Lecture 7

Tensor operators

Assume that $\vec{V}_a$ and $\bar{V}_b$ are independent vector operators

$$\mathcal{U}(R) V_a^i \mathcal{U}^\dagger(R) = \sum_{j=1}^{3} V_a^j R_{ji}$$

$$\mathcal{U}(R) V_b^i \mathcal{U}^\dagger(R) = \sum_{j=1}^{3} V_b^j R_{ji}$$

We consider the transformation properties of the product

$$V_a^i V_b^j$$

under rotations (we do not assume that $\bar{V}_a$ and $\bar{V}_b$ commute)

$$\mathcal{U}(R) V_a^i V_b^j \mathcal{U}^\dagger(R) =$$

$$\mathcal{U}(R) V_a^i \mathcal{U}^\dagger(R) \mathcal{U}(R) V_b^j \mathcal{U}^\dagger(R)$$

$$\sum_{k\ell} V_a^k V_b^\ell R_{ki} R_{\ell j}$$

Operators that transform like this under rotations are called rank 2 Cartesian tensors.

In general an operator

$$V^{i_1 \cdots i_N}$$

that transforms under rotation like

$$\mathcal{U}(R) V^{i_1 \cdots i_N} \mathcal{U}^\dagger(R) =$$

$$\sum V^{j_1 \cdots j_N} R_{i_1 j_1} \cdots R_{i_N j_N}$$

is called a rank N cartesian tensor.

Note

$$V_a^i V_b^j = \frac{\bar{V}_a \cdot \bar{V}_b}{3} \delta_{ij} + \frac{1}{2}\left(V_a^i V_b^j - V_a^j V_b^i\right)$$
$$+ \frac{1}{2}\left(V_a^i V_b^j + V_a^j V_b^i\right) - \frac{\bar{V}_a \cdot \bar{V}_b}{3} \delta_{ij}$$

The first term is a scalar, the second term is antisymmetric, and the third term is symmetric and traceless.

These properties are preserved under rotations —

The do not mix under rotations!

Recall $Y_1^m(\theta\varphi)$

$$Y_1^{-1}(\theta\varphi) = \sqrt{\frac{3}{8\pi}}\sin\theta(\cos\varphi - i\sin\varphi)$$

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

$$Y_1^1(\theta\varphi) = -\sqrt{\frac{3}{8\pi}}\sin\theta(\cos\varphi + i\sin\varphi)$$

$$\left.\begin{aligned} x &= r\sin\theta\cos\varphi \\ y &= r\sin\theta\sin\varphi \\ z &= r\cos\theta \end{aligned}\right\}$$ spherical polar coordinates

It follows that

$$Y_1^{-1}(\theta\varphi) = \sqrt{\frac{3}{4\pi}}\ \frac{x - iy}{\sqrt{2}\, r}$$

$$Y_1^{0}(\theta\varphi) = \sqrt{\frac{3}{4\pi}}\ \frac{z}{r}$$

$$Y_1^{1}(\theta,\varphi) = -\sqrt{\frac{3}{4\pi}}\ \frac{x + iy}{\sqrt{2}\, r}$$

We can extract the carte components of $\bar{x}$ from the three spherical harmonics with $\ell = 1$

If we treat $Y_\ell^m(\theta\varphi)$ as an operator

$$U(R)\, Y_\ell^m(\theta\varphi)\, U^\dagger(R) = \sum_{m'} Y_\ell^{m'}(\theta\varphi)\, D^{\ell}_{m'm}(R)$$

This leads to the definition of the spherical component of an arbitrary vector $\bar{v}$.

$$V_1^{-1} = \frac{1}{\sqrt{2}}(x - iy)$$

$$V_1^{0} = z$$

$$V_1^{1} = -\frac{1}{\sqrt{2}}(x + iy)$$

It follows that

$$\boxed{\mathcal{U}(R)\, V_1^{m}\, \mathcal{U}^{\dagger}(R) = \sum_{m'} V_1^{m'} D^{1}_{m'm}(R)}$$

