Problem 1 ("Lifetime of the Hydrogen Atom"): We mentioned in class that one of Bohr's postulates was that the electrons in the hydrogen atom were stuck in a stationary state. Why was this so radical?

For those of you that have taken advanced electromagnetism, one of the things you learn is that an accelerating point charge of charge q will lose energy in the form of electromagnetic radiation (light) at a rate of

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -\frac{q^2 a^2}{6\pi\epsilon_0 c^3}$$

where a is the acceleration and $c = 3 \times 10^8$ m/s is the speed of light. This is called the Larmor formula.

(a) If the electron is in a circular orbit around the proton at a radius r (ignore the effects of radiation for now!), find the energy E and the (magnitude of the) acceleration a as a function of r. Recall that the force between the electron and proton is simply given by Coulomb's Law, $\epsilon_0 \approx 8.85 \times 10^{-12}$ F/m, that the charge of the electron is $e \approx 1.6 \times 10^{-19}$ J, and that the mass of the electron $m \approx 9 \times 10^{-31}$ kg.

(b) Assuming that the orbit of the electron is circular, use the Larmor formula for $\mathrm{d}E/\mathrm{d}t$ to compute how much energy is lost in a period. Is this energy "negligible" in a single period?

(c) Work under the approximation that E, a and r are related as in part (a), but that these quantities are time dependent. Use the Larmor formula to find a formula for $\mathrm{d}E/\mathrm{d}t$ as a function of E.

(d) Suppose that at time $t = 0$, the energy of the atom is given by $-E_0$, the energy of the ground state of the hydrogen atom. Show that $r = 0$ at a finite time $t = t_\mathrm{f}$. Explain why it is valid to use the approximate result of part (c). This is the "classical lifetime" of the hydrogen atom. Compute the numerical value of t_f and comment on the result.

Problem 2 (Optical Molasses): One of the most amazing advances in physics in the last few decades has been our ability to cool down a gas to incredibly low temperatures. A major technique which aids in this capability is laser cooling. We will show in this problem how a cleverly designed laser trap can create an "optical molasses" which will cool atoms down to very low temperatures.

For simplicity, let us consider a single atom moving on the one dimensional line, of mass m, which can absorb radiation at frequencies of approximately ν_0 – we will shortly return to this point. Suppose that a laser to the right of this atom is emitting photons of frequency ν_L, which must be very close to ν_0 in order for absorption to occur It will re-emit the photon equally likely to the left or to the right, at frequency ν_0 – in its own rest frame.

(a) Suppose that the atom moves with velocity v, in the laboratory rest frame. v is positive when we move towards the laser. After the atom absorbs and re-emits a photon, what is the average change in the momentum of the atom?

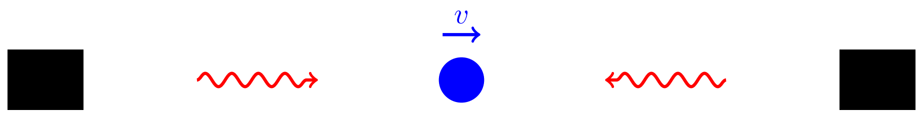
(b) One can show that the rate at which an atom will absorb photons is

$$\frac{\text{photons absorbed}}{\text{time}} \equiv R(\nu) = \frac{2\pi\Gamma\Omega^2}{\Gamma^2/4 + \Omega^2 + (\nu - \nu_0)^2}.$$

where Γ, Ω are constants. These constants are small, so this function is sharply peaked around $\nu \approx \nu_0$. Suppose that, as in the figure below, we have a pair of lasers emitting photons of frequency ν_L in the lab frame towards the atom, from opposite sides. Show that the force on the atom is approximately given by, as $v \to 0$:

$$F \approx \frac{8\pi\Gamma\Omega^2 h\nu_\mathrm{L}^2}{c^2\left(\Gamma^2/4 + \Omega^2 + (\nu_\mathrm{L} - \nu_0)^2\right)^2}(\nu_\mathrm{L} - \nu_0)v$$

Comment on this answer. If we want to use this laser setup to slow down the atoms, how should we pick ν_{L}? This technique is referred to as optical molasses.



Statistical mechanics tells us that the temperature associated with (a collection of many) atoms like the one above is

$$k_{\mathrm{B}}T = \frac{m}{2}\left\langle v^2 \right\rangle,$$

where $\langle \cdots \rangle$ denotes a thermal average, and $k_{\mathrm{B}} \approx 1.3 \times 10^{-23}$ J/K. The reason we're cooling down our gas of atoms to incredibly low temperatures is that the optical molasses makes the atoms move very slowly.

(c) Suppose we start with a cloud of sodium atoms ($m \approx 3 \times 10^{-26}$ kg) at temperature $T = 300$ K. How fast is the typical speed of an atom – let us denote it with $\bar{v}$?

(d) If an atom starts at speed $\bar{v}$, estimate how long will it take to (approximately) come to rest. Assume that $\lambda_0 = c/\nu_0 = 6 \times 10^{-7}$ m, and that $\mathit{\Gamma} \sim \mathit{\Omega} \sim |\nu_{\mathrm{L}} - \nu_0| \sim 10^8$ s^{-1}.

(e) How far will the atom travel before coming to rest? This gives you a sense of the size of an optical trap.

(f) It turns out that the minimum temperature acheivable through this method is (up to some experimental tricks!)

$$k_{\mathrm{B}}T_{\mathrm{min}} \sim h\mathit{\Gamma}.$$

Estimate T_{min} for our atomic gas.

Problem 3 (Material Properties of Crystalline Solids): Does quantum mechanics have any real relevance to everyday objects in our world? The answer is of course *yes* – almost all of chemistry relies on exclusively quantum mechanical phenomena, for example. But we can find quantum mechanical imprints on everyday life that are even simpler – knowledge of $\hbar$ alone allows us to make very successful back-of-the-envelope calculations about everyday materials!

The typical energy scale associated with the hydrogen atom is $\mathcal{E} \sim 2 \times 10^{-18}$ J; the typical mass scale is set by the mass of the proton: $\mathcal{M} \sim 2 \times 10^{-27}$ kg; the typical length scale is related to the Bohr radius, $\mathcal{L} \sim 5 \times 10^{-11}$ m.

(a) Postulate that the densest possible material on Earth consists of packing together hydrogen atoms. Using dimensional analysis, estimate the mass density of this material. Compare to the most dense known material, osmium, which has a mass density of about 2.2×10^4 kg/m^3. Note that many other crystalline solids have mass densities that are within an order of magnitude of osmium, but a bit smaller.

Remarkably, it turns out that even in a complicated quantum system such as a chemical bond, the energy scale associated with breaking that bond is still $\mathcal{E}$. And the length of chemical bonds is also of order $\mathcal{L}$.

(b) Consider taking a rectangular slab of solid of thickness A and length L, and stretching it lengthwise by a very small amount, $\mathit{\Delta} L \ll L$. This stretches the chemical bonds in the material, a process which exerts a force which tries to restore the solid, very much like a spring. One of the material properties of a solid is the Young's modulus E, defined as a proportionality coefficient of this force

$$F = -EA\frac{\mathit{\Delta} L}{L}.$$

It is universal to a material and independent of A and L. What are the dimensions of E? Estimate the value of E using dimensional analysis. In the appropriate SI units, the value of E is about 10^{11} to 10^{12} for many crystalline solids – compare your answer to this.

(c) Denoting the speed of sound in a material with c, show that the following equation is dimensionally correct:

$$c = \sqrt{\frac{E}{\rho}}.$$

Thus estimate the speed of sound in a crystalline solid. Compare to 6000 m/s, which is a reasonable estimate for many crystalline solids.

(d) Do you think a forward thinking physicist in the early 1900s could have estimated $\mathcal{E}$, $\mathcal{M}$, and $\mathcal{L}$, given simple material properties?

Problem 4 (The Distribution of Incomes): In this problem, we will explore a simple model for how incomes are distributed within a society, that turns out to match reasonably well with empirical data.

Let's suppose that we have an economy consisting of N people, who report their incomes Y_i ($i = 1, \ldots, N$) each year to the IRS. Then the IRS can go ahead and collect all this data and report back the distribution of incomes. For theoretical purposes, let's suppose that they reported back a smooth function $\rho(y)$, which is defined so that for most "reasonable" intervals,

$$\int\limits_{y_1}^{y_2} \mathrm{d}y\ \rho(y) = \frac{\text{number of people with income } Y_j \text{, such that } y_1 < Y_j < y_2}{N}.$$

We'll refer to the object on the left hand side of this equation as the probability that someone in our economy has an income in between y_1 and y_2.

(a) What is the probability that someone in our economy has income *exactly* equal to y_0?

Next, let us construct a very simple model that matches quite well with empirical data on the incomes of the rich in basically every single country. The full model is rather annoying to solve exactly, so we'll break it down into two parts. The basic idea is that the poor and the rich have two predominantly different mechanisms by which their incomes change from year to year. So we'll first study the poor, and then the rich.

