E-H_0}V|\psi\rangle \\ \Rightarrow (E-H_0)|\psi\rangle = (E-H_0)|\phi\rangle + V|\psi\rangle \\ \Rightarrow (H-H_0)|\psi\rangle = V|\psi\rangle = (E-E)|\phi\rangle + V|\psi\rangle \end{aligned}$$

also if we define $\Pi_{LS} = \dfrac{1}{E-H_0}$

$$\begin{aligned} |\psi\rangle &= |\phi\rangle + \Pi_{LS}V(|\phi\rangle + \Pi_{LS}V|\psi\rangle) \\ \Rightarrow |\psi\rangle &= |\phi\rangle + \Pi_{LS}V(|\phi\rangle + \Pi_{LS}V(|\phi\rangle + \Pi_{LS}V|\psi\rangle)) \\ \Rightarrow |\psi\rangle &= (I + \Pi_{LS}V + \Pi_{LS}V\Pi_{LS}V + \cdots)|\phi\rangle \end{aligned}$$

we often define the **transfer matrix** by $T|\phi\rangle = V|\psi\rangle$ then

$$T = V + V\Pi_{LS}V + V\Pi_{LS}V\Pi_{LS}V + \cdots$$

But $\Pi_{LS} = \frac{1}{E-H_0}$ is not defined since $E - H_0$ is **singular** in matrix form. So, we **add** $\pm i\epsilon$ for some $\epsilon > 0$ and $\Pi_{LS}^{(\pm)} = \dfrac{1}{E - H_0 \pm i\epsilon}$ and in the end we can apply $\epsilon \to 0$

$$|\psi^{(\pm)}\rangle = |\phi\rangle + \frac{1}{E - H_0 \pm i\epsilon} V|\psi^{(\pm)}\rangle$$

$$\begin{aligned}
|\psi^{(\pm)}\rangle &= |\phi\rangle + \int d^3\vec{p}'\,|\vec{p}'\rangle\langle\vec{p}'|\frac{1}{E - H_0 \pm i\epsilon} V|\psi^{(\pm)}\rangle \\
\langle\vec{p}|\psi^{(\pm)}\rangle &= \langle\vec{p}|\phi\rangle + \int d^3\vec{p}'\,\frac{1}{E - \frac{p'^2}{2m} \pm i\epsilon}\langle\vec{p}|\vec{p}'\rangle\langle\vec{p}'|V|\psi^{(\pm)}\rangle \\
&= \langle\vec{p}|\phi\rangle + \int d^3\vec{p}'\,\frac{1}{E - \frac{p'^2}{2m} \pm i\epsilon}\delta(\vec{p} - \vec{p}')\langle\vec{p}'|V|\psi^{(\pm)}\rangle \\
&= \langle\vec{p}|\phi\rangle + \frac{1}{E - \frac{p^2}{2m} \pm i\epsilon}\langle\vec{p}|V|\psi^{(\pm)}\rangle
\end{aligned}$$

as expected using $\langle\vec{p}|\psi^{(\pm)}\rangle = \langle\vec{p}|\phi\rangle + \langle\vec{p}|\Pi_{LS}^{(\pm)}V|\psi^{(\pm)}\rangle$. Note that $\langle\vec{p}|\vec{p}'\rangle = \delta(\vec{p} - \vec{p}') = Dirac \neq \text{Kronecker}$ as they are not normalizable. By defining $T^{(\pm)}|\phi\rangle = V|\psi^{(\pm)}\rangle$ we get $T_{\beta\alpha}^{(\pm)} = \langle\phi_\beta|T^{(\pm)}|\phi_\alpha\rangle = \langle\phi_\beta|V|\psi_\alpha^{(\pm)}\rangle$

$$\begin{aligned}
|\psi_\alpha^{(\pm)}\rangle &= |\phi_\alpha\rangle + \int d\beta\,\frac{|\phi_\beta\rangle\langle\phi_\beta|V|\psi_\alpha^{(\pm)}\rangle}{E_\alpha - E_\beta \pm i\epsilon} \\
&= |\phi_\alpha\rangle + \int d\beta\,\frac{T_{\beta\alpha}^{(\pm)}|\phi_\beta\rangle}{E_\alpha - E_\beta \pm i\epsilon}
\end{aligned}$$

