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Abstract

We discuss materials science examples of quantum phenomena embedded in a macroscopic, classical world. We present simple derivations showing the effects of the external world on gamma-ray emission (the Mössbauer effect), X-ray absorption (the overlap catastrophe), and on tunneling (macroscopic quantum tunneling and the Kondo effect). We draw some experimental lessons about the role of the external world in “collapsing” the wave function.

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Mössbauer, the X-ray Edge, and Macroscopic Quantum Effects

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Textbook quantum mechanics usually focuses on isolated systems: a hydrogen atom in empty space. Qualitatively new effects can occur when small quantum systems interact with the external world. The quantum mechanics of defects in solids are an ideal place to study these effects: the quantum system is embedded directly into the crystalline environment!

We discuss here classic examples of exotic quantum phenomena occurring for defects in solids. For perspective, we begin by outlining various philosophical approaches to the problem of quantum systems interacting with the external world. We then discuss four classic physical systems: the Mössbauer effect [1, 2] of gamma decay from nuclei in solids, the X-ray edge effect for absorption of X-rays by core states in metals, the Kondo effect of magnetic impurities in metals, and the problem of macroscopic quantum coherence in quantum tunneling. We attempt to explain the physics of these systems with a minimum of computation: we'll refer to results of more complete many-body calculations when appropriate.

1 Schrödinger's Cat

The profound mystery of quantum mechanics resolves around the “collapse of the wave function”. Quantum mechanics describes an electron as being in a superposition of many different possible states: the fact that we must use a wave function $\psi(x)$ for the electron represents the fact that it isn't in at any particular point x , but rather it is in many possible places with probability density $|\psi(x)|^2$. When an electron collides with a proton, or absorbs light, or diffracts off a crystal, one must treat the evolution of the wave-function as a whole to predict the behavior: the electron really is not in any one position, but is genuinely split between many. As far as we know, quantum mechanics describes all objects — indeed the universe as a whole — in precisely the same way.

How can we reconcile quantum mechanics, describing us as superpositions, with ordinary reality, where common objects have definite states? For example, consider the wave-function $\psi(r)$ of an α -particle being emitted by a radioactive nucleus (Figure 1). After one half-life of the nucleus, the wave-function is half inside the nucleus and half outside: schematically

$$|\psi(r, t_{1/2})\rangle = (|\text{Whole}\rangle + |\text{Decayed}\rangle)/\sqrt{2} \quad (1)$$

We have been forced by various experiments to conclude that the correct description of atomic and nuclear-scale phenomena must involve this kind of superposition. What happens, though, when we add a Geiger detector to our quantum system, guaranteed to trigger as soon as the nucleus decays? Or, as Schrödinger suggested, a Geiger counter connected to a fiendish device to do away with the scientist's cat (Figure 2)?

According to the original, Copenhagen interpretation of quantum mechanics [3], the wave-function of the α -particle would “collapse” into

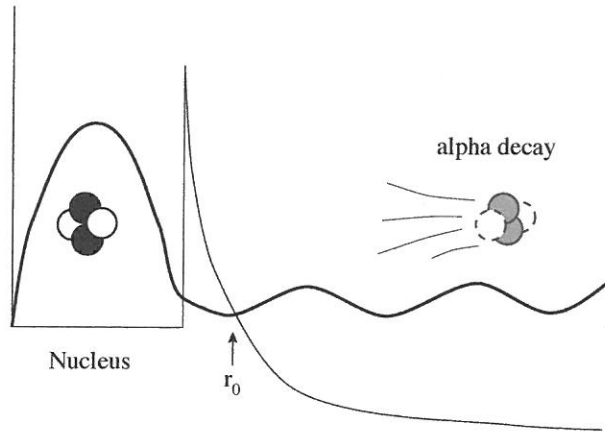


Figure 1: **Radioactive α decay.** The thick line represents the wavefunction $\psi(r)$ of the α -particle, as a function of the distance r from the center of the nucleus. The potential energy (thin line) is low and nearly constant inside the nucleus. The particle has an even lower energy outside the nucleus (hence the decay), but must cross a large barrier to depart (hence the long lifetime). Once the particle has leaked out to the point r_0 , it flies away: $\psi(r)$ becomes a outward-propagating wave. Details aside, the main point is that after a half-life of the particle, the wave-function ψ is half inside the nucleus and half outside.

