

Physics 143b: Quantum Mechanics II

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Multiparticle systems cont. (lec 9-10)

Ref: Griffiths 5.1.2-5.1.4

Exchange Force: Geometrical consequence of the symmetrization requirement. Consider the overlap integral:

$$\langle (x_1 - x_2)^2 \rangle = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2\langle x \rangle_a \langle x \rangle_b \mp 2|\langle a|x|b \rangle|^2.$$

Note that the $\mp 2|\langle a|x|b \rangle|^2$ term is the **quantum correction**:

- identical **bosons** take the upper sign and tend to be somewhat closer together
- identical **fermions** take the lower sign and tend to be somewhat farther apart
- distinguishable particles have no quantum correction

Spin: The complete state of a particle includes both the position wave function and the **spinor** (orientation of the spin). For example,

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \psi(\mathbf{r}_1, \mathbf{r}_2) \chi(1, 2).$$

Then, the overall wavefunction must satisfy the symmetrization requirements. The singlet combination is *antisymmetric* while the triplet states are *symmetric*.

Generalized symmetrization principle: the *symmetrization axiom* for identical particles states that the state is required to satisfy

$$|(1, 2)\rangle = \pm |(2, 1)\rangle$$

where we have the upper sign for bosons and lower sign for fermions. For n particles, the state must satisfy symmetry requirements under interchange of any **two** particles

$$|(1, 2, \dots, i, \dots, j, \dots, n)\rangle = \pm |(1, 2, \dots, j, \dots, i, \dots, n)\rangle.$$

The **Slater determinant** allows us to compute the satisfying wavefunction efficiently (Griffiths Problem 5.8). For **three particles** in states ψ_a, ψ_b, ψ_c , the matrix is given by

$$\Psi(x_1, x_2, x_3) = \frac{1}{\sqrt{3!}} \det \begin{bmatrix} \psi_a(x_1) & \psi_b(x_1) & \psi_c(x_1) \\ \psi_a(x_2) & \psi_b(x_2) & \psi_c(x_2) \\ \psi_a(x_3) & \psi_b(x_3) & \psi_c(x_3) \end{bmatrix}.$$

Ref: Problem Set 2.4

Approximation methods (lec 11)

Ref: Griffiths 5.2.1, Tong 6.1.2

We have that the respective Hamiltonians of the Hydrogen and Helium atoms are ($Z = 1, 2$ respectively):

$$H_H = \frac{p_1^2}{2m} - \frac{e^2}{4\pi\epsilon_0} \frac{Z}{r_1}$$

$$H_{He} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \frac{e^2}{4\pi\epsilon_0} \frac{Z}{|\mathbf{r}_1|} - \frac{e^2}{4\pi\epsilon_0} \frac{Z}{|\mathbf{r}_2|} + \frac{e^2}{4\pi\epsilon_0} \frac{Z}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

where the final term in the Helium Hamiltonian accounts for Coulombic repulsion between the two electrons. While we can directly solve the Hydrogen atom, we wish to approximate the ground state energy of the Helium atom.

First, we try the **independent particle approximation**, where we ignore the e - e interactions. Then, the two effects are 1) the nucleus charge is enhanced and 2) the Bohr radius shrinks. Thus, each of the two electrons has four times the Bohr energy, so the ground state energy is

$$E_{gs, IPA} = -2Z^2 R_y = -8R_y = 8(-13.6 \text{ eV}) = -109 \text{ eV}$$

where R_y is the Rydberg constant.

Now, we compute the ground state with a **perturbative e - e interaction**. Using first-order perturbation theory, we obtain a ground state energy of

$$E_{gs, PI} = \left(-2Z^2 + \frac{5Z}{4} \right) R_y = -74.8 \text{ eV}.$$

Ref: Problem Set 3.3

Variational principle (lec 12-13)

Ref: Tong 6.1, Griffiths Ch. 8

The variational principle provides a simple method to compute an *upper bound* for the ground state energy. It utilizes the principle that

$$E_{gs} \leq \langle \psi | H | \psi \rangle \equiv \langle H \rangle$$

for any **normalized function** ψ . With a clever ansatz that realistically approximates the true wavefunction, we can achieve miraculously accurate results.