Green's function

$$\begin{aligned}
\langle\vec{x}|\psi^{(\pm)}\rangle &= \langle\vec{x}|\phi\rangle + \int d^3\vec{x}'\,\langle\vec{x}|\frac{1}{E - H_0 \pm i\epsilon}|\vec{x}'\rangle\langle\vec{x}'|V|\psi^{(\pm)}\rangle \\
\langle\vec{x}|\psi^{(\pm)}\rangle &= \langle\vec{x}|\phi\rangle - \frac{2m}{\hbar^2}\int d^3\vec{x}'\,\frac{e^{\pm ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|}\langle\vec{x}'|V|\psi^{(\pm)}\rangle
\end{aligned}$$

Let $G^{(\pm)}(\mathbf{x}, \mathbf{x}') = \frac{\hbar^2}{2m}\langle\mathbf{x}|\Pi_{LS}^{(\pm)}|\mathbf{x}'\rangle$ then $G^{(\pm)}(\mathbf{x}, \mathbf{x}') = -\dfrac{e^{\pm ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|}$

$$(\nabla^2 + k^2)G^{(\pm)}(\mathbf{x}, \mathbf{x}') = \delta^{(3)}(\mathbf{x} - \mathbf{x}')$$

The cross section

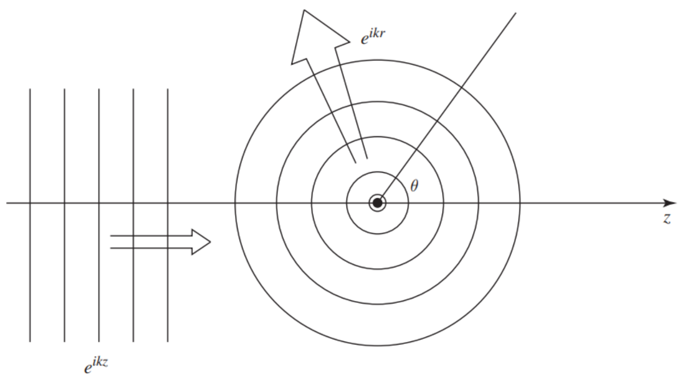

Figure 10.4: Scattering of waves; an incoming plane wave generates an outgoing spherical wave.

The general solution for a scattering is

$$\psi(\mathbf{x}) = e^{i\vec{k}\cdot\vec{x}} + f(\vec{k}, \vec{k}')\frac{e^{ikr}}{r}\ ,$$

here $f(\vec{k}, \vec{k'})$ is **the scattering amplitude**.
In writing above eqn we have used the elasticity of the scattering, imposing the condition that the outgoing wave has the same momentum, $k = |\vec{k}|$, as the incoming wave.
Differential cross section is $\frac{d\sigma}{d\Omega} = |f(\vec{k}, \vec{k'})|^2$

$$f(\vec{k}, \vec{k'}) = -\frac{m}{2\pi\hbar^2}\langle\phi|V|\psi^{(\pm)}\rangle = -\frac{m}{2\pi\hbar^2}\int d^3\vec{x}'\, e^{\mp i\vec{k'}\cdot\vec{x}'}\, V(\vec{x}')\langle\vec{x}'|\psi^{(\pm)}\rangle$$

$$\phi(\vec{x}) = e^{i\vec{k}\cdot\vec{x}}$$

Spherically symmetric

Optical theorem

Derived by Werner Heisenberg.