Suppose that you have income $Y(t)$ in year t, and income $Y(t+1)$ in year $t+1$. We're interested in

$$\mathit{\Delta} Y = Y(t+1) - Y(t).$$

When you are poor, changes in your income are predominantly random, and so you're probably equally likely to see your salary go up and go down in an average year. However, because of the effects of inflation, it turns out that you're more likely to lose money (in real terms) in any given year. The simplest possible model that accounts for this is simply to say that

$$\mathrm{P}(\mathit{\Delta} Y = -\alpha) = \mathrm{P}(\mathit{\Delta} Y = \beta) = \frac{1}{2},$$

with $\alpha > \beta$. Half the time you lose income α, and half the time you gain income β.

Now, we want to construct $\rho(y)$ for an economy where approximately everybody is poor. To do this, we can use the following logic. Let us consider a fixed income y. We need to count the probability $p_+(y)$ that an individual started out below income y in year t, and ended up above income y in year $t+1$; and $p_-(y)$, the probability that we started out above y in year t and ended up below y in year $t+1$. In order for the distribution $\rho(y)$ to be stationary, we must have $p_+(y) = p_-(y)$ for every y.

(b) Assume that α and β are small enough so that ρ is very smoothly varying on these income scales, and may be treated as an approximately linear function for the purposes of computing $p_\pm(y)$. Use the condition $p_+ = p_-$ to find a differential equation for $\rho(y)$.

(c) Let us assume that nobody in our economy can have income $y < 0$. Solve the ODE for $\rho(y)$, restrict to the interval $0 < y < \infty$, and find the normalized solution to the ODE. You should find

$$\rho(y) \sim \mathrm{e}^{-\lambda y}.$$

What is λ in terms of α and β?

(d) Among the poor, compute $\langle y \rangle$ and σ_y, the mean and standard deviation of the income distribution.

Next, let us consider the economy of the rich. Incomes of the rich are often tied to investments and the stock market, and as such grow proportionally to the amount of income they currently have: e.g., if the stock market doubles, then your income doubles no matter how high it was to begin with. So this time, we say that

$$\mathrm{P}(\mathit{\Delta} Y = -ay) = \mathrm{P}(\mathit{\Delta} Y = by) = \frac{1}{2},$$

namely that half the time incomes grow by by, and half the time they fall by ay.

(e) Repeat the analyses of parts (b) and (c), this time for the economy of the rich. You should find that the solution to the resulting differential equation is

$$\rho(y) \sim y^{-\gamma}.$$

What is γ in terms of a and b?

(f) Realistic distributions for the incomes of the rich are always normalizable in the interval $y_0 < y < \infty$. What are the constraints on γ?

(g) Compute $\langle y \rangle$ and σ_y. Show that they may be infinite.

(h) Focus on the interesting case where $1 < \gamma < 2$. If the economy has N_r rich people, estimate the highest income among the rich, in a typical realization of random incomes drawn from $\rho(y)$. Compare to the result of part (g), and comment.

Empirical income distributions tend to have $\gamma \sim 2.2$.

Problem 5 (The Classical Limit): We know from everyday experience that classical Newtonian mechanics ($F = ma$) is a very good way to describe the motion of big, "classical" objects that we see around us. It is not at all obvious how to recover this as any limit of the quantum Schrödinger equation, which we've learned for a point particle of mass m in one dimension.

The basic intuition is that classical physics occurs when $\hbar \to 0$. However, we can't just go ahead and set $\hbar = 0$ above, because that trivializes the entire equation! We have to try a bit harder. A helpful place to start is to re-write the wave function as

$$\mathit{\Psi} = \sqrt{\rho}\mathrm{e}^{\mathrm{i}\theta},$$

where $\rho \geq 0$ and θ are real-valued fields.

(a) Plug in the ansatz for Ψ into the Schrödinger equation. Show that taking the real and imaginary parts of the resulting answer, and after performing a few more basic manipulations, you find the pair of equations

$$\partial_t\rho + \partial_x(\rho v) = 0,$$
$$\partial_t v + v\partial_x v = -\frac{1}{m}\partial_x\left(V - \frac{\hbar^2}{2m}\frac{\partial_x^2\sqrt{\rho}}{\sqrt{\rho}}\right).$$

where

$$v \equiv \frac{\hbar}{m}\partial_x\theta.$$

(b) The equations above may remind you of the equations of motion of a compressible fluid, up to the remnant of $\hbar$ in the second equation. Explain the physical content contained in each of these equations. How have we managed to "hide" $\hbar$?

It now suffices to show that these fluid-like equations reduce to Newton's Law $F = ma$. We still need to make a physical assumption – namely, that the quantum particle is approximately localized at the point X, but is spread out over a small length scale l. For example, you might think $\rho \approx \mathrm{e}^{-|x-X|/l}/\sqrt{2\pi}l$. l is effectively an input parameter, and there is no forced relationship between l and any other parameter in the problem, though later on in the course we'll see that l would typically be at least as big as some "minimum" l_0.

(c) Suppose that a classical point particle at point X would feel a force F. How large must l be in order for us to neglect the $\hbar^2$ term in the equations of part (a)?[1]

From now on, we'll take l to be much larger than the required value found in part (c).

The classical limit will really consist of $\hbar \to 0$ first, and $l \to 0$ second. What we really care about is that V is approximately constant on the length scale l: namely, that $|V|/l \gg |\partial_x V|$.

(d) Justify defining the approximate position of our classical point mass to be

$$X(t) \equiv \int \mathrm{d}x\; x\rho(x,t).$$

(e) Manipulate the equations of part (a), and show that under reasonable approximations

$$m\frac{\mathrm{d}^2X}{\mathrm{d}t^2} \approx -\left.\frac{\partial V}{\partial x}\right|_{x=X}.$$

This is, of course, another way of saying that $F = ma$.

On the homework, you are supposed to prove an exact theorem of quantum mechanics that, using the same approximations we have made, reduces to a derivation of Newton's Laws. You may use very similar logic to this problem if you wish, but it will probably be easier to work directly with Ψ and Ψ^*, and integrate by parts.

Problem 6: Sometimes there can be subtleties in trying to take classical limits in quantum mechanics.

(a) Suppose we had a free classical particle of mass m in a box of width a, at energy E. Describe the motion as a function of time. If we wait for a very long time, what is the limiting probability distribution for where we will find the particle?

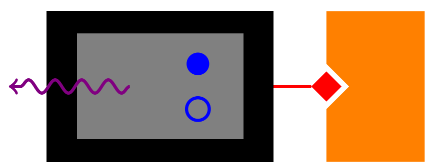
[1] We may crudely estimate $\partial_x\rho \sim \rho/l$ for the purposes of estimating whether terms are big or small.

(b) Now suppose we have a quantum particle in a box. Choose $\Psi(x,0)$ to be a real-valued quantum wave function with the same probability density as in part (a). Be sure to normalize $\Psi(x,0)$. Compute $c_n(0)$, the overlap of Ψ with the n^{th} stationary state at $t=0$. Conclude by stating $\Psi(x,t)$.

(c) What is $\langle H\rangle$ – the expected energy we observe on measurement. Explain the result you find.

(d) Consider a particle in stationary state ψ_n. Sketch the probability distribution of where it is most likely to be found if $n=1$. What about $n \gg 1$? Compare to the classical case. Does the probability distribution limit to the classical one as $n\to\infty$? There are various mathematics answers here – what about physically?

Problem 7 (Quantum Dots): One of the practical uses of the particle in the box in the laboratory is to serve as a mobile, robust and precise emitter of light. A very important use for this technology is as follows: a nanoscale semiconductor arrangement called a quantum dot, consisting of various layers of semiconducting materials, is attached to a molecule with a "flag" on the end. This flag will consist of a molecular group that is heavily attracted to certain receptors on proteins – for example, a toxin or other unwanted substance. By releasing these quantum dot flags into a cell, we can track down and image (in real time) where all the bad proteins are, by observing the photons emitted from the quantum dots. A cartoon of this setup is below.



We can model this system as a particle in the box (with some complications) of length $a \approx 5$ nm. When a photon of the right frequency hits this dot, it excites an electron out of the filled energy levels of the metal – this costs an energy $\Delta \approx 2.5\times 10^{-19}$ J. This electron becomes confined in the inner part of the semiconductor, and behaves as though it is a particle in a box. Unfortunately, the hole left behind (the absence of an electron in the filled band of the metal) behaves as a positively charged particle, and so we'll approximately have to double the required energy of the photon necessary to excite our electron, to account for the quantum behavior of this hole as well.

(a) How much energy does the photon need to kick both the electron and the hole into the ground state of the box? Does Δ or the ground state energy of the particle in the box dominate this energy requirement?

(b) Suppose that we re-emitted a photon at about the same wavelength at which we absorbed a photon. What would the wavelength λ of these photons be? In the lab, you would easily be able to detect light being strongly emitted by the dot at wavelengths of about λ.

(c) How should we change the width of the quantum dot a if we want to make the emitted photon redder? Bluer?

