Two Lectures on Quantum Mechanics

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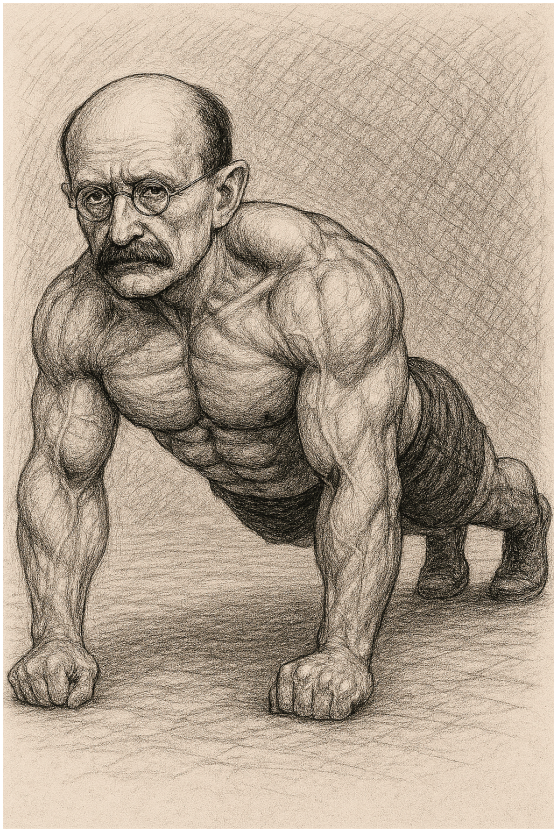


Planck Power

Max Planck's discovery of the fundamental constant $\hbar$ made it possible to express all the quantities in mechanics as multiples of fundamental scales. G and c were already known, and since

$$G \propto M^{-1}\ L^{+3}\ T^{-2}$$
$$c \propto M^{\,0}\ \ L^{+1}\ T^{-1}$$
$$\hbar \propto M^{+1}\ L^{+2}\ T^{-1}$$

have linearly independent exponents for mass (M) length (L) and time (T), suitable products of powers of the three fundamental constants will express any quantity with M, L and T in its units. The corresponding fundamental scale is identified by the prefix "Planck." In the case of power, since

$$\frac{c^5}{G} \propto \frac{M\,(L/T)^2}{T}$$

has units of power, the **Planck power** is defined as

$$P_{\rm P} = \frac{c^5}{G} = 3.6 \times 10^{52}\ {\rm W}.$$

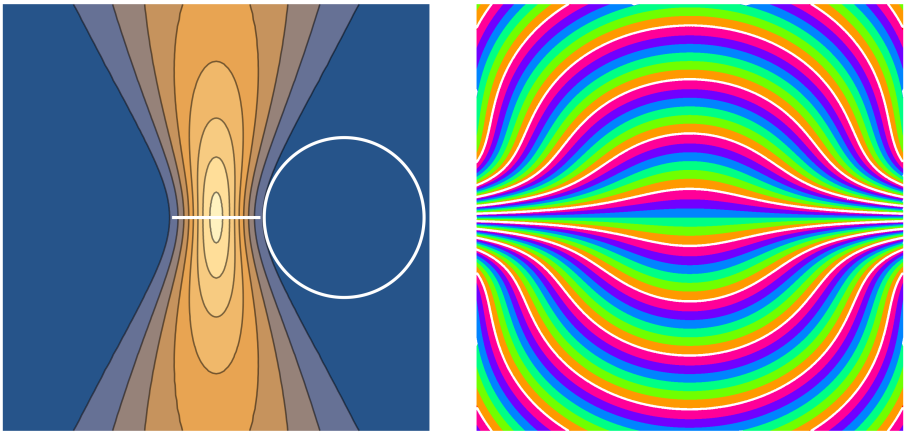
This exceeds even the peak power output of a supernova. There's nothing quantum-mechanical about this power—$\hbar$ is conspicuously absent—and perhaps an odd way to start a course on that subject!