$$\sigma_{tot} = \oint_{4\pi} \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\,\mathrm{d}\Omega = \int_0^{2\pi}\int_0^{\pi} \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\varphi.$$

$$\mathrm{Im} f(\vec{k}, \vec{k}) = \mathrm{Im} f(\theta = 0) = \frac{k\sigma_{tot}}{4\pi}$$

Born approximation

The above semi-blue equation for local (i.e. $\langle\mathbf{x}'|V|\mathbf{x}''\rangle = V(\mathbf{x}')\,\delta^{(3)}(\mathbf{x}' - \mathbf{x}'')$) potentials will become:

$$\langle\vec{x}|\psi^{(\pm)}\rangle = \langle\vec{x}|\phi\rangle - \frac{2m}{\hbar^2}\int d^3\vec{x}'\,\frac{e^{\pm ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|}V(\vec{x}')\langle\vec{x}'|\psi^{(\pm)}\rangle$$

For large $r = |\vec{x}|$

$$\langle\vec{x}|\psi^{(\pm)}\rangle = \langle\vec{x}|\phi\rangle - \frac{2m}{\hbar^2}\int d^3\vec{x}'\,\frac{e^{\pm ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|}V(\vec{x}')\langle\vec{x}'|\psi^{(\pm)}\rangle$$

In the above blue equation we can substitute $\langle\vec{x}'|\psi^{(\pm)}\rangle = \psi^{(\pm)}(\vec{x}') \approx \phi(\vec{x}') = e^{i\vec{k}\cdot\vec{x}'}$ up to the 0th order and we will get the 1sr order solution. We can go on similarly to get higher order solutions.

1st order

$$\langle\vec{x}|\psi^{(\pm)}\rangle = \langle\vec{x}|\phi\rangle - \frac{2m}{\hbar^2}\int d^3\vec{x}'\,\frac{e^{\pm ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|}V(\vec{x}')e^{i\vec{k}\cdot\vec{x}'}$$

$$f^{(1)}(\vec{k}, \vec{k'}) = -\frac{m}{2\pi\hbar^2}\int d^3\vec{x}'\,e^{-i\vec{k'}\cdot\vec{x}'}\,V(\vec{x}')\langle\vec{x}'|\phi\rangle$$

$$f^{(1)}(\vec{k}, \vec{k'}) = -\frac{m}{2\pi\hbar^2}\int d^3\vec{x}'\,e^{i(\vec{k}-\vec{k'})\cdot\vec{x}'}\,V(\vec{x}')$$

Spherical

$$\begin{aligned} f^{(1)}(\theta) &= -\frac{1}{2}\frac{2m}{\hbar^2}\frac{1}{iq}\int_0^\infty \frac{r^2}{r}V(r)\left(e^{iqr} - e^{-iqr}\right)dr \\ &= -\frac{2m}{\hbar^2}\frac{1}{q}\int_0^\infty rV(r)\sin qr dr \end{aligned}$$

2nd order

$$
\begin{aligned}
f^{(2)} = & -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3 \int d^3x' \int d^3x'' \langle \mathbf{k}' \mid \mathbf{x}' \rangle V(\mathbf{x}') \\
& \times \left\langle \mathbf{x}' \left| \frac{1}{E - H_0 + i\varepsilon} \right| \mathbf{x}'' \right\rangle V(\mathbf{x}'') (\mathbf{x}'' \mid \mathbf{k}) \\
= & -\frac{1}{4\pi}\frac{2m}{\hbar^2} \int d^3x' \int d^3x'' e^{-i\mathbf{k}'\cdot\mathbf{x}'} V(\mathbf{x}') \\
& \times \left[\frac{2m}{\hbar^2} G_+(\mathbf{x}', \mathbf{x}'')\right] V(\mathbf{x}'') e^{i\mathbf{k}\cdot\mathbf{x}''}
\end{aligned}
$$

Validity

- If the potential is strong enough to develop a bound state, the Born approximation will probably give a misleading result.
- Quite generally, the Born approximation tends to get better at higher energies.