Problem 8 (Carbon Dioxide): One of the concerns with greenhouse gas emissions – primarily CO_2, carbon dioxide – is that they can lead to global warming via the greenhouse effect. A physical cartoon of this is as follows. Imagine that you have a CO_2 molecule in the atmosphere, and a photon comes up from the Earth's surface, carrying away energy. If the molecule can absorb this photon, it will re-emit it towards space half the time, but half the time emit it back down to Earth, where it gets reabsorbed. This process repeats many times until the photon escapes, but more energy is trapped on Earth while this process occurs, and this leads to a rise in temperature. In this problem we will ask whether this process is likely to occur frequently, based on microscopic estimates.

(a) The energy scale associated with a chemical bond is about 10^{-18} J, and the length of a chemical bond is about 10^{-10} m. Estimate from dimensional analysis what the spring constant k should be for a typical chemical bond.

(b) Using your estimate of k from above, and the mass of hydrogen at $m \approx 2 \times 10^{-27}$ kg, estimate the angular frequencies of photons which the harmonic oscillator(s) associated with vibrations of the CO_2 molecule will effectively absorb (and emit).

(c) Estimate the angular frequency of the "typical" photon emitted from Earth's surface, and compare to the result in part (b).

The absorption spectrum of real gases is far more complicated, of course – some molecules absorb lots of photons, and others don't. But this gives you a sense that the numbers make the greenhouse effect possible.

Problem 9 (Bogoliubov Quasiparticles): Let a and $a^\dagger$ be the annihilation and creation operators for a harmonic oscillator in one dimension, and let ψ_n denote the stationary states associated with the n^{th} energy state of the harmonic oscillator. Consider the Hamiltonian

$$H = \epsilon a^\dagger a + \eta \left(aa + a^\dagger a^\dagger \right).$$

ϵ and η are real parameters. More complicated Hamiltonians – but with the essential feature of η-like terms – arise in the Hamiltonians describing superfluids and superconductors.

(a) Show that ψ_n is not a stationary state of H for any n.

(b) Consider the Bogoliubov creation and annihilation operators given by

$$b = a\cosh\theta + a^\dagger \sinh\theta, \quad b^\dagger = a^\dagger \cosh\theta + a\sinh\theta.$$

Show that $[b, b] = [b^\dagger, b^\dagger] = 0$, and that $[b, b^\dagger] = 1$.

(c) Find the value of θ such that

$$H = \zeta b^\dagger b + E_0,$$

for constants ζ and E_0; also determine ζ and E_0. Conclude by determining the energy spectrum of the Hamiltonian.

(d) Discuss the nature of the stationary states of H – though you do not need to give exact expessions for all of them, at least show clearly how to compute them. In particular, comment physically on what has happened by writing the ground state in terms of the wave functions ψ_n – the stationary states of the original oscillator when $\eta = 0$.

Problem 10 (Hermite Polynomials): In this problem we're going to properly understand the Hermite polynomials by exploiting the beautiful harmonic oscillator algebra. For simplicity we work in dimensionless units: "we set $\hbar = m = \omega = 1$". So

$$a = \frac{x + \mathrm{i}p}{\sqrt{2}}, \quad a^\dagger = \frac{x - \mathrm{i}p}{\sqrt{2}}, \quad p = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}.$$

Note that $[a, a] = [a^\dagger, a^\dagger] = 0$ and $[a, a^\dagger] = 1$, and

$$a\psi_n = \sqrt{n}\psi_{n-1}, \qquad a^\dagger\psi_n = \sqrt{n+1}\psi_{n+1}.$$

In these units, the harmonic oscillator wave functions are

$$\psi_n(x) = \frac{\mathrm{e}^{-x^2/2}}{\pi^{1/4}2^{n/2}\sqrt{n!}}\mathrm{H}_n(x),$$

where $\mathrm{H}_n(x)$ is the n^{th} Hermite polynomial ($n = 0, 1, 2, 3, \ldots$).

(a) Begin with the fact that $\mathrm{H}_0(x) = 1$. By constructing ψ_n from the creation operators, derive the Rodrigues formula:

$$\mathrm{H}_n(x) = \mathrm{e}^{x^2}\left(-\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \mathrm{e}^{-x^2}.$$

(b) It is not obvious from the Rodrigues formula that $\mathrm{H}_n(x)$ is a polynomial. Derive the following recursion relation:

$$\mathrm{H}_{n+1}(x) = 2x\mathrm{H}_n(x) - \frac{\mathrm{dH}_n(x)}{\mathrm{d}x}.$$

and show how H_n is always a polynomial.

(c) Use the relations between x, p, a and $a^\dagger$, acting on the wave function ψ_n, to derive the following pair of identities:

$$x\mathrm{H}_n(x) = \frac{1}{2}\mathrm{H}_{n+1}(x) + n\mathrm{H}_{n-1}(x), \qquad \frac{\mathrm{dH}_n(x)}{\mathrm{d}x} = 2n\mathrm{H}_{n-1}(x).$$

(d) A generating function for Hermite polynomials is defined as

$$G(x; z) \equiv \sum_{n=0}^{\infty} \frac{z^n}{n!}\mathrm{H}_n(x),$$

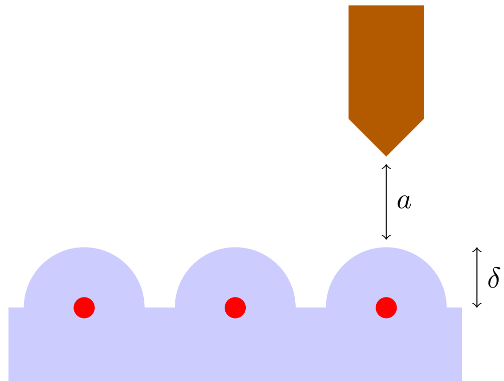
as

$$\left.\frac{\partial^n G}{\partial z^2}\right|_{z=0} = \mathrm{H}_n(x).$$

Show that the generating function for Hermite polynomials is

$$G(x; z) = \mathrm{e}^{2xz - z^2}.$$

Problem 11 (Scanning Tunneling Microscope): A scanning tunneling microscope (STM) is used to determine where electrons are on the surface of a material. The basic idea is as follows: a thin metal tip is placed a distance a from the "surface" of a metal. In reality, the surface of the metal is not entirely smooth – electronic wave functions stick out farther in some places than in others. As we'll compute in this problem, it is possible, though unlikely, for an electron from the metal to tunnel into the STM tip. Not surprisingly, the closer the tip is to the electronic wave function, the larger the rate of tunneling events will be. So we scan the STM tip over the surface of the metal and, by measuring the rate of these tunneling we can tell how much the electronic wave functions stick out from the surface of the metal.



We end up with the following cartoon. For simplicity, we only model the dynamics of the electrons perpendicular to the surface, and assume that electrons are approximately bound in place along the surface, due to the presence of attractive Coulomb interactions with a nearby ion. An electron of mass m moves in the following potential:

$$V(x) = \begin{cases} -\Delta & x < 0 \\ 0 & 0 < x < a \\ -\varphi & x > a \end{cases},$$

with $0 < \Delta < \varphi$. The former constraint ensures that it takes some energy to pull an electron out of a metal, and the latter "ensures" that tunneling events from the STM tip into the metal are essentially negligble (we won't worry about this point, as a lab set-up is more complicated and would avoid this issue entirely). The electron starts at $x < 0$, in the metal of interest.

(a) Approximately find the scattering states where the electron is incident on the barrier from the left, in the limit where $a \to \infty$, if the electron has incident wave number k, assuming that[2]

$$\frac{\hbar^2 k^2}{2m} \ll \Delta.$$

(b) Approximate that the incident energy of the electrons is comparable to Δ, and estimate the width of the vacuum gap a_c necessary before the likelihood of a tunneling event occuring is "high". Obtain both an analytic estimate, as well as a numerical estimate, using that for a typical metal, $\Delta \approx 5 \times 10^{-19}$ J ~ 3 eV, and the mass of the electron is $m \sim 10^{-30}$ kg.

(c) Typical STM measurements work at $a \sim 10a_\mathrm{c}$, so that the probability of tunneling events is very low. Approximate that whenever an electron gets reflected, it must travel about an atomic distance before another electron is incident on the barrier. Using dimensional analysis, and noting that the interatomic distance scale in a metal is about $\delta \sim 0.3$ nm, estimate the time required before we can see a single electron tunnel into our STM.

(d) Now suppose that we move the STM tip to another location on the surface where the thickness of the distance between the STM tip and the surface electrons has grown to $a + \delta$. By how much will the electric current flowing through the STM tip reduce?

(e) To what extent does the answer in this problem depend on φ? What if φ was a function of x?

[2]Remember that physically, the probability that the particle can tunnel through the barrier becomes extremely small as $a \to \infty$. What does this imply about the dominant contribution to the wave function in the region $0 < x < a$?

In reality, the net electric current flowing is sensitive to "φ". But calculating the electric current requires a bit more solid-state physics, and the most dramatic effect is the low probability for tunneling, which we're already able to calculate fairly reliably.