Even though quantum mechanics plays no role in the origin of the fundamental scale of power, we can use the quantum formalism to analyze a scenario where the Planck power is relevant. In the late 1970s a group of undergraduates—who choose to remain anonymous—asked Richard Feynman whether gravity could reverse the effects of diffraction. NASA astronauts had placed a corner-reflector-array on the moon that could be used to precisely measure the variation in the earth-moon distance. But because of diffraction, the laser beam's cross section is enormous and attenuated by the time it arrives on the moon! Could the gravitational self-attraction of the laser beam's energy density keep the beam focused?

Rather than try to reconstruct Feynman's analysis, we will consider the simpler scenario of a *focused beam*. Can self-gravitation reduce the size of the focus? And if so, how much power is needed for the radiation-collapse to be turned into a factory for miniature black holes?

We are only interested in working out estimates, such as how things depend on geometrical characteristics of the focus, and also the power in the beam. On the next page are plots of the magnitude (left) and phase (left) of the electromagnetic field in a plane through the focus (when gravity is switched off). The white line in the magnitude plot, of length $2\sigma_0$, gives the scale of the "waist" of the beam at the tightest focus. The white circle of radius r characterizes the curvature of the trajectories of energy-density elements at the periphery of the beam at the waist. You know from wave mechanics that the smallest achievable σ_0 is of order the wavelength λ of the light. And since this is the only length scale around, it should not surprise you that $r \sim \lambda$. This will be one of the outcomes of our analysis later in the chapter. The perpendiculars to the phase contours give the local propagation direction of the energy density. Far from the focus the phase contours become curved and the energy-density trajectories approach straight lines. This will also emerge from our "quantum analysis" of the wave propagation.

The electromagnetic energy density elements are moving with speed c. When forced—by Maxwell's equations!—to move along the circle of radius r at the



waist, they experience an outward acceleration

$$a = \frac{c^2}{r} \sim \frac{c^2}{\lambda}. \tag{1}$$

We are counting on gravity to oppose this acceleration, to the point where the net acceleration is inward. We can estimate the required power in the beam P as follows. Consider a cubic region with sides $2\sigma_0 \sim \lambda$ centered at the focus. The energy E in this region is equal to the product of P and the time λ/c needed to fill the region with energy density:

$$E \sim \frac{P\lambda}{c}.$$

Using $E = Mc^2$ for the mass equivalent in the region, and

$$g \sim G\,\frac{M}{\lambda^2} \sim G\,\frac{(P\lambda)/c^3}{\lambda^2}$$

for the scale of the gravitational acceleration at distance λ from the center of the mass, the criterion

$$\begin{aligned} a &\sim g \\ \frac{c^2}{\lambda} &\sim G\,\frac{(P\lambda)/c^3}{\lambda^2} \end{aligned}$$

leads us to the conclusion that the required scale of P is the Planck power P_{P}.

Schrödinger wave model of beam dynamics

To keep our analysis of beam dynamics simple, there is just one transverse dimension, with coordinate x. The generalization to a second transverse dimension is straightforward and doesn't add much. The propagation axis has coordinate y. We choose to express $\mathbf{E}$ and $\mathbf{B}$ in the standard way, in terms of a complex function Ψ. In particular,

$$\mathbf{E} = \mathrm{Re}\left(\Psi(x,y)\right)\,\hat{\mathbf{z}}$$

describes a beam where the electric field has a constant linear polarization. We will use the "paraxial approximation," where the phase contours are not too strongly curved, so that the local propagation direction (Poynting vector) is always close to the y axis. In this approximation the polarization of $\mathbf{B}$ is also nearly constant and we can write

$$\mathbf{B} \approx \mathrm{Im}\left(\Psi(x,y)\right)\,\hat{\mathbf{x}}.$$

We have no further need for these definitions other than the fact that

$$u(x,y) \propto |\Psi(x,y)|^2$$

is the electromagnetic energy density.