In general, we will consider a family of states $|\psi(\alpha)\rangle$ and observe that

$$E(\alpha) = \langle \psi(\alpha) | H | \psi(\alpha) \rangle \psi \geq E_0, \quad \forall \alpha.$$

Then, we can minimize $E(\alpha)$ with respect to α to obtain the most stringent upper bound on the ground state energy, solving

$$\frac{\partial E}{\partial \alpha} = 0$$

for the critical α_* and computing the upper bound $E(\alpha_*)$.

Example (Helium atom): We pick the trial wavefunction $\Psi(\mathbf{r}_1, \mathbf{r}_2) = \psi(\mathbf{r}_1, \mathbf{r}_2)$, where

$$\psi(\mathbf{r}; \alpha) = \sqrt{\frac{\alpha^3}{\pi a_0^3}} e^{-\alpha r/a_0}$$

with α the variational parameter and a_0 the Bohr radius.

To compute $E(\alpha)$, we further know that the trial wavefunction is the eigenfunction of H_H with $Z = \alpha$, with known energy. Then we just need to compute the expectation of the interaction term as $\frac{5\alpha}{8a_0}$, so

$$E(\alpha) = \left(-2\alpha^2 + 4(\alpha - Z)\alpha + \frac{5}{4}\alpha \right) R_y$$

this energy is minimized at $\alpha_* = Z - \frac{5}{16}$, so

$$E(\alpha_*) = -2 \left(Z - \frac{5}{16} \right)^2 = -77.5 \text{ eV}$$

which is remarkably close to the experimental value of -79 eV. We can further interpret the nucleus to have $(Z - \frac{5}{16})e$ charge, with an effect from electron screening.

Ref: Problem Set 3.2, Griffiths 8.2, Tong 6.1.2

Bound States in 1D: **Ref:** Tong 6.1.3, lec 12

If $\int_{-\infty}^{\infty} V(x) dx = V_0 < 0$ for a 1D potential with $V(\pm\infty) = 0$, a **bound state** always occurs (the ground state).

Excited States: **Ref:** Tong 6.1.4, sec 7

If a given Hamiltonian has some **symmetry** with a known quantum number for the ground state under the symmetry, then we can construct a trial wavefunction with a different quantum number, guaranteeing that it is orthogonal to the ground state (so the variational energy has no contribution from the ground state component).

Often, this theory is applied to **parity states**: if a given Hamiltonian is invariant under parity $x \rightarrow -x$, the ground state is even under parity. Then we can bound the *first excited state* by constructing an odd-parity trial wave function.

Ref: Problem Set 3.4

Hydrogen molecule (ion) H_2^+ , H_2 : **Ref:** Griffiths 8.3, 8.4

H_2^+ has a bound state (covalent bond) and is stable. H_2 has two electrons, singlet has a bound state. Variational wavefunction also (over)estimates bond length.

Ref: Problem Set 4.1, Griffiths 8.3, 8.4, lec 13

WKB approximation (lec 13-16)

Ref: Tong 6.2, Griffiths Ch. 9

The WKB method allows us to approximate solutions to the TISE in 1D, with particular applications in calculating **bound state energies** and **tunneling rates**.