Let us assume that a "typical" value for the potential energy $V(x)$ is V_0 and that it acts within some "range" a. Writing $r' = l\vec{x} - \vec{x}' l$

$$
\left| \frac{2m}{\hbar^2} \left(\frac{4\pi}{3} a^3\right) \frac{e^{ikr'}}{4\pi a} V_0 \frac{e^{i\mathbf{k}\cdot\mathbf{x}'}}{L^{3/2}} \right| \ll \left| \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{L^{3/2}} \right|
$$

Partial-wave analysis

The Free Particle in Spherical Coordinates

Let $\psi_{Elm}(r,\theta,\phi) = R_{El}(r) Y_l^m(\theta,\phi)$ and $R_{El} = \frac{U_{El}}{r}$ then

$$
\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2}\right] U_{El} = 0, \quad k^2 = \frac{2\mu E}{\hbar^2}
$$

if $\rho = kr$ then

$$
\left[-\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2}\right] U_l = U_l
$$

Now analogous to harmonic oscillator we define

$$
d_l = \frac{d}{d\rho} + \frac{l+1}{\rho}, \quad d_l^\dagger = -\frac{d}{d\rho} + \frac{l+1}{\rho}
$$

Note that $\frac{d}{d\rho}$ is anti-Hermitian since $i\frac{d}{d\rho}$ is Hermitian.

$$
\begin{aligned}
d_l d_l^\dagger &= \left[-\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2}\right] \\
d_l^\dagger d_l &= d_{l+1} d_{l+1}^\dagger \\
\Rightarrow d_l d_l^\dagger U_l &= U_l \\
\Rightarrow d_l^\dagger d_l d_l^\dagger U_l &= d_l^\dagger U_l \\
\Rightarrow d_{l+1} d_{l+1}^\dagger d_l^\dagger U_l &= d_l^\dagger U_l \\
\Rightarrow d_l^\dagger U_l &= c_l U_{l+1}
\end{aligned}
$$

choose $c_l = 1$, for it can always be absorbed in the normalization. We can find the following two independent solutions for U_0

$$
U_0^A(\rho) = \sin\rho, \quad U_0^B = -\cos\rho
$$

Now U_0^B is unacceptable at $\rho = 0$ since it should go to 0. If, however, one is considering the equation in a region that excludes the origin, U_0^B must be included. Using the definition of U_l we can find R_l

$$R_l = (-\rho)^l \left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\right)^l R_0$$

$$R_0^A = \frac{\sin\rho}{\rho}, \quad R_0^B = \frac{-\cos\rho}{\rho}$$

$$R_l^A \equiv j_l = (-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \left(\frac{\sin\rho}{\rho}\right)$$

$$R_l^B \equiv n_l = (-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \left(\frac{-\cos\rho}{\rho}\right)$$

j_l and n_l are the spherical Bessel functions and Neumann functions of order l respectively.

$$j_0(\rho) = \frac{\sin\rho}{\rho} \quad n_0(\rho) = \frac{-\cos\rho}{\rho}$$
$$j_1(\rho) = \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho} \quad n_1(\rho) = -\frac{\cos\rho}{\rho^2} - \frac{\sin\rho}{\rho}$$
$$j_2(\rho) = \left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\sin\rho - \frac{3\cos\rho}{\rho^2} \quad n_2(\rho) = -\left(\frac{3}{\rho} - \frac{\partial}{\rho}\right)^l \left(\frac{-\cos\rho}{\rho}\right)$$

j_l are regular and n_l are irregular since

$$j_l(\rho) \xrightarrow[\rho\to 0]{} \frac{\rho^l}{(2l+1)!!}$$

$$n_l(\rho) \xrightarrow[\rho\to 0]{} -\frac{(2l-1)!!}{\rho^{l+1}}$$

$$\int_0^\infty j_l(kr) j_l(k'r) r^2 dr = \frac{2}{\pi k^2}\delta(k-k')$$

$$\psi_{Elm}(r,\theta,\phi) = j_l(kr) Y_l^m(\theta,\phi), \quad E = \frac{\hbar^2 k^2}{2\mu}$$

$$\iiint \psi^*_{Elm}\psi_{E'l'm'} r^2 dr d\Omega = \frac{2}{\pi k^2}\delta(k-k')\delta_{ll'}\delta_{mm'}$$