Our beam is monochromatic of wavelength λ and automatically satisfies Maxwell's equation when constructed as a superposition of plane-wave modes

$$\Psi_k(x,y) = e^{ikx + i\sqrt{k_0^2 - k^2}\,y}, \tag{2}$$

where $k_0 = 2\pi/\lambda$ is the wavenumber associated with λ. The transverse wave vectors of our modes have the restriction $|k| < k_0$. The modes at the limits, with wavelengths close to λ, are required to make the most compact transverse wave packets. You might object that the use of such modes undercuts the paraxial approximation, and you would be correct! However, let's not forget we are ultimately working out an estimate, and the *scales* we identify in that analysis are mostly immune to such details.

We can turn beam formation into a dynamical process by interpreting the y axis as time with the definition $y = ct$. The plane wave modes thereby acquire mode frequencies ω_k defined by

$$\begin{aligned} -\omega_k t &= \sqrt{k_0^2 - k^2}\,y \\ &\approx \left(k_0 - \frac{k^2}{2k_0}\right) ct, \end{aligned}$$

where we used the paraxial approximation in the second line. The energy associated with the mode frequency can be written in the following suggestive way:

$$\hbar\omega_k = \frac{\hbar^2}{2m}k^2 - \hbar\omega_0.$$

Here $\omega_0 = k_0 c$ is the frequency of the light and

$$m = \frac{\hbar k_0}{c}$$

is a parameter having dimension mass. Writing the mode (2) as

$$\Psi_k(x,t) = e^{ikx - i\omega_k t},$$

we see that it satisfies the following partial differential equation

$$i\hbar \frac{\partial \Psi_k}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi_k}{\partial x^2} + V_0 \Psi_k$$

if we define $V_0 = -\hbar\omega_0$. Notice that all the terms are independent of k, so the same equation applies to arbitrary superpositions of modes (all of frequency ω_0). Using Ψ for that arbitrary superposition, we've found that the transverse evolution of the electromagnetic field as a function of y is equivalent to the time evolution of the wave function Ψ of a quantum particle of mass m in a constant potential V_0.

You might be disappointed that the Schrödinger equation corresponding to laser beams is the most boring one imaginable, the free-particle (constant potential) case. That could be because in the past you have mostly been interested in stationary state wave functions, where the time-dependence is the most boring imaginable! The free-particle equation is quite interesting when we consider initial conditions, and that is what's important in this application of the equation. Let's not forget that at some negative y there is a lens that "initializes" the electromagnetic wave!

Here is the free-particle wave function that has the right initial conditions for our application:

$$\Psi(x,t) = \frac{1}{\sqrt{b^2(t)}} e^{-x^2/b^2(t) + i\omega_0 t}. \tag{3}$$

The function

$$b^2(t) = \sigma_0^2 + 2i\frac{\hbar}{m}t$$

provides a time dependence beyond that of stationary states and includes the wave function's single free parameter σ_0, a length. In the exercises you confirm that this does indeed satisfy the free-particle Schrödinger equation and that up to a time-dependent normalization factor

$$|\psi(x,t)|^2 \propto e^{-2x^2/\sigma^2(t)},$$

where

$$\sigma(t) = \sqrt{\sigma_0^2 + \left(\frac{2\hbar t}{m\sigma_0}\right)^2} \tag{4}$$

is the time-dependent Gaussian width of the energy density distribution in x. Using $t = y/c$, at large or small y,

$$\sigma(t) \approx \tan\theta \; |y|,$$

where

$$\theta = \tan^{-1}\left(\frac{2}{k_0\sigma_0}\right)$$

is the angle of the asymptotic linear growth of the width with $|y|$. This establishes that our wave function has converging-lens initial conditions, and gives us another interpretation of the parameter σ_0. The paraxial approximation is valid when θ is small, or when σ_0 is not much smaller than the scale of the wavelength λ (in order that $k_0\sigma_0$ is not too small).

Near the waist (small $|t|$) the Gaussian width expression (4) can be approximated as

$$\sigma(t) \approx \sigma_0 + \frac{1}{2}at^2$$

in which the quadratic-in-time growth is parametrized by the "acceleration"

$$a = \frac{4\hbar^2}{m^2\sigma_0^3}.$$

Recalling the definition of the mass m, and using $\sigma_0 \sim \lambda$, we confirm our earlier guess (1).