In the *classical regime*, ($E > V(x)$), we have

$p(x) = \sqrt{2m(E - V(x))}$ and can approximate the wave function as a plane wave

$$\psi(x) \sim A e^{ip(x)x/\hbar}.$$

In the **semi-classical limit**, we assume that the phase $W(x) = p(x)x$ has a small second derivative:

$$\hbar|W''| \ll |W'|^2 \implies \lambda \left| \frac{dV}{dx} \right| \ll \frac{p^2}{2m}.$$

Equivalently, the potential varies slowly with respect to the de Broglie wavelength $\lambda = \frac{\hbar}{p}$. The characteristic potential length scale satisfies

$$\Delta x \gg \lambda \sim \frac{\hbar}{p} \implies p\Delta x \gg \hbar$$

This gives us the interpretation that \hbar is “small.” With the series expansion of W to first order in \hbar , we can derive $\psi(x) \approx$

$$\psi_1(x) \approx \frac{A}{\sqrt{p(x)}} e^{\pm \frac{i}{\hbar} \int dx p(x)}, \quad \psi_2(x) \approx \frac{C}{\sqrt{|p(x)|}} e^{\pm \frac{1}{\hbar} \int dx |p(x)|}.$$

for ψ_1 **classical** ($E > V(x)$) and ψ_2 **non-classical** ($E < V(x)$) regimes respectively, where $p(x) = \sqrt{2m(E - V(x))}$.

Ref: Griffiths 9.47, Tong 6.2.2

At the turning point between the two regions ($E = V$), the WKB approximation breaks down. We derive the **connection formulas** by matching the WKB solutions on either side of the turning point x_2 with the Airy functions. Using the connection formulas, we have the WKB wave function given by

$$\psi(x) \approx \begin{cases} \frac{2D}{\sqrt{p(x)}} \sin \left[\frac{1}{\hbar} \int_x^{x_2} dx' p(x') + \frac{\pi}{4} \right], & x < x_2 \\ \frac{D}{\sqrt{|p(x)|}} \exp \left[-\frac{1}{\hbar} \int_x^{x_2} dx' |p(x')| \right], & x > x_2 \end{cases}$$

where D is some normalization constant.

Application: Tunneling

Ref: Griffiths 9.2, Tong 6.2.5

We consider the 1D tunnelling problem, a purely quantum phenomenon where a particle with low energy can tunnel through a barrier of higher potential. Using the theory of bound and scattering states, we can derive the **transmission probability** as

$$T \approx e^{-2\gamma}, \quad \gamma \equiv \frac{1}{\hbar} \int_0^a dx |p(x)|.$$

The canonical example of this effect is Gamow's theory of alpha decay. In this case, the **lifetime** is

$$\tau = \frac{2r_1}{v} e^{2\gamma}.$$

Ref: Problem Set 4.2

Application: Bound states

Ref: Tong 6.3.3

To find the **bound state energies**, we evaluate by substituting $p(x) = \sqrt{2m(E - V(x))}$

$$\int_a^b dx' p(x') = \hbar\pi \left(n + \frac{1}{2} \right), \quad n = 0, 1, 2, \dots$$

where a, b are the boundary points of the potential at $E = V(x)$. We can then use the LHS result in terms of E to find the energy spectrum E_n .

Ref: Problem Set 4.3

Quantum dynamics (lec 16-21)

Ref: Griffiths Ch. 11, Tong 6.3

We will consider a time-dependent potential energy function $V(\mathbf{r}, t)$. This allows for **transitions** or **quantum jumps** from one energy level to another. If the time-dependent part of the Hamiltonian is small compared to the time-independent part, we can treat it as a perturbation. That is, we can write

$$H(t) = H_0 + H'(t)$$

where H_0 is a time-independent Hamiltonian, and $H'(t)$ contains the time-dependence.

Note that computing the time-evolution operator when the Hamiltonian is time-dependent requires us to evolve the operator as a function of time. In general, this operator is non-commutative, so we introduce the **time-ordered operator** \mathcal{T}_t to allow us to write

$$U(t) = \mathcal{T}_t e^{-\frac{i}{\hbar} \int_0^t dt' H(t')}$$

Two-level system (lec 16-18)

Ref: Griffiths 11.1

We will suppose that there are only *two* states of the unperturbed system ψ_a, ψ_b , eigenstates of the unperturbed Hamiltonian H_0 , $\langle \psi_i | \psi_j \rangle = \delta_{ij}$, ($i, j = a, b$).