Connection with the Solution in Cartesian Coordinates

Consider now the case of a particle moving along the z axis with momentum $\mathbf{p}$. Since $\frac{\mathbf{p}\cdot\mathbf{r}}{\hbar} = kr\cos\theta$

$$\psi_E(x,y,z) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}, \quad E = \frac{p^2}{2\mu} = \frac{\hbar^2 k^2}{2\mu}$$

$$\Rightarrow \psi_E(r,\theta,\phi) = \frac{e^{ikr\cos\theta}}{(2\pi\hbar)^{3/2}}$$

Partial wave expansion

The incoming wave can be written as

$$e^{i\vec{k}\cdot\vec{r}} = e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos\theta)$$

$$e^{ikz} \xrightarrow[r\to\infty]{} \frac{1}{2ik}\sum_{l=0}^{\infty} i^l (2l+1)\left(\frac{e^{i(kr-l\pi/2)}}{r} - \frac{e^{-i(kr-l\pi/2)}}{r}\right) P_l(\cos\theta)$$

the full wave can be expressed as

$$\psi(r,\theta) = \sum_{l=0}^{\infty} b_l R_{kl}(r) P_l(\cos\theta)$$

$$\psi(r,\theta) \underset{r\to\infty}{\longrightarrow} -\frac{e^{-ikr}}{2ikr}\sum_{l=0}^{\infty} b_l i^l e^{-i\delta_l} P_l(\cos\theta) + \frac{e^{ikr}}{2ikr}\sum_{l=0}^{\infty} b_l (-i)^l e^{i\delta_l} P_l(\cos\theta)$$

the full wave can **also** be expressed as

$$\psi(r,\theta) \simeq \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos\theta) + f(\theta)\frac{e^{ikr}}{r}$$

$$\psi(r,\theta) \underset{r\to\infty}{\longrightarrow} -\frac{e^{-ikr}}{2ikr}\sum_{l=0}^{\infty} i^{2l}(2l+1)P_l(\cos\theta)$$
$$+\frac{e^{ikr}}{r}\left[f(\theta) + \frac{1}{2ik}\sum_{l=0}^{\infty} i^l (-i)^l (2l+1) P_l(\cos\theta)\right]$$

comparing the asymptotic coefficients we get

$$b_\ell = i^\ell (2\ell+1) e^{i\delta_\ell}$$

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

$$\boxed{\begin{aligned} f(\theta) = \sum_{l=0}^{\infty} f_l(\theta) &= \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)\left(e^{2i\delta_l}-1\right) \\ &= \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin\delta_l P_l(\cos\theta) \end{aligned}}$$

$$f(\theta,k) = \sum_{l=0}^{\infty}(2l+1)a_l(k)P_l(\cos\theta)$$

$$a_l(k) = \frac{e^{2i\delta_l}-1}{2ik} = \frac{e^{i\delta_l}\sin\delta_l}{k}$$

$$\boxed{f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin\delta_l P_l(\cos\theta)}$$

$$\boxed{f(\theta) = \sum_{\ell=0}^{\infty}\frac{2\ell+1}{2ki}P_\ell(\cos\theta)\left(e^{2i\delta_\ell}-1\right)}$$