The power of the STM is that – as shown in part (d) – it is an extraordinarily sensitive measurement. We are thus able to "image" the electronic wave functions on the surface of a metal.

Problem 12 (Quantum Decay Processes): In this problem we will write down a very simple cartoon for a variety of quantum decay processes: e.g., emisssion of α or β radiation. Let us consider a particle of mass m, trapped in a 1d δ well, but where the strength of the δ well abruptly changes in time:

$$H = \frac{p^2}{2m} - \alpha(t)\delta(x),$$

$$\alpha(t) \equiv \begin{cases} \alpha_1 & 2nT \le t < (2n+1)T \\ \alpha_2 & (2n+1)T \le t < 2(n+1)T \end{cases}.$$

Of course, we take $\alpha_1 \neq \alpha_2$. At time $t = +\epsilon$ (ϵ small), the particle is in the sole bound state of the Hamiltonian with α_1. We'll begin by focusing on whether or not particles remain bound to the well as it evolves.

(a) At time $t = T$, the "strength" of the well switches suddenly to α_2. Describe qualitatively what the wave function will look like for $T < t < 2T$. What is the probability that the particle will remain "bound" near $x = 0$?

(b) Is $\langle H\rangle(T-\epsilon) = \langle H\rangle(T+\epsilon)$? (Here ϵ is infinitesimal.) Why or why not?

(c) At time $t = 2T$, the strength switches back to α_1. Assuming that T is "long enough", argue that the only part of the wave function localized around $x = 0$ is the "bound part" of the wave function, and that this is the only part of the wave function altered by the switch-over. Calculate the probability that the particle is bound after $t = 2T$.

(d) What do we mean by T being a "long time"? Dimensional analysis will help you here.

(e) Argue that, on time scales $t \gg T$, we may approximate that the probability P that the particle is "bound" to the well obeys the differential equation

$$\frac{\mathrm{d}P}{\mathrm{d}t} = -\lambda P.$$

and compute λ.

However weak the disturbance to the δ well, there is always a finite probability that the particle becomes unbound. This is in contrast to classical physics, where a finite amount of energy must be added before a particle becomes unbound.

Now, let's focus on the dynamics when the particle becomes unbound. For this case, let us consider the following simplified problem:

$$H = \frac{p^2}{2m} - \begin{cases} \alpha\delta(x) & t < 0 \\ 0 & t > 0 \end{cases}.$$

Again, we assume that the particle is in the bound state of the well for $t < 0$.

(f) Calculate $\Psi(x,t)$, up to evaluating an integral. Qualitatively describe what you think the dynamics of the resulting wave packet will be.

Problem 13 (Vector Spaces of Polynomials): This problem is meant to provide a healthy refresher and warm-up in linear algebra. We will focus on vector spaces of functions, which are of great importance in quantum mechanics. In particular, in this problem we will study the vector space $\mathbb{P}_n$, which is the vector space of all polynomials of degree $\leq n$: namely,

$$a_0 + a_1 x + \cdots + a_n x^n \in \mathbb{P}_n, \quad \text{for any } a_0, \ldots, a_n \in \mathbb{R}.$$

(a) Explain why $\mathbb{P}_n$ is a real vector space. What is its dimension?

(b) Is the subset of $\mathbb{P}_n$ consisting of all polynomials with $a_0 = 5$ a vector space? If so, construct a basis.

(c) Is the subset of $\mathbb{P}_n$ consisting of all polynomials $p(x)$ with $p(1) = 0$ a vector space? If so, construct a basis.

(d) We can, of course, arrange the coefficients $a_0, \ldots, a_n$ into a column vector:

$$\mathbf{a} \equiv \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{pmatrix}.$$

Explain why the derivative operator $\mathrm{d}/\mathrm{d}x$ acts as a linear transformation on $\mathbb{P}_n$. Denote the matrix associated with this linear transformation with D. Compute D^m for all (positive) m. Is D invertible?

(e) Does multiplication by x act as a linear transformation on $\mathbb{P}_n$ for any finite n? What about $\mathbb{P}_\infty$ (defined in the obvious way)? If your answer is yes, then find the matrix X associated with this transformation.

In quantum mechanics, we always want to work with an inner product space. Namely, we wish to find a function $\langle \circ, \circ \rangle : \mathbb{P}_n \times \mathbb{P}_n \to \mathbb{R}$ which appropriately defines the "length" of a polynomial. Remember that this function is not arbitrary, and must satisfy certain axioms! A "natural guess" is

$$\langle p, q \rangle = \int_\alpha^\beta \mathrm{d}x \; F(x) p(x) q(x),$$

where $\alpha < \beta$ are the limits of integration, and $F(x)$ is some fixed function.

(f) Pick $\alpha = 0$, $\beta = 1$ and $F(x) = 1$. Using the Gram-Schmidt procedure, construct an orthonormal basis for $\mathbb{P}_2$ with respect to this inner product.

(g) Is this a satisfactory definition of inner product for arbitrary F? If yes prove it, and if no find a counterexample.

(h) Now pick $\alpha = -\infty$, $\beta = +\infty$, and $F(x) = \mathrm{e}^{-x^2}$. Can you think of an orthogonal basis for $\mathbb{P}_\infty$ with respect to this inner product?

Problem 14 (Canonical Transformation of Momentum): While Schrödinger "guessed" at his wave function, Dirac was a much more mathematical physicist. It might surprise you that the way he tried to justify the new quantum theory to the old people of his time, in his influential textbook, was to actually state the fundamental "equation" of quantum mechanics as

$$[x, p] = \mathrm{i}\hbar.$$

This is called the canonical commutation relation. There is a classical analogue to this formula, called a Poisson bracket, and the analogy resonated with his audience. The "obvious" choice of operator p that satisfies this equation is

$$p = -\mathrm{i}\hbar\frac{\partial}{\partial x}.$$

(a) Let us define the operator

$$q = p + Q(x)$$

where Q is a function of x. Show that $[x, q] = \mathrm{i}\hbar$. Under what conditions is the operator q Hermitian – explicitly use the definition of a Hermitian operator to check this. Henceforth we take q to be Hermitian. q is called a canonical transformation of the momentum.

(b) Find the eigenvalues and eigenvectors of q in the position basis. Normalize them and check that they are orthonormal.

(c) Suppose we have a quantum system with Hamiltonian

$$H = \frac{q^2}{2m}$$

Discuss the general solution $\Psi(x,t)$ to the time-dependent Schrödinger equation. Show that there is a one-to-one map between $\Psi(x,t)$, and an analogous solution of the time-dependent Schrödinger equation with $H = p^2/2m$ (the free particle). Are the wave functions identical? Can one physically distinguish between these two Hamiltonians in a meaningful way?

Problem 15 (BB84 Quantum Cryptography): Quantum mechanics gives us a way to send a string of bits `01001`, etc., to a friend, with the absolute confidence that nobody else has read the message. The clever trick that we use is based on the disruptive nature of quantum measurement.

Suppose that Alice wants to send her string of bits to her friend Bob, across a possibly insecure line of communication. However, suppose that she can send quantum bits. The basic idea is that Alice will send 4 bits, each with equal 1/4 probability, at times $t = 0, 1, 2, \ldots$:

$$|\psi_1\rangle = |0\rangle, \quad |\psi_2\rangle = |1\rangle, \quad |\psi_3\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}, \quad |\psi_4\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}.$$

Now, Bob recieves this string of quantum bits. He has no idea what to expect, and so with equal probability he makes a measurement with one of the two Hermitian operators:

$$\sigma_z = |0\rangle\langle 0| - |1\rangle\langle 1|, \quad \sigma_x = |0\rangle\langle 1| + |1\rangle\langle 0|.$$

(a) What are the eigenvalues and eigenvectors of σ_z and σ_x? (Try the quantum states above!)

(b) There are 8 possibilities: Alice has sent $|\psi_{1,2,3,4}\rangle$ and Bob measures with $\sigma_{z,x}$. Each is equally likely. Describe what quantum states Bob will have after the measurement, with what probability. Show that Bob does not alter the quantum state if Alice has sent $|\psi_{1,2}\rangle$ and Bob measures with σ_z, or if Alice has sent $|\psi_{3,4}\rangle$ and Bob measures with σ_x.

The next step in the protocol is that Alice publicly sends Bob a string of zs and xs. The n^{th} letter in the string is a z if she sent $|\psi_{1,2}\rangle$ at time n, and an x otherwise. Bob compares Alice's string with what he measured, and he returns to her a list of all times n at which he measured with the appropriate $\sigma_{z,x}$ operator. As we showed in part (b), if Bob has directly received a quantum state from Alice, then it is these states which are unaltered. Bob now sends a list of the quantum states he has measured to Alice.

Now, however, suppose that at each time step, Bob does not receive a bit directly from Alice. Instead, there's a quantum eavesdropper Eve who has been "listening in". For our purposes, that means that at each time step, Eve makes a measurement on Alice's quantum state before Bob does. She uses the same two operators. As Eve also won't know which random states Alice is sending, she must, like Bob, choose her operators randomly.