With a *time-dependent potential*, any state can be written as

$$\Psi(t) = c_a(t) \psi_a e^{-iE_a t/\hbar} + c_b(t) \psi_b e^{-iE_b t/\hbar},$$

$$|c_a(t)|^2 + |c_b(t)|^2 = 1.$$

Assuming the diagonal matrix elements vanish $H'_{aa} = H'_{bb} = 0$, we can solve and obtain

$$\dot{c}_a = -\frac{i}{\hbar} H'_{ab} e^{-i\omega_0 t} c_b, \quad \dot{c}_b = -\frac{i}{\hbar} H'_{ba} e^{i\omega_0 t} c_a.$$

where $H'_{ij} \equiv \langle \psi_i | H' | \psi_j \rangle$, $\omega_0 \equiv \frac{E_b - E_a}{\hbar}$. The **probability of transitioning** to state ψ_i is given by $|c_i(t)|^2$.

Time-dependent perturbation

We begin with the zeroth order initial state

$$c_a^{(0)} = 1, \quad c_b^{(0)} = 0.$$

To calculate subsequent order approximations, we insert the previous order approximations into the right side of the differential equations above. We can see the general results in Griffiths equations 11.20, 11.21, 11.22.

Ref: Problem Set 5.4

Sinusoidal perturbations

Ref: Griffiths 11.1.3

We assume the perturbation follows a sinusoidal time dependence:

$$H'(\mathbf{r}, t) = V(\mathbf{r}) \cos(\omega t) \implies H'_{ab} = V_{ab} \cos(\omega t),$$

$$V_{ab} \equiv \langle \psi_a | V | \psi_b \rangle.$$

Under these assumptions, we can solve for the transition probability, given by

$$P_{a \rightarrow b}(t) = |c_b(t)|^2 \approx \frac{|V_{ab}|^2}{\hbar^2} \frac{\sin^2[(\omega_0 - \omega)t/2]}{(\omega_0 - \omega)^2}$$

where $\omega_0 \equiv \frac{E_b - E_a}{\hbar}$ is the “natural” frequency.

Observe that the transition probability oscillates sinusoidally in time, with a maximum at

$$p_b(t) = \frac{|V_{ab}|^2}{\hbar^2} (\omega_0 - \omega)^2 \ll 1.$$

At times $t_n = 2n\pi/|\omega_0 - \omega|$ the particle is certainly in the lower state. At the resonance, $\omega = \omega_0$, we have

$$p_b(t) = \sin^2 \Omega t, \quad \Omega = \frac{V_{ab}}{2\hbar}.$$

Ref: Problem Set 5.1, Griffiths Problem 11.9, 11.29, Tong 6.3.5 **Rabi Oscillation and Nuclear Magnetic Resonance**.

Fermi's Golden Rule (lec 19-20)

Ref: Griffiths 11.4, Example 11.2

The **interaction representation** is an efficient way to do perturbation theory. Time ordering is natural in the path integral formulation. We use the interaction picture to help with derivations.

We have previously solved for the transition amplitude between two discrete energy states. Now, we consider consider a transition from E_i to an energy in some finite range ΔE of E_f in a *continuum*, we can take an integral over all final states and obtain the transition rate

$$R = P_{i \rightarrow f} = \frac{2\pi}{\hbar} \left| \frac{V_{if}}{2} \right|^2 \rho(E_f)$$

where $V_{if} \equiv \langle \psi_i | V | \psi_f \rangle$ and $\rho(E_f)$ is the density of states.

Note that if the perturbation is constant, we replace $\frac{V_{if}}{2}$ with V_{if} .