Exercises

1. By working out the derivatives by hand, confirm that (3) is a solution to the free-particle Schrödinger equation.

2. Derive expression (4) for the Gaussian width of the energy density.

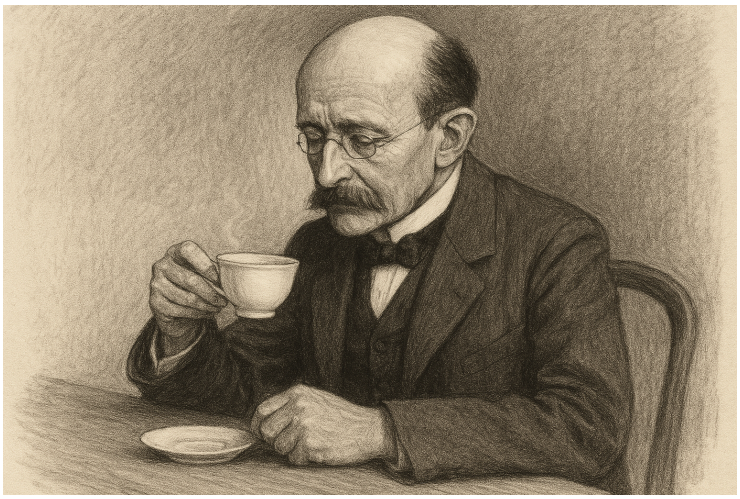
3. In making the paraxial approximation, our model for the focusing of light does not correspond to initial conditions where the incoming and outgoing phase contours are spherical (circular) far from the focus. Consider the phase contour that intersects the y-axis at $y = R$. If the contours are truly spherical, then

   $$y_R(x) = \sqrt{R^2 - x^2}$$

   is the y coordinate of that contour as a function of the distance x away from the axis. The curvature of the contour, where it intersects the axis, is then

   $$\left.\frac{d^2y_R}{dx^2}\right|_{x=0} = -\frac{1}{R}.$$

   Calculate this quantity for the phase contours given by the wave function (3). Only work out the limiting case where $R/k_0 \gg \sigma_0^2$. You will find that the curvature even has a different dependence on R.



Ordinary Matter

It's a remarkable fact that all ordinary matter has a single, universal, smallest length scale—and it's not Planck's! Think of the world of ordinary matter as an enormous digital image. While the image has features spanning many length scales, below a certain length scale all you see is pixels. The pixels of ordinary matter are better known as atoms. Their length scale, named after Niels Bohr, is derived from two properties of the electron: its mass m and its charge e.

Bohr's length and energy scale

Because we are going to go crazy writing $4\pi\epsilon_0$ every time we need the electric potential of a point charge, we will briefly use the cgs electron-charge unit $\tilde{e}$ defined by

$$\frac{e^2}{4\pi\epsilon_0} = \tilde{e}^2 \ .$$

For example, the potential energy of an electron separated from a proton by distance r is simply

$$-\frac{\tilde{e}^2}{r} \ .$$

From the MKS Coulomb's law number[1]

$$\frac{1}{4\pi\epsilon_0} \approx 9 \times 10^9 \ \frac{\mathrm{N\,m^2}}{\mathrm{C^2}} \ ,$$

you can work out

$$\begin{aligned} \tilde{e} &\approx \left(1.6 \times 10^{-19}\ \mathrm{C}\right) \sqrt{9 \times 10^9 \times 10^9 \ \frac{\mathrm{dyn\,cm^2}}{\mathrm{C^2}}} \\ &= 4.8 \times 10^{-10} \ \sqrt{\mathrm{dyn\,cm^2}} \ . \end{aligned}$$

The square-root entity is the cgs counterpart of the Coulomb, called esu (for "electrostatic unit") and

$$\frac{(1\ \mathrm{esu})^2}{1\ \mathrm{cm}} = 1\ \mathrm{erg} \ .$$

But as we'll see, as soon as we introduce Bohr's scale of length, called the *Bohr radius*, and an associated energy scale, called the *Hartree*, we will never have to write another e or $\tilde{e}$!