(c) What is the probability that Alice has sent the state $|\psi_i\rangle$, and Bob receives the state (before his measurement) $|\psi_j\rangle$? Make a table of these probabilities, $\mathbb{P}(i \to j)$. (You should be able to exploit results from part (b) to do this quickly!)

(d) What is the probability ρ that Alice has sent $|\psi_{1,2}\rangle$ and Bob measured with σ_z, or that Alice has sent $|\psi_{3,4}\rangle$ and Bob measured with σ_x, and Bob's measurement of the quantum state disagrees with what Alice prepared?

If Alice and Bob disagree on (at least) a fraction ρ of the quantum states when they compare, then Alice knows that there is an eavesdropper in the channel. Otherwise she knows that nobody has been listening, and the channel is secure. She may now securely send her message to Bob across this channel.

Problem 16 (The Energy-Time Uncertainty Principle, Redux): Let $|\Psi(0)\rangle$ be the initial state of some quantum system with Hamiltonian H. Suppose that at some time τ, $\langle\Psi(\tau)|\Psi(0)\rangle = 0$.

(a) Show that τ obeys the following inequality, where C is an O(1) number:

$$\sigma_H \tau \geq C\hbar,$$

where σ_H is the uncertainty in the Hamiltonian of the state $|\Psi(0)\rangle$. The simplest way to proceed is as follows: consider $X(t) \equiv \mathrm{e}^{-\mathrm{i}\langle H\rangle t/\hbar}\langle\Psi(t)|\Psi(0)\rangle$, and find an upper bound for $\mathrm{Re}(X(t))$.

(b) A more serious calculation gives $C = \pi/2$. Construct a quantum state $|\Psi(0)\rangle$ and a Hamiltonian H such that the inequality above is realized with this value of C.

Problem 17 (Quantum Wires): Consider a very thin strip of a semiconductor, with a square cross section of side length a. Electrons of mass $m \sim 10^{-30}$ kg are approximately constrained to move in the three dimensional potential

$$V(x, y, z) \approx \begin{cases} 0 & |z|, |y| \leq a/2 \\ \infty & \text{otherwise} \end{cases}.$$

There will be electrons in energy eigenstates for every $E < \mu$ in the system; $\mu > 0$. For a typical semiconductor we can estimate $\mu \sim 1$ eV $\sim 2 \times 10^{-19}$ J.

(a) What are the eigenvectors and eigenvalues of the Hamiltonian?

(b) For what value of a will the dynamics of all electrons be describable by the Hamiltonian of a one dimensional free particle in the potential $V(x) =$ constant? Compare your answer to the typical interatomic spacing, 0.2 nm.

Wires of width smaller than this, made of "typical" materials, will behave as effectively one dimensional quantum systems. This width is too small to be fabricated cleanly in most labs. But recent materials such as carbon nanotubes have allowed for realistic, effectively one dimensional quantum systems to be created and used for engineering purposes.

Problem 18 (Binding to an Impurity in a Metal): Consider a particle of mass m in three dimensions in the potential

$$V(\mathbf{r}) = -\alpha\delta(r-R),$$

where $\alpha, R > 0$. This is a crude model for attractive interactions between a free electron and an impurity in a metal.

(a) Find all bound states of this potential with $l = 0$ angular momentum, including both the stationary state and the energy. Does a bound state always exist?

(b) Compare to what happens for the δ well in one dimension.

This is a crude model that suggests the following result, which turns out to be rigorous. In one dimension, any amount of impurities at all can trap electrons in a metal and localize them, which means that it is very hard to maintain an electrical current – namely, a one dimensional metal becomes an insulator for any impurity density. However, we must have a finite "strength" of impurities (modeled by α) in a three dimensional metal before we get an insulator.

Problem 19 ($Z > 1$ Atoms): Consider the Schrödinger equation for an electron of mass m_e, bound by the Coulomb interaction to a heavy nucleus of charge Ze, with $Z > 1$. Z counts the number of protons in the nucleus of the atom. Find the bound states of this Hamiltonian, and the allowed energies. (Feel free to express the answers in terms of the known results for the hydrogen atom, at $Z = 1$.)

Problem 20 (Do Chemists Need Relativity?): Schrödinger ignored special relativity when developing quantum mechanics, and Dirac famously dismissed the possibility that relativity would be meaningful for quantum chemistry. Is this really true?

(a) Estimate the typical speed v of an electron in the ground state of the Coulomb potential of an atom with $Z > 1$.

(b) Whenever $v \sim c \approx 3 \times 10^8$ m/s, relativistic effects become important. For what value of Z do relativistic effects matter? Are such nuclei present (anywhere) on Earth (and thus of interest to at least some chemists)? Determine whether Schrödinger and Dirac were correct.

Problem 21 (Tritium Decay): Tritium is an isotope of hydrogen where the nucleus consists of two neutrons and one proton, so it has a charge $Z = 1$. It is radioactive and will decay to a helium-3 nucleus (two protons, one neutron) (with $Z = 2$) after (on average) 12 years. The decay process emits an energetic electron which can escape the pull of the Coulomb potential. Let us suppose that during the decay process, the wave function of tritium's bound electron is approximately constant.

(a) Denote with P_{nlm} the probability that the electron is found in the nlm state of the $Z = 2$ nucleus after the radioactive decay. Compute P_{100} and P_{200}. Use the fact that for the $Z = 1$ atom:

$$\psi_{100} = \frac{\mathrm{e}^{-r/a_0}}{\sqrt{\pi a_0^3}}, \qquad \psi_{200} = \frac{\mathrm{e}^{-r/2a_0}}{\sqrt{32\pi a_0^3}}\left(2 - \frac{r}{a_0}\right)$$

(b) For what values of n, l and m may $P_{nlm} \neq 0$?

(c) Is it absolutely necessary that

$$\sum_{nlm} P_{nlm} = 1?$$

Why or why not?

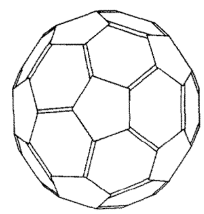
(d) Suppose that, for simplicity, the electron ends up decaying into the state

$$|\Psi(0)\rangle = c_1|100'\rangle + c_2|200'\rangle,$$

with $|nlm'\rangle$ the eigenstates of the $Z = 2$ nucleus. Assume c_1 and c_2 are arbitrary. What is $|\Psi(t)\rangle$, for times $t > 0$?

(e) Compute $\langle r(t)\rangle$ for times $t > 0$. You may assume that $|\Psi(t)\rangle$ from the previous part is normalized.

Problem 22 (Buckyball): The buckyball, C_{60} is an exotic, approximately spherical, arrangement of 60 carbon atoms.



(a) We can approximately model the electronic structure of buckyballs by assuming that electrons of mass $m \approx 10^{-30}$ kg are constrained to move on a sphere of radius R, but otherwise free. Argue that the Hamiltonian describing the electrons is

$$H = \frac{\mathbf{L}^2}{2mR^2},$$

and determine the eigenvalues, and their degeneracy.

(b) If the lowest energy photon that buckyballs can absorb has wavelength $\lambda = 404$ nm, and induces a transition between angular momentum $l = 5$ and $l = 6$ states, what is the radius R of the buckyball?

Problem 23 (Rotational Spectroscopy): Consider the rotation of a molecule which is rotationally symmetric about a single axis, which we label the z-axis. The rotational dynamics of this molecule is described by the Hamiltonian

$$H = \frac{L_x^2 + L_y^2}{2I_0} + \frac{L_z^2}{2I_z}.$$

(a) Find the eigenvalues and eigenvectors of the Hamiltonian.

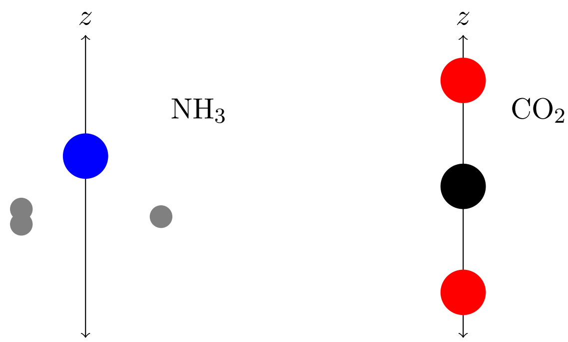
(b) Consider the molecule ammonia, NH_3. The lowest frequencies of photons that can[3] be absorbed by transitions between rotational states of ammonia are $\nu \approx 97,\ 291,\ 388$ GHz. What does this tell you about I_0 and I_z?

(c) Some further possible transitions for ammonia are at $\nu \approx 469,\ 566,\ 841,\ 1035,\ 1132$ GHz. Conclude the values of I_0 and I_z from this data.

(d) Estimate the length of the N-H bond in ammonia.