Ref: Problem Set 6.2c

Adiabatic Approximation (lec 20)

Ref: Griffiths 11.5, Tong 6.3.3

In the **sudden approximation**, the Hamiltonian changes very fast, $\hbar\omega_0 \gg \hbar\omega$. Then, if the original ground state wavefunction is ψ_0 we can write the new wavefunction $\tilde{\psi}_0$ simply by incorporating the change in the potential. Then, the overall wavefunction is

$$\psi(t) = \sum_n c_n \tilde{\psi}_n e^{-iE_n t/\hbar}, \quad c_n = \langle \tilde{\psi}_n | \psi_0 \rangle.$$

Ref: Problem Set 5.3

We now consider if the Hamiltonian changes gradually from some initial form $H(0)$ to some final form $H(T)$ with $\hbar\omega_0 \ll \hbar\omega$. Then the **adiabatic theorem** states that if the particle was initially in the n th eigenstate of $H(0)$, it will be carried into the n th instantaneous eigenstate of $H(T)$ (i.e. there is no crossing of eigenstates).

For a *constant* Hamiltonian, the wave function picks up a phase $e^{-iE_n t/\hbar}$. If the eigenvalue E_n is a function of time, the wiggle factor generalizes to a **dynamic phase**:

$$e^{i\theta_n(t)}, \quad \theta_n(t) \equiv -\frac{1}{\hbar} \int_0^t dt' E_n(t').$$

Berry's phase (lec 20-21)

Ref: Griffiths 11.5

In addition to the classically determined dynamic phase, there may be an additional phase factor $\gamma_n(t)$ and the wave function can take the form

$$\psi_n(t) = e^{i\theta_n(t)} e^{i\gamma_n(t)} \psi_n(t).$$

The **geometric phase** around an **adiabatic closed cycle** depends *only on the path* taken and is time-independent. In this case, we have that the **Berry's phase** is

$$\gamma_n(T) \equiv \gamma(T) - \gamma(0) = i \int_0^T dt \langle \psi_n(t) | \frac{\partial}{\partial t} \psi_n(t) \rangle.$$

Parallel transport on a sphere is a non-holonomic process.

Ref: Problem Set 5.2, Griffiths Example 11.4

Scattering theory (lec 21-23)

Ref: Griffiths Ch. 10, Tong Ch. 10

Classical vs. quantum scattering (lec 21)

The **differential cross-section** is defined as

$$D(\theta) \equiv \frac{d\sigma}{d\Omega} = \frac{b}{\sin \theta} \left| \frac{db}{d\theta} \right|,$$

where b is the impact parameter.

The **total cross-section** is the integral of $D(\theta)$ over all solid angles:

$$\sigma \equiv \int d\Omega D(\theta).$$

Example (Classical hard sphere): We calculate

$$\begin{aligned} b = R \cos \frac{\theta}{2} &\implies \left| \frac{db}{d\theta} \right| = \frac{R}{2} \sin \frac{\theta}{2} \implies \frac{d\sigma}{d\Omega} = \frac{R^2}{4} \\ &\implies \sigma_{tot} = \int \frac{d\sigma}{d\Omega} d\Omega = \frac{R^2}{4} \cdot 4\pi = \pi R^2, \end{aligned}$$

which is just the cross-sectional area of the sphere.

In the **quantum scattering** case, we use **Fermi's Golden Rule**; for constant potential V we have

$$P_{i \rightarrow f} = \frac{2\pi}{\hbar} |V_{if}|^2 \rho(E_f)$$

We write the initial and final states with box normalization, that is

$$\psi_i(r) = \frac{1}{\sqrt{l^3}} e^{ik' \cdot r}, \quad \psi_f(r) = \frac{1}{\sqrt{l^3}} e^{ik \cdot r}$$

With these states, we can compute the matrix element V_{if} . Further, we can compute the density of states as

$$\rho(E) = \left(\frac{l}{h} \right)^3 \sqrt{2m^3 E} d\Omega$$

Combining these results with Fermi's Golden Rule, we derive

$$R_{i \rightarrow d\Omega} = \left(\frac{l}{h} \right)^3 \frac{2\pi}{\hbar} \frac{1}{l^6} \sqrt{2m^3 E} \left| \int e^{i(k' - k) \cdot r} V(r) \right|^2 d\Omega.$$