V_1^m is called a rank 1 spherical tensor operator

This can be generalized

Def: A rank j spherical tensor operator has $2j+1$ components that transform like

$$\boxed{\mathcal{U}(R)\, V_\mu^{j}\, \mathcal{U}^{\dagger}(R) = \sum_{\nu=-j}^{j} V_\nu^{j} D^{j}_{\nu\mu}(R)}$$

$j=0$ is a scalar

$j=1$ is a vector

$j=2$ has the same content as a traceless symmetric tensor

Exercise:

Express $Y^2_m(\theta\phi)$ in terms of cartesian coordinates

The important property of the spherical components of a tensor operator is that they transform irreducibly

i.e. If you have 1 component you can get the others by a rotation

One of the most useful results involving spherical tensor operators is the Wigner–Eckart Theorem

The essential content is that matrix elements of the form

$$\langle j_a\, \mu_a |\, V^{j_b}_{\mu_b} \,| j_c\, \mu_c \rangle$$

is proportional to

$$C^{j_a\ \ j_b\ \ j_c}_{\mu_a\ \mu_b\ \mu_c}$$

The result is normally written

$$\boxed{\langle j_a\, \mu_a |\, V^{j_b}_{\mu_b} \,| j_c\, \mu_c \rangle = \frac{C^{j_a\ \ j_b\ \ j_c}_{\mu_a\ \mu_b\ \mu_c} \langle j_a \| V^{j_b} \| j_c \rangle}{\sqrt{2j_a+1}}}$$

The value of this result is that selection rules for $\langle j_a \mu_a | V^{j_b}_{\mu_b} | j_c \mu_c \rangle$

follow from the selection rules for the Clebsch-Gordan coefficients - i.e. this vanishes unless

$$|j_b - j_c| \leq j_a \leq |j_b + j_c|$$

$$\mu_a = \mu_b + \mu_c$$

Furthermore

$$\frac{\langle j_a \mu_a | V^{j_b}_{\mu_b} | j_c \mu_c \rangle}{\langle j_a \nu_a | V^{j_b}_{\nu_b} | j_c \nu_c \rangle} = \frac{C^{j_a j_b j_c}_{\mu_a \mu_b \mu_c}}{C^{j_a j_b j_c}_{\nu_a \nu_b \nu_c}}$$

This allows one to get all non 0 matrix elements if you know only one of them.

Proof of Theorem

we use $\int dR = 1$

and $\mathcal{U}(R)\mathcal{U}^\dagger(R) = I$

$$\langle j_a \mu_a | V^{j_b}_{\mu_b} | j_c \mu_c \rangle =$$

$$\int dR \langle j_a \mu_a | \mathcal{U}^\dagger(R)\mathcal{U}(R) V^{j_b}_{\mu_b} \mathcal{U}^\dagger(R)\mathcal{U}(R) | j_c \mu_c \rangle =$$

$$\sum \int dR\, D^{j_a *}_{\nu_a \mu_a}(R) \langle j_a \nu_a | V^{j_b}_{\nu_b} | j_c \nu_c \rangle \times \underbrace{D^{j_b}_{\nu_b \mu_b}(R)\, D^{j_c}_{\nu_c \mu_c}(R)}_{\sum_{j \nu \mu} C^{j\ j_b\ j_c}_{\nu\ \nu_b\ \nu_c}\, D^{j}_{\nu \mu}(R)\, C^{j\ j_b\ j_c}_{\mu\ \mu_b\ \mu_c}} =$$

use $\int D^{j *}_{\mu \nu}(R)\, D^{j'}_{\mu' \nu'}(R)\, dR = \dfrac{\delta_{jj'}\delta_{\mu\mu'}\delta_{\nu\nu'}}{2j+1}$

$$\boxed{\text{gives} \quad C^{j_a j_b j_c}_{\mu_a \mu_b \mu_c} \sum_{\nu_a \nu_b \nu_c} \frac{C^{j_a j_b j_c}_{\nu_a \nu_b \nu_c} \langle j_a \nu_a | V^{j_b}_{\nu_b} | j_c \nu_c \rangle}{2 j_a + 1}}$$