(e) Consider the molecule carbon dioxide, CO_2. The longest wavelength of light that this molecule can absorb is $\lambda = 2.56$ cm. What do you think the next longest wavelength of light that can be absorbed is? Explain your arguments carefully!

[3] Ignoring conservation of angular momentum between the ammonia and photons...



Problem 24 (Covalent Bonds): Let us consider a covalent bond in the H_2 molecule – though the same principles apply to more generic chemical bonds as well (at least to decent approximation). For simplicity we ignore electron-electron Coulomb repulsion and just focus on qualitative considerations. The Hamiltonian is

$$H = \frac{\mathbf{p}^2}{2m_\mathrm{e}} - \frac{e^2}{4\pi\epsilon_0\sqrt{s^2+(z+a/2)^2}} - \frac{e^2}{4\pi\epsilon_0\sqrt{s^2+(z-a/2)^2}}.$$

where $s^2 = x^2 + y^2$.

(a) Show that $[H, L_z] = 0$.

(b) We may thus label eigenstates $|\psi\rangle$ of H by their eigenvalue of L_z: $L_z|\psi\rangle = \Lambda\hbar|\psi\rangle$. It is conventional to label the $\Lambda = 0$ state with σ and a $|\Lambda| = 1$ state with π (the higher states are rare in nature). Which Λs do you think have the lowest energy, at least for this molecule?

(c) Sketch the electron's probability density in a σ bond and a π bond.

Problem 25 (Quantum Random Number Generator): Consider a spin-1/2 state, in an eigenstate of S_x.

(a) What is the operator S_x written in terms of bras and kets of the eigenstates of S_z, $|+\rangle$ and $|-\rangle$? What are the possible quantum states $|\psi\rangle$?

(b) We now make a measurement of S_z. What are the possible measurements, what will the quantum state be after each measurement, and what is the probability of each? Does the answer depend on $|\psi\rangle$?

(c) We now make a measurement of S_x. What are the possible measurements, what will the quantum state be after each measurement, and what is the probability of each? Are the answers sensitive to the previous measurement of S_z?

Alternating back and forth between measuring S_x and S_z forms the simplest example of a quantum random bit generator. Unlike pseudorandom number generators on your computer, say, these numbers are truly random.

Problem 26 (Mesons and Baryons): In this problem, we will consider some properties of the lighter elementary particles. Many of the lightest elementary particles can be made up of combining up quarks (u), down quarks (d), and their anti-particles ū and d̄. These quarks have a mass of $mc^2 \approx 330$ MeV (in particle physics, everything is measured in units of MeV, GeV, etc., by tacking on appropriate factors of $\hbar$ and c!). One can model a surprising amount of properties of this particles by supposing that there is a fictitious spin called "isospin", such that the up quark is associated with spin up, and the down quark is associated with spin down. "Rotational invariance" in isospin space then provides many experimentally testable constraints on particle physics, some of which we will explore in this problem.

We begin by considering the mesons, which are made by combining a quark and an antiquark. In terms of the isospin up and down states, we have the conversion:

$$|\mathrm{u}\rangle \to |+\rangle, \quad |\mathrm{d}\rangle \to |-\rangle; \qquad |\bar{\mathrm{u}}\rangle \to |-\rangle, \quad |\bar{\mathrm{d}}\rangle \to -|+\rangle.$$

And we have operators J_x, J_y, J_z and $\mathbf{J}^2$, which obey the commutation relations $[J_x, J_y] = \mathrm{i}J_z$ (we just ignore the factors of $\hbar$...), and act exactly as angular momentum or spin operators in the theory of angular momentum, but just switch around up and down isospin states: for example: $J_x|\uparrow\rangle = |\downarrow\rangle$. With these "conversions" between isospin and quark states at hand, we can now create mesons by "adding together" the isospins of constituent quarks.

(a) How many mesons would you predict to exist? The "physical basis" in which we observe elementary particles is diagonal in $\mathbf{J}^2$ and J_z, with $\mathbf{J}$ the total isospin.[4] What are the eigenvalues of $\mathbf{J}^2$ and J_z for each meson? Write down the quantum states for each particle.

(b) The electric charge on the up quark is $2e/3$, on the down quark is $-e/3$, and the charge on antiquarks is opposite of on quarks. What are the charges of each of the elementary particles so far?

Each quark is also a spin-1/2 particle in *actual* spin $\mathbf{S}$. Let's denote a $+1/2$-spin state (in the z-basis) state with $|\uparrow\rangle$, and a $-1/2$-spin state with $|\downarrow\rangle$. And so to form a meson, we really need to add together states of the form $|\mathrm{u}\uparrow\rangle$ with $|\bar{\mathrm{u}}\downarrow\rangle$ (for example). Both isospin and actual spin add together using the rules of angular momentum addition.

(c) How many physically observable mesons do we predict so far? Assume that we can only measure the quantum number s – the "total spin" of the particle – isospin invariance is approximate however, because we can measure electric charge (as in part (b))!

(d) Rather surprisingly, it turns out that the mass of these mesons, M, is determined (approximately) through the following formula:

$$Mc^2 = mc^2 + mc^2 + \frac{A}{(mc^2)^2}\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle,$$

where $\mathbf{S}_{1,2}$ are the physical spin states associated with the constituent quark/anti-quark, and A is a constant. Experimentally, one measures one set of mesons at mass $Mc^2 \approx 140$ MeV, and a second set at mass $Mc^2 \approx 780$ MeV. What is the spin s of each set of particles? What is the value of A?

Another way we can get elementary particles that are light is to combine together three quarks and zero anti-quarks. These states are called baryons – the proton and neutron are two such states.

(e) How many baryons do we expect, and what are their isospin and spin states? Do not worry anymore about writing down the exact wave functions. In particular, predict the existence of an exotic particle (called the Δ^{++}) with charge $+2e$. When this particle was observed it was a great triumph for the (early) model of quarks.

(f) $j = 3/2$ particles called Δs decay extremely fast into other particles of smaller total isospin j: pions, protons and neutrons. Approximately, we can use the fact that

$$|j = 3/2, J_z\rangle \to \sum C^{j_1 j_2, 3/2}_{m_1 m_2 J_z} |j_1 m_1\rangle |j_2 m_2\rangle.$$

[4] This has to do with the fact that isospin is not a true symmetry of nature, only an approximate one.

where $j_{1,2}$ and $m_{1,2}$ are the net and z-isospins of the elementary particles at the end of the decay, and the Cs are the Clebsch-Gordon coefficients. We assume that $j_{1,2} < 3/2$ as the end state particles are more stable. Which of the Clebsch-Gordon coefficients (i.e., which values of j and ms) are non-zero? The rates of these decay channels are proportional to $|C|^2$ – predict (up to an overall constant with the units of s^{-1}) the rates of all decays from $j = 3/2$ particles into lower j particles.

The result of part (f) has been confirmed beautifully in experiments.

There is one final mystery that we can now understand, just based on our simple models. Recall that we have seen how a spinning elementary charged relativistic particle has a magnetic moment:

$$\mu_z = \frac{q}{m} S_z,$$

with q and m the charge and mass of the elementary particle. This formula clearly predicts that the uncharged neutron has no magnetic moment, but in fact a magnetic moment is observed! This was an early clue that the neutron must be a composite object. As the proton (p) and neutron (n) are both baryons, the wave functions of the proton and neutron are[5]:

$$|\mathrm{p}\uparrow\rangle = \frac{2|\mathrm{u}\uparrow\mathrm{u}\uparrow\mathrm{d}\downarrow\rangle - |\mathrm{u}\uparrow\mathrm{u}\downarrow\mathrm{d}\uparrow\rangle - |\mathrm{u}\downarrow\mathrm{u}\uparrow\mathrm{d}\uparrow\rangle}{\sqrt{6}}.$$

$$|\mathrm{n}\uparrow\rangle = \frac{2|\mathrm{d}\uparrow\mathrm{d}\uparrow\mathrm{u}\downarrow\rangle - |\mathrm{d}\uparrow\mathrm{d}\downarrow\mathrm{u}\uparrow\rangle - |\mathrm{d}\downarrow\mathrm{d}\uparrow\mathrm{u}\uparrow\rangle}{\sqrt{6}}.$$

Each spin direction in the quantum states on the right hand side is associated with the quark state directly to its left. If we have a particle made up of three quarks (1,2,3), then the magnetic moment operators of each quark simply add together:

$$\mu_z = \mu_{1z} + \mu_{2z} + \mu_{3z}.$$

You may assume that the formula for the magnetic moment of a quark is what has been given above – remember to use the proper formulas for the mass and charge of each quark.

(g) Define μ_p and μ_n to be the magnetic moment of the up spin state of the proton or neutron, respectively (these are the quantum states given above!) – namely, $\langle \mu_z \rangle$. Predict the value of $\mu_\mathrm{p}/\mu_\mathrm{n}$ based on the quark model, and compare to the experimental value of -1.46.