We also have the relation

$$\frac{d\sigma}{d\Omega} = \frac{R_{i \rightarrow d\Omega}}{J_i d\Omega}, \quad J_i = -\frac{i\hbar}{m} \psi^* \nabla \psi = \frac{1}{l^3} \frac{\hbar k'}{m}$$

where J_i is the probability current of incident particles. Thus, our differential cross-section for this case is

$$\frac{d\sigma}{d\Omega} = \left| -\frac{m}{2\pi\hbar^2} \int d^3 r e^{i(k' - k) \cdot r} V(r) \right|^2$$

Ref: Problem Set 6.2(c), Griffiths Example 11.2, 10.3

Born approximation (lec 21)

Ref: Griffiths 10.4, Shang Section 12

Above, we have derived the Born approximation with Fermi's Golden Rule. The **Born approximation** supposes that the incoming wave is not substantially altered by the potential, so the potential is small $\frac{mV_0 a^2}{\hbar^2} \ll 1$, where we use

$\psi(r_0) \approx \psi_0(r_0) = A e^{i\mathbf{k}' \cdot \mathbf{r}_0}$, $\mathbf{k}' \equiv \hbar \hat{\mathbf{z}}$. We have

$$f(\theta, \phi) \approx -\frac{m}{2\pi\hbar^2} \int d^3 r e^{i(k' - k) \cdot r} V(r).$$

In the **low-energy (long-wavelength) limit** $\frac{2\pi}{k} = \lambda \gg a$, we can further simplify the scattering amplitude

$$f(\theta, \phi) \approx -\frac{m}{2\pi\hbar^2} \int d^3 r V(r).$$

For a **spherically symmetric** potential, we have

$$f(\theta) \approx -\frac{2m}{\hbar^2 \kappa} \int_0^\infty dr r V(r) \sin \kappa r, \quad \kappa \equiv 2k \sin \theta/2.$$

Ref: Problem Set 6.1, Griffiths Example 10.5, 10.6

1D scattering (lec 22)

Ref: Tong 10.1

Consider a 1D potential with an incoming wave. When the wave sees the potential, it will reflect or transmit.

The 1D analog of the differential cross sectional area is

$$D(\theta) \implies D(\pi) = |r|^2 = R$$

where r is the amplitude for the reflected wave and t for the transmitted wave.

If we have a wave coming from the left producing r, t and a wave coming from right producing r', t' , we can write the **scattering matrix**

$$S = \begin{pmatrix} t & r \\ r' & t' \end{pmatrix}$$

for real potentials, we have $t' = t$, $r' = -\frac{r^* t}{t^*}$. We can note that S is unitary:

$$S^\dagger S = \begin{pmatrix} |t|^2 + |r|^2 & t r'^* + r t'^* \\ t^* r' + t' r^* & |t'|^2 + |r'|^2 \end{pmatrix} = 1.$$

Note that if S were a number, we must have $S^\dagger S = 1 \implies S = e^{2i\delta}$, a pure phase.

Symmetric Potentials

For a symmetric potential, we can do a change of basis into the **parity basis** and see that

$$S^P = \mathcal{M} S \mathcal{M}^{-1} = \begin{pmatrix} t + (r + r')/2 & (r - r')/2 \\ (r' - r)/2 & t - (r + r')/2 \end{pmatrix}.$$

For symmetric potentials, $r = r', t = t'$ and S^P is **diagonal**, with $S_{++} = t + r = e^{i2\delta+(k)}$, $S_{--} = t - r = e^{-i2\delta-(k)}$.