The invariant matrix element

$$\langle j_a \| V^{j_b} \| j_c \rangle \equiv$$

$$\frac{1}{\sqrt{2j_a+1}} \sum_{\nu_a \nu_b \nu_c} C^{j_a j_b j_c}_{\nu_a \nu_b \nu_c} \langle j_a \nu_a | V^{j_b}_{\nu_b} | j_c \nu_c \rangle$$

which gives the advertised result

$$\boxed{\langle j_a \mu_a | V^{j_b}_{\mu_b} | j_c \nu_c \rangle = C^{j_a j_b j_c}_{\mu_a \mu_b \mu_c} \frac{\langle j_a \| V^{j_b} \| j_c \rangle}{\sqrt{2j_a+1}}}$$

which is the conventional form of the theorem

The next topic is approximation methods

* WKB approximation
* Rayleigh Schrödinger perturbation theory
* Variational Methods
* Feynman Hellman Theorem – Virial Theorem
* Born Oppenheimer approximation
* Time dependent perturbation theory

WKB

Consider the Schrödinger equation for a linear potential

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - Fx\right)\psi(x) = E\psi(x)$$

(here I keep $\hbar$ explicity in order to investigate the accuracy of the approximation

(In this equation F is a constant force)

step 1: write the Schrodinger equation as

$$\boxed{\frac{d^2\psi}{dx^2} = -\left(\frac{2m}{\hbar^2}\right)(E + Fx)}$$

we simplify this by defining

$$\sigma = -\left(\frac{2mF}{\hbar^2}\right)^{1/3}\left(x + \frac{F}{E}\right)$$

$$\frac{d}{dx} = \frac{d\sigma}{dx}\frac{d}{d\sigma} = -\left(\frac{2mF}{\hbar^2}\right)^{1/3} \cdot \frac{d}{d\sigma}$$

$$\frac{d^2}{dx^2} = \left(\frac{2mF}{\hbar^2}\right)^{2/3}\frac{d^2}{d\sigma^2}$$

Then the equation $\boxed{}$

becomes

$$\cancel{\left(\frac{2mF}{\hbar^2}\right)^{2/3}}\frac{d^2\psi}{d\sigma^2} = \cancel{\left(\frac{2mF}{\hbar^2}\right)^{2/3}}\underbrace{\left(-\left(\frac{2mF}{\hbar^2}\right)^{1/3}\left(x+\frac{E}{F}\right)\right)}_{\sigma}\psi$$

canceling the constants that appear in both sides and using the definition of σ gives

$$\boxed{\frac{d^2\psi}{d\sigma^2} = \sigma\psi}$$

This is a second order ordinary differential equation. It has 2 linearly independent solutions

$$\boxed{\psi(\sigma) = Ai(\sigma),\ Ai\left(e^{\frac{2\pi i}{3}}\sigma\right)}$$

where $Ai(\sigma)$ is called an <u>Airy function</u>

where

$$Ai(\sigma) = \int_{-\infty}^{\infty} \frac{ds}{2\pi} e^{-is\sigma - i\frac{s^3}{3}}$$

$$= \int_{0}^{\infty} \frac{ds}{\pi} \cos\left(\sigma s + \frac{s^3}{3}\right)$$

The Airy function has the following properties

(*) $Ai(\sigma) = \frac{1}{\sqrt{\pi}}\sqrt{\frac{\sigma}{3}}\, K_{1/3}\left(\frac{2}{3}\sigma^{3/2}\right)$

K is an analytic continuation of a Bessel

(*) $\int_{-\infty}^{\infty} Ai(\sigma)\, d\sigma = 1$

(*) $\int_{-\infty}^{\infty} Ai(\sigma - x)\, Ai(\sigma - y)\, d\sigma = \delta(x-y)$