Problem 27: Suppose that we have two spinless particles of the same mass m, and a Hamiltonian:

$$H = \frac{\mathbf{p}_1^2}{2m} + \frac{\mathbf{p}_2^2}{2m} + V(\mathbf{r}_1, \mathbf{r}_2).$$

(a) Define the exchange operator P, such that $P\Psi(\mathbf{r}_1, \mathbf{r}_2) = \Psi(\mathbf{r}_2, \mathbf{r}_1)$, for an arbitrary function Ψ. Show that $P^2 = 1$. What are the eigenvalues of P?

(b) Under what circumstances does $[P, H] = 0$?[6]

(c) Suppose that $[P, H] = 0$, and that at time $t = 0$:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, 0) = \sigma\Psi(\mathbf{r}_2, \mathbf{r}_1, 0)$$

where $\sigma = \pm 1$. Show that

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = \sigma\Psi(\mathbf{r}_2, \mathbf{r}_1, t).$$

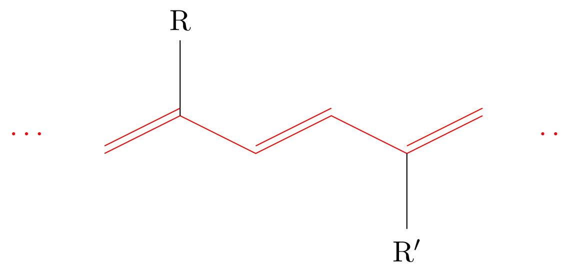
[5] Up to an overall symmetrization in the order in which we write u and d, unimportant for this problem...

[6] It may help to multiply by a test function to evaluate this commutator! Be careful with the momentum terms in H!

A bosonic/fermionic wave function will stay bosonic/fermionic for all times, and thus it makes sense to demand symmetry/antisymmetry of the wave function.

(d) Does it make sense to talk about a pair of bosons or fermions if $[P, H] \neq 0$?

Problem 28 (Pigments): A typical pigment molecule has a structure sketched below. The bonds highlighted in red are special: they are called conjugated π bonds. Suppose there are N conjugated π bonds: then each bond contributes one "free" spin-1/2 electron, of mass m, which may move up and down the chain of bonds freely. If each bond has length a, when N is large, we may thus approximate these electrons as moving in a particle in a box of width $L = a(N-1) \approx Na$.



(a) Suppose N is an even number. Using the Pauli exclusion principle and the results for the particle in a box, describe which energy levels in the box are filled and which are empty. Ignore electron-electron interactions.

(b) How much energy does it take to place all of these fermions in the ground state of this quantum system? Approximate your answer in the $N \gg 1$ limit.

(c) Now, suppose we send a photon of wavelength λ at the pigment molecule. What is the largest value of λ such that the photon can be absorbed by an electron in the pigment molecule? When the photon is absorbed, the electron must be able to jump to an unoccupied state in the box. You should find that

$$\lambda \approx KN$$

in the limit when $N \gg 1$ – what is the value of K?

(d) Evaluate numerically the value of K, given that $m \approx 9 \times 10^{-31}$ kg and $a \approx 10^{-10}$ m. A typical pigment molecule might have a chain with $N \approx 20$. Does λ correspond to a photon in the visible spectrum?

(e) Suppose I give you 2 pigment molecules, one of which is red, and one of which is blue. Which pigment molecule do we expect has a longer chain of conjugated π bonds?

Problem 29 (Repulsive Bosons): Suppose that we have N identical bosons of mass m in a one dimensional box of length $L = Na$ $(0 < x < Na)$, with the Hamiltonian

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{\lambda}{2} \sum_{i \neq j} \delta(x_i - x_j).$$

We are interested in the $N \gg 1$ limit. This problem can be solved exactly, but we will not attempt to do so here.

(a) Suppose $\lambda = 0$. What is the ground state wave function? Call your answer $\Psi_0(x_1, \ldots, x_N)$. What is the energy of this state, $E_0(0)$?

(b) Now, let us suppose that $\lambda > 0$, so that these bosons tend to repel each other. Calculate

$$E_0(\lambda) = \langle \Psi_0 | H | \Psi_0 \rangle$$

and comment on your answer. What is happening physically?

(c) Let us temporarily consider that we had N *fermions* in the box. What would be the ground state $\tilde{\Psi}_0(x_1, \ldots, x_N)$, if $\lambda = 0$?

(d) What is the energy of the state $\tilde{\Psi}_0$? Call it $\tilde{E}$, and verify that it is independent of λ.

(e) Show that the function

$$\tilde{\Psi}(x_1, \ldots, x_N) = \tilde{\Psi}_0(x_1, \ldots, x_N) \prod_{i>j} \mathrm{sign}(x_i - x_j)$$

is a symmetric, normalized wave function. What is $\langle \tilde{\Psi} | H | \tilde{\Psi} \rangle$? This is provably the exact ground state at $\lambda = \infty$.

(f) Give a heuristic argument for what should happen to the ground state of H as we increase the parameter λ.

Problem 30 (Metallic Junction): Suppose that we have a junction between two different metals: metal 1 for $x < 0$, and metal 2 for $x > 0$. A simple model for the conduction of an electron between these two metals is as follows. An electron of mass m, propagating perpendicular to the area of contact, sees an effective 1d Hamiltonian

$$H = \frac{p^2}{2m} + \alpha\delta(x) - \left\{ \begin{array}{ll} \mu_1 & x < 0 \\ \mu_2 & x > 0 \end{array} \right. .$$

where α, μ_1 and μ_2 are real numbers. Crudely speaking, $\mu_{1,2}$ are the Fermi energies of metals 1 and 2. The parameter α represents the fact that the interface might be dirty (e.g., higher concentration of impurities). Without loss of generality we take $\mu_1 > \mu_2$.

(a) Under what circumstances will a bound state exist? If so, how many are there? If they exist, find their energies – up to the solution of a equation for E, expressed only in terms of $\hbar$, α, m and $\mu_{1,2}$.

(b) Suppose we have an electron wave packet of energy $\approx E$ incident on the barrier from $x \to -\infty$. What is the probability $P(E)$ that the electron will, after a long time, be found propagating towards $x \to \infty$ in metal 2? Explain how impurities affect $P(E)$ and justify the effect on physical grounds.

Problem 31 (Particle Mixing): In quantum field theory, it is possible for 2 particles of "species 1" to "collide" and become a pair of 2 particles of "species 2" – and vice versa. We will explore a toy model of this effect in this problem. Let a_1 and $a_1^\dagger$ be the annihilation and creation operators for a 1d harmonic oscillator, and a_2 and $a_2^\dagger$ for an independent oscillator:

$$[a_1, a_1^\dagger] = 1, \quad [a_2, a_2^\dagger] = 1, \quad [a_1, a_2] = [a_1, a_2^\dagger] = [a_2, a_1^\dagger] = [a_1^\dagger, a_2^\dagger] = 0.$$

The Hilbert space of this system consists of $|n_1 n_2\rangle$, with $n_{1,2} = 0, 1, 2, \ldots$. n_1 can be interpreted as the number of type 1 particles, and n_2 as the number of type 2 particles, in our universe.

Now consider the Hamiltonian

$$H = \epsilon\left(a_1^\dagger a_1 + a_2^\dagger a_2\right) - \eta\left(a_1^\dagger a_1^\dagger a_2 a_2 + a_2^\dagger a_2^\dagger a_1 a_1\right).$$

with $\epsilon, \eta > 0$ real parameters.

(a) Show that H is Hermitian.

(b) Define the total number operator $N = a_1^\dagger a_1 + a_2^\dagger a_2$. What are the eigenvalues of N? Show that $[N, H] = 0$.

(c) Prove that if we start in a quantum state $|\Psi(0)\rangle$ with $N|\Psi(0)\rangle = n|\Psi(0)\rangle$, then at any time $t > 0$, $N|\Psi(t)\rangle = n|\Psi(t)\rangle$.

(d) Use the result of part (c) to conclude that if we start in a state with eigenvalue $N = 2$, while H is non-diagonal in an infinite-dimensional Hilbert space, we need only worry about the dynamics in a subspace of dimension 3. Give a simple basis for this subspace.

(e) Write down H, in Dirac notation, in the basis of part (d), for all states with $N = 2$. Diagonalize H and find the eigenvalues and eigenvectors.

(f) Suppose that at time $t = 0$, $|\Psi(0)\rangle = |20\rangle$ – namely, we start in a state of 2 type 1 particles. Find $|\Psi(t)\rangle$ exactly and comment on its physical interpretation.

(g) Suppose we measure $N_2 = a_2^\dagger a_2$ at time t_0, given the initial state of part (f). What values could we measure and with what probabilities? What is the maximum of this probability, and at what time does it occur?

Problem 32 (Constant Forces): Consider a non-relativistic particle of mass m in the potential

$$V(x) = -Fx.$$

(a) Does this potential have any bound states?

(b) Write down the momentum space time dependent Schrödinger equation for $\Phi(p, t)$. Find the exact solution given initial conditions $\Phi(p, 0) = \Phi_0(p)$.

(c) Evaluate $\langle p(t)\rangle$ and comment on your result. From this result, compute $\langle x(t)\rangle$.