Ref: Problem Set 6.2(ab)

3D Scattering (lec 23)

In three dimensions, a solution for $D(\theta)$ is given by

$$\psi(r) = e^{ikz} + f(\theta, \phi) \frac{e^{ikr}}{r}$$

Given $V(r)$, k , we wish to find the **scattering amplitude** $f(\theta, \phi)$, because

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

Assuming a **central potential**, $f(\theta, \phi) = f(\theta)$. Note that we can write

$$f(\theta) = \frac{1}{k} \sum_\ell f_\ell P_\ell(\cos \theta) (2\ell + 1) \implies \sigma_{tot} = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} |f_\ell|^2 (2\ell + 1)$$

Partial wave analysis (low-energy approximation)

Ref: Griffiths 10.2, Tong 10.2.3

For low energy scattering $\lambda > R \implies kR \ll 1$, the scattering is **dominated by the lowest angular momentum** $\ell = 0$, and so σ_{tot} is dominated by f_0 :

$$\sigma_{tot} \approx \frac{4\pi}{k^2} |f_0|^2, \quad D(\theta) = \frac{d\sigma}{d\Omega} = |f(\theta)|^2.$$

Phase shifts

Ref: Griffiths 10.3, Tong 10.2.3

By considering the lowest partial wave (s-wave), we can project out the angular momentum ($\ell = 0$); that is, $P_0(\cos \theta) = 1$. Then we can calculate the ratio of the outgoing and incoming waves to calculate the phase shift

$$e^{2i\delta_0} = 1 + 2ikf_0, \quad f_0 = \frac{e^{i\delta_0}}{k} \sin \delta_0.$$

The scattering cross section is then given by

$$\sigma_{tot} = 4\pi |f_0|^2 = \frac{4\pi}{k^2} \sin^2 \delta_0.$$

Radial projection (3D \rightarrow 1D)

We can calculate δ_0 by specializing $\psi(r) = R_0(r)$ where we consider only the radial component from the approximation.

In 3D, we have $\psi(r) = R(r)$.

We can map this 3D solution to 1D by first noting that we need to map the domain $r \in \{0, \infty\} \rightarrow \{-\infty, \infty\}$. From the boundary condition in 3D, we must solve the 1D scattering problem with $\psi(0) = 0$, which is satisfied by **odd-parity** wavefunctions.

Example (Quantum scattering from hard sphere): We will use partial wave analysis and project into $\ell = 0$, with solution $\psi = \sin k(r - R)$. Solving for the scattering state, we have

$$\psi(r) = \frac{i}{2} e^{ikR} \left\{ \frac{e^{-ikr}}{r} - \frac{e^{ikr}}{r} e^{-2ikR} \right\} = e^{-i2kR}$$

$$\implies \delta_0 = -kR \implies \sigma_{tot} = \frac{4\pi}{k^2} \sin^2 kR \approx 4\pi R^2$$

where we used $kR \ll 1$ for the approximation to hold. Note that this is **four times** larger than the classical result.

Ref: Problem Set 6.3, Griffiths Example 10.3

Entanglement (lec 24)

Ref: Griffiths 12.3, Tong 9.3

We can define the **density operator**

$$\rho \equiv |\Psi\rangle\langle\Psi| = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \quad \rho_{ij} = \langle e_i | \rho | e_j \rangle = \langle e_i | \Psi \rangle \langle \Psi | e_j \rangle.$$

We have $\rho^2 = \rho \iff \Psi$ is a **pure state**. Analogously, a pure state must have one eigenvalue 1 and all others 0. Otherwise, it is a **mixed state**. The density matrix is also Hermitian $\rho^\dagger = \rho$ and unit trace $\text{tr}(\rho) = 1$ (i.e. probability distribution is normalized). Moreover, ρ is positive semi-definite. The **reduced density matrix** ρ_A completely contains all

information about the subsystem A , and is defined as

$$\rho_A \equiv \text{tr}_B(\rho) = \langle \uparrow | \rho | \uparrow \rangle_B + \langle \downarrow | \rho | \downarrow \rangle_B = p_1 |\uparrow\rangle\langle\uparrow| + p_2 |\downarrow\rangle\langle\downarrow|$$

The expectation of an observable A is given by $\langle A \rangle = \text{tr}(\rho_A A)$.