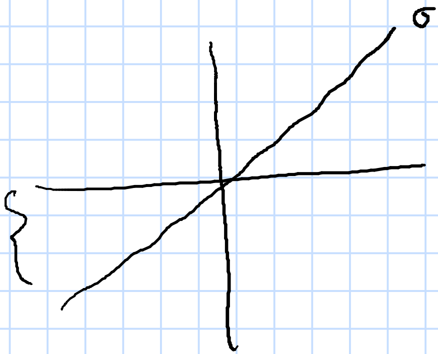
(*) $Ai(0) = \frac{1}{2\pi}(3)^{-1/3}\,\Gamma\left(\frac{1}{3}\right)$

where $\Gamma(x)$ is the Gamma function

consider

$$-\frac{d^2\psi}{dx^2} + \sigma\psi = 0$$

(T + V) $\quad \sigma$ = potential



$\sigma > 0$
wave function should fall off

$\sigma < 0$

wave function should oscillate

one can show

$$\lim_{\sigma \to +\infty} Ai(\sigma) \to \frac{1}{\sqrt{\pi}} |\sigma|^{-1/4} e^{-\frac{2}{3}\sigma^{3/2}}$$

$$\lim_{\sigma \to -\infty} Ai(\sigma) \to \frac{1}{2\sqrt{\pi}} |\sigma|^{-1/4} \cos\left(\frac{2}{3}|\sigma|^{3/2} - \frac{\pi}{4}\right)$$

There are 2 reasons to study this potential

(1) A linear radial potential for $\ell = 0$ has this form. quarks + antiquarks experience a force that behaves approximately like a linear potential for large x

(2) The system determines how to impose boundary conditions in a semiclassical approximation due to Wentzel Kramers and Brillouin

For the second application the classical energy is

$$\frac{p_{cl}^2}{2m} - Fx = E$$

solving for the classical momentum gives

$$p_{cl} = \sqrt{2m(E+Fx)}$$

solving for x in terms of the classical momentum gives

$$x = \left(\frac{p_{cl}^2}{2m} - E\right)/F$$

recall

$$\sigma = -\left(\frac{2mF}{\hbar^2}\right)^{1/3}\left(x + \frac{E}{F}\right)$$

$$= -\left(\frac{2mF}{\hbar^2}\right)^{1/3}\left(\frac{p_{cl}^2}{2m}\right)$$

$$= -\frac{p_{cl}^2(x)}{(2mF\hbar)^{2/3}}$$

This means

$$Ai(\sigma) = Ai\left(-\frac{p_{cl}^2}{(2mF\hbar)^{2/3}}\right)$$

note that by definition p_{cl}^2 is not necessarily positive

positive is associated with classically allowed region while negative corresponds to the classically forbidden region

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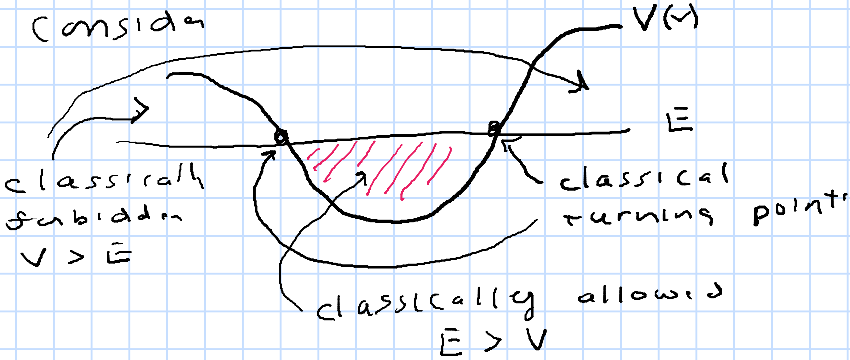
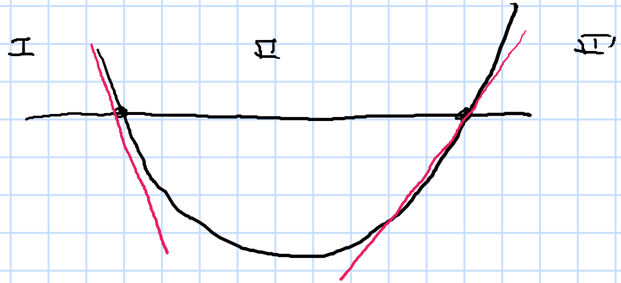
This will be use to formulate the WKB approximation