Today we have a better way of introducing the atomic length scale than Bohr's. Because we already know about wavefunctions, operators, expectation values, and so on, we will freely draw on these mathematical ideas. So let's start by considering a point charge—a nucleus of charge $Z\tilde{e}$—at the origin, and an electron described by a wavefunction Ψ, localized near the origin. The only thing we care about Ψ is its length scale, a. We will determine a starting with the electron's Hamiltonian in the presence of the nucleus:

$$H = \frac{p^2}{2m} - \frac{Z\,\tilde{e}^2}{r} \ .$$

Besides the positive integer Z, the only physical parameters are the mass m and electron charge $\tilde{e}$.

Without having to do hardly any thinking, we know that the expectation value

$$\langle\Psi|p^2|\Psi\rangle = c_1 \ \frac{\hbar^2}{a^2}$$

varies as the inverse square of the length scale, and c_1 is a positive numerical constant that depends on details other than the scale. That's because

$$\langle\Psi|p^2|\Psi\rangle = \int d^3\mathbf{r} \ \left(+ i\hbar\,\nabla\Psi\right) \cdot \left(- i\hbar\,\nabla\Psi\right) = \hbar^2 \int d^3\mathbf{r} \ |\nabla\Psi|^2$$

after we do the integration by parts and make note of the fact that the boundary term is zero because Ψ vanishes far from the origin. With even less thinking we know that

$$\langle\Psi| \ \frac{1}{r} \ |\Psi\rangle = -c_2 \ \frac{1}{a}$$

[1] Throughout these lectures we limit precision in these situations to a level that can be committed to memory.

where c_2 is another positive constant unrelated to the scale. Combining the two expectation values we arrive at

$$\begin{aligned} \langle \Psi | \, H \, | \Psi \rangle &= c_1 \, \frac{\hbar^2}{2m \, a^2} - c_2 \, \frac{Z \, \tilde{e}^2}{a} \\ &= E(a) \; . \end{aligned} \tag{5}$$

Modern-day Bohr would be taking a victory lap upon arriving at the result (5). It already resolves the awkward problem of the electron spiraling ever closer to the nucleus, with no bound on how low its energy can get. That corresponds to the second term of (5), when the scale a gets smaller without bound. But this is countered by the first term: it grows positively through the increase in kinetic energy as the wave function shrinks in size. Minimizing $E(a)$ with respect to a, the optimum scale

$$a^* = \frac{c_1}{c_2} \frac{1}{Z} \frac{\hbar^2}{m \tilde{e}^2}$$

gives the total energy

$$\begin{aligned} E(a^*) &= c_1 \left(\frac{\hbar^2}{2m \, a^*} \right) \frac{1}{a^*} - c_2 \, \frac{Z \, \tilde{e}^2}{a^*} \\ &= c_1 \left(\frac{1}{2} \frac{c_2}{c_1} Z \, \tilde{e}^2 \right) \frac{1}{a^*} - c_2 \, \frac{Z \, \tilde{e}^2}{a^*} \\ &= -\frac{1}{2} c_2 \, \frac{Z \, \tilde{e}^2}{a^*} \; . \end{aligned}$$

At the optimum scale, the positive kinetic energy is exactly half the magnitude of the negative potential energy, resulting in a net negative energy. The electron is bound, because were it to escape from the nucleus it would only have kinetic energy, which is positive.

The combination of electron parameters

$$a_{\rm B} = \frac{\hbar^2}{m \tilde{e}^2} \; , \tag{6}$$

in the expression for a^*, has units of length and defines the Bohr radius. The term "radius" is historical and something we will return to later. What's interesting is that *all* the terms of the Hamiltonian can be expressed in terms of this one scale. Introducing the symbols $\bar{p}$ and $\bar{r}$ for the corresponding dimensionless momentum and distance operators,

$$\begin{aligned} p &= (\hbar / a_{\rm B}) \, \bar{\nabla} \\ r &= a_{\rm B} \, \bar{r} \; , \end{aligned}$$

the Hamiltonian takes the form

$$\begin{aligned} H &= \left(\frac{\hbar^2}{m a_{\rm B}^2} \right) \frac{1}{2} \bar{\nabla}^2 - \left(\frac{\tilde{e}^2}{a_{\rm B}} \right) \frac{Z}{\bar{r}} \\ &= E_{\rm H} \left(\frac{1}{2} \bar{\nabla}^2 - \frac{Z}{\bar{r}} \right) \; , \end{aligned}$$

where

$$E_{\rm H} = \frac{\hbar^2}{m a_{\rm B}^2} = \frac{\tilde{e}^2}{a_{\rm B}}$$

are the two ways of writing the Hartree unit of energy.