(d) Without performing an explicit computation, do you think that $\sigma_x\sigma_p$ will increase or decrease in time? Explain your answer qualitatively.

Problem 33: Consider a non-relativistic particle of mass m in an eigenstate of an unknown Hamiltonian in three spatial dimensions. The state is

$$\psi = N(x + y + 2z)r^{s-1}\exp[-r/\xi],$$

where N is a normalization factor, and s and ξ are positive constants. You may find helpful:

$$\mathrm{Y}_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\frac{x \pm \mathrm{i}y}{\sqrt{x^2 + y^2 + z^2}}, \qquad \mathrm{Y}_1^0 = \mp\sqrt{\frac{3}{4\pi}}\frac{z}{\sqrt{x^2 + y^2 + z^2}}.$$

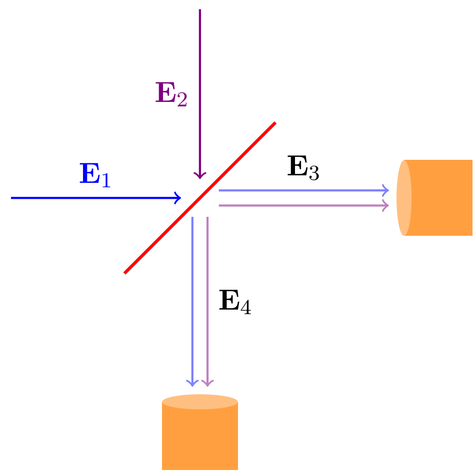
(a) If we make a measurement of L^2, what could we measure, and with what probability?

(b) If we make a measurement of L_z, what could we measure, and with what probability?

(c) Suppose that we now learn that the potential is spherically symmetric. What is the potential $V(r)$ associated with this state, and what is its energy? Assume that $V(r \to \infty) = 0$.

(d) If we put 3 bosons in a state with this wave function, what are the possible values of L^2_{tot} and $L_{\text{tot},z}$ that we could measure? You do not need to determine the probabilities.

Problem 34 (Measuring Quantum Light): One of the ways to detect the quantum nature of light in an experiment is to rely on a trick called **photon antibunching**. Experimentally, we consider the following set-up:



In classical electrodynamics, the first beam of light has electric field $\mathbf{E}_1 = E_1(t)\hat{\mathbf{x}}$, and the second beam has electric field $\mathbf{E}_2 = E_2(t)\hat{\mathbf{y}}$.[7] We pass these beams through a 50:50 beam splitter, which converts these beams into beams 3 and 4 with electric fields

$$\mathbf{E}_3 = \frac{\mathbf{E}_1 + \mathbf{E}_2}{\sqrt{2}}, \quad \mathbf{E}_4 = \frac{\mathbf{E}_1 - \mathbf{E}_2}{\sqrt{2}}.$$

We then measure the intensity of light $I_{3,4}(t)$ associated with each one of these beams at time t at a photodetector (the orange boxes in the figure). The object we will focus on is the correlation function

$$g \equiv \frac{\langle I_3(t) I_4(t)\rangle}{\langle I_3(t)\rangle\langle I_4(t)\rangle},$$

with $\langle \cdots \rangle$ denoting the appropriate averages (either classical or quantum).

(a) In classical electrodynamics the intensity of a beam of light is given by (up to an unimportant dimensional factor $\mathcal{I}_{\text{cl}}$):

$$I_{\text{cl}} = \mathcal{I}_{\text{cl}} \mathbf{E}^2.$$

Show that for any arbitrary (real-valued) $E_{1,2}(t)$, $I_3 = I_4$. Conclude that $g \geq 1$, classically.

Let us now revisit this problem from a quantum perspective. In quantum electrodynamics, we simply associate a (1d) quantum harmonic oscillator to each mode of the electromagnetic field; thus if $\mathbf{E}_{1,2}$

[7] Note for simplicity we have dropped the spatial variations of $\mathbf{E}_{1,2}$. These can rigorously be included but play no role in the physics we're interested in.

correspond to simple propagating waves, we simply have a pair of oscillators with creation operators $a^\dagger_{1,2}$ and annihilation operators $a_{1,2}$, obeying

$$[a_1, a_1^\dagger] = [a_2, a_2^\dagger] = 1, \quad [a_1, a_2^\dagger] = [a_2, a_1^\dagger] = 0.$$

The creation operators create single photons in that mode; the Hilbert space is spanned by $|n_1, n_2\rangle$ with $n_{1,2} = 0, 1, 2, \ldots$. After passing through the beam splitter, we have a new pair of oscillators with creation operators $a^\dagger_{3,4}$ with

$$a_3 = \frac{a_1 + a_2}{\sqrt{2}}, \quad a_4 = \frac{a_1 - a_2}{\sqrt{2}}.$$

It turns out that the proper quantum mechanical definition of g is

$$g \equiv \frac{\langle a_3^\dagger a_4^\dagger a_4 a_3 \rangle}{\langle a_3^\dagger a_3 \rangle \langle a_4^\dagger a_4 \rangle}.$$

(b) Find the commutation relations between $a_{3,4}$ and $a^\dagger_{3,4}$. Is the definition of g sensitive to the labeling of beams 3 and 4?

(c) In a seminal experiment, only beam 1 was turned on. What is the value of g – express it in terms of the quantum state $|\psi\rangle$ and the operator $N_1 \equiv a_1^\dagger a_1$? Show explicitly that it is possible to obtain $g < 1$; this was observed quite conclusively in experiment.

Problem 35: A pair of interacting spin-1/2 fermions of mass m feels an effective Hamiltonian of the form

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \left(A + \frac{B}{\hbar^2} \mathbf{S}_1 \cdot \mathbf{S}_2 \right) (x_1 - x_2)^2$$

For simplicity, we only consider the (position) dynamics in one spatial dimension. These sorts of Hamiltonians arise when considering nucleon-nucleon interactions inside of the nucleus.

(a) Show that $\mathbf{S}_1 + \mathbf{S}_2 \equiv \mathbf{S}$ commutes with H. What does this imply about the eigenvectors of H?

(b) Under what conditions will there be a well defined ground state?[8]

(c) Give an example of an A and B for which the particles bind together in a spin-1 state, but unbind in a spin-0 state.

(d) Is it possible to pick an A and B such that the spin-0 state is bound but the spin-1 state is unbound?

For the remainder of the problem, assume that the condition of part (b) holds, but do not make any further assumptions on the values of A or B.

(e) Write down all ground state wave functions $\psi_0(x_1, s_1, x_2, s_2)$. Be careful to consider all possibilities in A and B.

Problem 36 (Mass of a Meson): Consider two quarks of mass m, which interact via the potential

$$V(x_1, x_2) = T|x_1 - x_2|.$$

For simplicity, we do not consider the dynamics in three dimensions, but only in one. T is equal to the tension of the "flux tube" that must stretch from one quark to the other. If these two quarks (really, one of them is an antiquark) make up a meson, then a crude model for the mass M of the meson is that Mc^2 is the ground state energy of the quantum mechanical problem. Do not worry about the spin of the quarks in this problem.

[8] We need that $V(x)$ is bounded from below!

(a) Suppose that the quarks can be treated non-relativistically. Argue that the ground state energy is determined entirely by the one particle Schrödinger equation in the potential $V = T|x|$. What is the mass of this particle?

(b) Explain why $\langle x \rangle = 0$ for a stationary state. What does this imply about $\langle p \rangle$?

(c) Estimate M by using Heisenberg's uncertainty principle to estimate the ground state energy.

(d) In reality, the quarks may be ultra-relativistic, so that $E \approx c|p|$. (Continue to approximate, however, that the one particle description is valid.) Again use Heisenberg's uncertainty principle to estimate M.

(e) A typical meson has $M \sim 10^{-27}$ kg. Using $c = 3 \times 10^8$ m/s and $\hbar \approx 10^{-34}$ J/s, estimate the tension T of the flux tubes binding quarks, assuming they behave ultrarelativistically. Compare to best estimates of $T \sim 10^5$ N.

Problem 37 (Nuclear Magic Numbers): It is an empirical fact that, at least for light nuclei consisting of A nucleons (either protons or neutrons), nuclei are particularly stable if $A = 2, 8, 20, 28, 50$, etc. For simplicity, suppose that all the nucleons were neutrons, which are spin-1/2 fermions. A simple model to try and understand this effect would be to approximate the nucleus as a quantum mechanical system with Hamiltonian

$$H = \sum_{i=1}^{A} \left[\frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} m\omega^2 \mathbf{r}_i^2 \right].$$

(a) Describe the eigenvectors and eigenvalues of H in the case $A = 1$. What is the degeneracy of each energy level?

(b) Describe how to write down the ground state of H for any A. (You do not need to carry out the procedure explicitly.)

(c) A heuristic argument – similar to that used for atoms – is that we might expect the nucleus to be particularly stable when the ground state is unique. What are the nuclear magic numbers that we predict? Is this a good model?