The role of the Airy function

Consider



The WKB approximation breaks down near the classical turning points, but near those points the potential can be approximated by a linear potential



The Airy functions connect the solutions in regions I, II and II, III near the classical turning points – this results in matching conditions that determine approximate energy eigenvalues

WKB Approximation

* Start by assuming a wave function of the form

$$\psi(x) = A(x)\, e^{iS(x)}$$

where $A(x)$ is a real amplitude and $S(x)$ is a phase

To use this in the Schrodinger equation we need to compute

$$\frac{d^2\psi}{dx^2}$$

(1) $$\frac{d\psi}{dx} = \frac{dA}{dx} e^{iS(x)} + iA(x)\frac{dS}{dx} e^{iS(x)}$$

(2) $$\frac{d^2\psi}{dx^2} = \frac{d^2A}{dx^2} e^{iS(x)} + 2i\frac{dA}{dx}\frac{dS}{dx} e^{iS(x)} + iA(x)\frac{d^2S}{dx^2} e^{iS(x)} - A(x)\left(\frac{dS}{dx}\right)^2 e^{iS(x)}$$

using the shorthand

$$\frac{d^2\psi}{dx^2} = \psi'' \quad \frac{dA}{dx} = A' \quad \frac{d^2A}{dx^2} = A''$$

$$\frac{dS}{dx} = S' \quad \frac{d^2S}{dx^2} = S''$$

the equation on the last page becomes

$$\psi''(x) = [A'' + 2iA'S' + iAS'' - A(S')^2] \times e^{iS(x)}$$

$$= -\frac{2m}{\hbar^2}(E-V)\psi =$$

$$= -\frac{P_{cl}^2}{\hbar^2} A(x) e^{iS(x)}$$

equating the real an imaginary parts gives

$$(1) \quad A'' - A(S')^2 = -\frac{P_{cl}^2}{\hbar^2} A$$

$$(2) \quad 2A'S' = -AS''$$

This replaces the Schrodinger equation by a pair of coupled non linear equations

The second equation gives

$$* \quad \frac{S''}{S'} = -2\frac{A'}{A} = \ln S' = -2\ln A + \text{const}$$

$$S' A^2 = \text{const} \qquad \boxed{S'(x) = \frac{C}{A(x)^2}}$$

This can ubstituted into the first equation to get

$$** \quad \frac{A''}{A} = (S')^2 - \frac{P_{cl}^2}{\hbar^2}$$

differentiate $*$ to get

$$\left(\frac{S''}{S'}\right)' = -2\frac{A''}{A} + 2\left(\frac{A'}{A}\right)^2$$

use $**$ in the above equation to get

$$\left(\frac{S''}{S'}\right)' = -2\left[(S')^2 - \frac{P_{cl}^2}{\hbar^2}\right] + 2\left(\frac{1}{2}\frac{S''}{S'}\right)^2$$

which is a nonlinear equation for S which we write as

$$\boxed{(S')^2 = \frac{P_{cl}^2}{\hbar^2} - \frac{1}{2}\left(\frac{S''}{S'}\right)' + \frac{1}{4}\left(\frac{S''}{S'}\right)^2}$$

if $\frac{p^2}{\hbar^2} >> \frac{1}{4}\left(\frac{S''}{S'}\right)^2 ; \frac{1}{2}\left(\frac{S''}{S'}\right)'$

and we can ignore the small term we get a very simple equation

$$(S')^2 = \frac{P_{cl}^2}{\hbar^2} \qquad S'(x) = \pm \frac{P_{cl}(x)}{\hbar}$$

$$\boxed{\begin{aligned} S(x) &= \pm \int_c^x \frac{P_{cl}(x')}{\hbar}\, dx' \\ A(x) &= \frac{C}{\sqrt{S'}} = \frac{C}{\sqrt{P_{cl}}} \end{aligned}}$$

which expressed the amplitude and phase in terms of the classical momentum

** At the classical turning points $P_{cl}(x) = 0$ and the approximation breaks down