Now, if you're doing a calculation on paper, or something more ambitious on a computer, and it involves atoms or molecules (to which we'll get later), then set up your Hamiltonian in dimensionless momenta and positions. Because your wave functions will be functions of the dimensionless position coordinates, anything that involves distance 1 in those coordinates corresponds to the physical distance

$$a_{\rm B} \approx 0.529 \text{ Å} .$$

And if the energy (expectation value or eigenvalue) of that wave function happens to be, say -1, the physical energy is

$$E_{\rm H} \approx -27.2 \text{ eV} .$$

As an example, the dimensionless Hamiltonian you would be working with when studying the helium atom is

$$H = \frac{1}{2}(\nabla_1^2 + \nabla_2^2) - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}} ,$$

where we have dropped the over-bars and $r_{12} = \|\mathbf{r}_1 - \mathbf{r}_2\|$ is the dimensionless operator for the distance between the electrons.

Shaken, not stirred

Particle physicists will tell you the energy scale associated with the electron is

$$mc^2 \approx 0.511 \text{ MeV} ,$$

which is fine because ordinary matter is not their purview. The ratio with the Hartree defines the following dimensionless combination of physical constants:

$$\frac{E_{\rm H}}{mc^2} = \frac{\tilde{e}^2}{a_{\rm B}} \frac{1}{mc^2} = \tilde{e}^2 \, \frac{m\,\tilde{e}^2}{\hbar^2} \, \frac{1}{mc^2} \, = \left(\frac{\tilde{e}^2}{\hbar\, c} \right)^2 .$$

For historical reasons, the square-root

$$\alpha = \frac{\tilde{e}^2}{\hbar\, c}$$

is called the *fine structure constant*. A better name, based on its value

$$\alpha \approx .007 ,$$

is the *Bond constant*. The number α shows up all the time. We follow up with two instances of α that are important in approximations.

When an atom or molecule makes a transition between two *electronic* energy levels and in the process emits a photon, how does the wavelength, of the corresponding light, compare with the atomic scale? Starting with $a_{\rm B}$, through which we define the scale of electronic energy levels, we define the wavenumber $k_{\rm B}$ of the associated light like this:

$$\Delta E = \frac{\tilde{e}^2}{a_{\rm B}} = \hbar\omega_{\rm B} = \hbar c k_{\rm B} \ .$$

The dimensionless product

$$k_{\rm B}\ a_{\rm B} = \left(\frac{\tilde{e}^2}{a_{\rm B}}\frac{1}{\hbar c}\right) a_{\rm B} = \alpha$$

comes up when calculating the photon emission process. Because α is small, one can neglect higher order terms in the "multipole expansion" of the phase factor $e^{i\mathbf{k}\cdot\mathbf{r}}$ of the electromagnetic field. Since $k_{\rm B} = 2\pi/\lambda_{\rm B}$, it means that the wavelength of light associated with electronic transition is enormous compared to the size of atoms.

Thanks to the electron's kinetic energy, the electron never gets too close to the nucleus (in an average sense). But how sure are we that its speed is well below c, so that special relativity can be neglected? Here's how that estimate works out:

$$\frac{\langle v\rangle}{c} \sim \frac{\langle p\rangle/m}{c} \sim \frac{\frac{\hbar}{a_{\rm B}}\frac{1}{m}}{c} = \alpha \ .$$

Because $\alpha \approx .007$ is small, neglecting relativity is a good approximation. On the other hand, α is not all that small, and the effects of relativity can be confirmed when calculations are carried out to higher order in this small quantity.