Formulas used to derive $f(\theta)$

$$jl(kr) \underset{r\to\infty}{\longrightarrow} \frac{\sin(kr - l\pi/2)}{kr}$$

$$n_l(kr) \underset{r\to\infty}{\longrightarrow} -\frac{\cos(kr - l\pi/2)}{kr}$$

$$R_{kl}(r) \underset{r\to\infty}{\longrightarrow} A_l\frac{\sin(kr - l\pi/2)}{kr} - B_l\frac{\cos(kr - l\pi/2)}{kr}$$

$$R_{kl}(r) \underset{r\to\infty}{\longrightarrow} C_l\frac{\sin\left(kr - l\pi/2 + \delta_l\right)}{kr}$$

$$\int_0^\pi P_l(\cos\theta)P_{l'}(\cos\theta)\sin\theta d(\theta) = \frac{2}{2l+1}\delta_{ll'}$$

Optical theorem

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

The Hard Sphere

$V(r)=\infty, \quad r<r_0$ and $=0, \quad r>r_0$

$$\begin{aligned} R_l\left(r_0\right)&=0\\ \Rightarrow \frac{B_l}{A_l}&=-\frac{j_l\left(kr_0\right)}{n_l\left(kr_0\right)}\\ \Rightarrow \delta_l=\tan^{-1}\left(\frac{-B_l}{A_l}\right)&=\tan^{-1}\left[\frac{j_l\left(kr_0\right)}{n_l\left(kr_0\right)}\right]=-kr_0 \end{aligned}$$

The hard sphere has pushed out the wave function, forcing it to start its sinusoidal oscillations at $r=r_0$ instead of $r=0$. In general, **repulsive** potentials give **negative** phase shifts (since they slow down the particle and reduce the phase shift per unit length) while **attractive** potentials give **positive** phase shifts (for the opposite reason).

If $k\to 0$

$$\tan\delta_l \cong_{k\to 0} \delta_l \propto \left(kr_0\right)^{2l+1}$$

Resonances

Near resonance δ_l will be of the form

$$\delta_l=\delta_b+\tan^{-1}\left(\frac{\Gamma/2}{E_0-E}\right)$$

Now neglect δ_b then

$$\begin{aligned} \sigma_l&=\frac{4\pi}{k^2}(2l+1)\sin^2\delta_l\\ &=_{E\cong E_0}\frac{4\pi}{k^2}(2l+1)\frac{(\Gamma/2)^2}{\left(E_0-E\right)^2+(\Gamma/2)^2} \end{aligned}$$

σ_l is described by a bell-shaped curve, called the **Breit-Wigner form**, with a maximum height σ_l^{max} (the unitarity bound) and a half-width $\Gamma/2$. This phenomenon is called a **resonance**.

Appendix

$$\langle\vec{x}|\vec{k}\rangle=\frac{1}{(2\pi\hbar)^{3/2}}e^{i\vec{k}\cdot\vec{x}}$$

Dirac Delta

$$\delta(x-y)=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{ip(x-y)}\,dp$$

$$\delta(\vec{x}-\vec{y})=\frac{1}{(2\pi)^3}\int_{-\infty}^{\infty}e^{i\vec{p}\cdot(\vec{x}-\vec{y})}\,d^3\vec{p}$$

$$\begin{aligned} \delta\left(\vec{r}-\vec{r}'\right)&=\frac{1}{r^2}\delta\left(r-r'\right)\delta\left(\cos\theta-\cos\theta'\right)\delta\left(\varphi-\varphi'\right)\\ &=\frac{1}{r^2\sin\theta}\delta\left(r-r'\right)\delta\left(\theta-\theta'\right)\delta\left(\varphi-\varphi'\right) \end{aligned}$$

Cauchy integration formula

$$f(a) = \frac{1}{2\pi i} \oint_\gamma \frac{f(z)}{z-a}\, dz.$$

To calculate a integral on the real line we can extrapolate it into a closed integral extending to the side of $i\infty$ or $-i\infty$ depending on whether it goes to zero on $i\infty$ or $-i\infty$.