one of the two states $|\text{Whole}\rangle$ or $|\text{Decayed}\rangle$ as soon as the particle hits the quasi-classical Geiger detector. According to some authors [4, 5], the wave-function is collapsed only when it is observed by an “intelligent being” (presumably the cat). One can avoid introducing this additional “collapse” operation into quantum mechanics by turning to the many-worlds interpretation of quantum mechanics. So long as the system remains perfectly isolated from the rest of the world, the cat is in a superposition of states perfectly correlated with those of the particle:

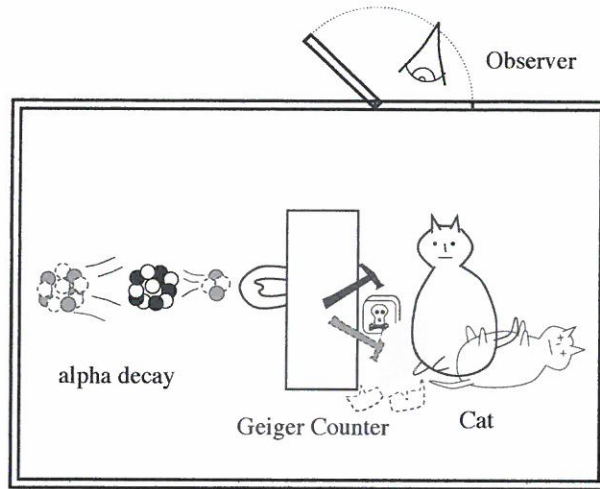


Figure 2: Schrödinger’s cat is in a box completely isolated from the rest of the world. When the Geiger counter detects that the nucleus has decayed, it triggers a hammer which “shatters a little flask of prussic acid.”

$$|\Psi(\mathbf{X}_{\text{cat}}, r, t_{1/2})\rangle = (|\text{Whole}\rangle|\text{Alive}\rangle + |\text{Decayed}\rangle|\text{Dead}\rangle)/\sqrt{2} \quad (2)$$

The “many worlds” occur when the box is opened, and the experimentalist’s clean-up becomes contingent on the quantum state of the nucleus:

$$|\Psi(\mathbf{X}_{\text{cat}}, r, t_{1/2})\rangle = (|\text{Whole}\rangle|\text{Alive}\rangle|\text{BuyKittyLitter}\rangle + |\text{Decayed}\rangle|\text{Dead}\rangle|\text{RIP}\rangle)/\sqrt{2}. \quad (3)$$

Even though the many-worlds and wavefunction-collapse formulations are essentially equivalent, they are psychologically and philo-

sophically opposed to one another. A reformulation which bypasses these tensions has been formulated by Mermin [6] as the “Ithaca interpretation” of quantum mechanics. He states that quantum mechanics is best considered a theory of correlations, which have physical reality. One may ask only whether burying the cat is *correlated* with the decay of the nucleus, for which the answer is both unambiguous and uncontroversial.

Are these questions physics or philosophy? Experimentally, is there a difference between the “collapse” and the “many-worlds” views? Can we do a further experiment to see if the Geiger counter and the cat collapsed the wavefunction? According to quantum mechanics, if one repeats an experiment many times, the average result can always be described by the expectation values of an operator O : $\langle O \rangle = \langle \Psi(\mathbf{X}_{\text{cat}}, r, t_{1/2}) | O | \Psi(\mathbf{X}_{\text{cat}}, r, t_{1/2}) \rangle$. So long as our experiment O is probing the nucleus (and not the Geiger counter, the cat, or the experimenter), this quantity splits into four parts:

$$\begin{aligned}
 \langle O \rangle &= (1/2) && \langle \text{Whole} | O | \text{Whole} \rangle \langle \text{Alive} | \text{Alive} \rangle \\
 &+ (1/2) && \langle \text{Decayed} | O | \text{Decayed} \rangle \langle \text{Dead} | \text{Dead} \rangle \\
 &+ (1/2) && \langle \text{Whole} | O | \text{Decayed} \rangle \langle \text{Alive} | \text{Dead} \rangle \\
 &+ (1/2) && \langle \text{Decayed} | O | \text{Whole} \rangle \langle \text{Dead} | \text{Alive} \rangle
 \end{aligned} \tag{4}$$

$$\begin{aligned}
 &= (1/2) (\langle \text{Whole} | O | \text{Whole} \rangle + \langle \text{Decayed} | O | \text{Decayed} \rangle) \\
 &+ (1/2) \langle \text{Whole} | O | \text{Decayed} \rangle \langle \text{Alive} | \text{Dead} \rangle \\
 &+ (1/2) \langle \text{Decayed} | O | \text{Whole} \rangle \langle \text{Dead} | \text{Alive} \rangle.
 \end{aligned} \tag{5}$$

Copenhagen

Many Worlds

The first two terms are easy to understand. We’ve waited for one half-life, so we measure on average half the decayed value of O and half of the value of O for the whole nucleus. If we subscribe to the “collapse” view, this is the end of the calculation: as soon as the presence or absence of the α particle is detected by the outside world,

More details on Fock space, different Hilbert spaces. $(a^\dagger a a^\dagger a \dots)$ $|Dead\rangle$ all finite orthogonal Hilbert space convergent series \rightarrow also orthogonal

the wavefunction of the nucleus is projected onto the corresponding state: $(|Whole\rangle + |Decayed\rangle)/\sqrt{2}$ becomes $(|Whole\rangle$ or $|Decayed\rangle)$ each with probability $1/2$. If we subscribe to the "many-worlds" point of view, we must calculate the other two terms, involving the overlap $\langle Dead|Alive\rangle$. These terms represents the interference between the two branches of the wave function. The two views agree in practice because the overlap is zero:

$$\langle Dead|Alive\rangle = 0. \quad (6)$$

Because the cat has so many atoms, death is unambiguously identifiable: gas diffusion, body temperature, and other forensic evidence clearly distinguish $|Dead\rangle$ from $|Alive\rangle$.

$|Dead\rangle$ and $|Alive\rangle$ not only have zero overlap: they live in different Hilbert spaces. More precisely, in the approximation that the number of particles N in the cat goes to infinity (the cat has $N \sim 10^{26}$) the overlap $\langle Dead|Q|Alive\rangle = 0$ for any operator Q involving finite numbers of single-particle excitations. (Rearranging six atoms or 10^6 atoms won't make a dead cat come alive again.) Mathematically, this means that one can start with the two states $|Dead\rangle$ and $|Alive\rangle$, build in all the particle excitations (Fock space), and get two entirely different, non-overlapping Hilbert spaces for the wavefunctions. What this means is that experiments which observe quantities $\langle O\rangle$ which involve the Geiger counter and the cat also can't show interference.

Once a macroscopic detector or being is involved in an essential way in the experiment, the wave function splits into non-interfering pieces. Whether you describe this with a collapse into one piece, or as multiple non-interfering future worlds, makes no difference when cats are involved.

An isolated ~~atom~~ nucleus/ α -particle can exhibit quantum interference. An ~~atom~~ nucleus/ α -particle coupled to a cat does not. Can experiments be performed in between, to explore the mystery of the collapse of the wavefunction? There are indeed

through a Geiger counter

can \rightarrow no cat particles
 $\langle Dead|Q|Alive\rangle$
 $\langle Alive|Q|Dead\rangle$
 no interference
 Q can raise the dead.

many experimental systems where a quantum system is coupled to an external environment. We'll study atoms and electrons which are stuck directly inside a solid. None of these systems behaves like Schrödinger's thought experiment! Nature is far more imaginative than philosophy: the coupling to the solid produces fascinating, unanticipated results that took decades to untangle.

The key to understanding the effects of the environment on the quantum system turns out to be precisely the analogue of the overlap $\langle \text{Dead} | \text{Alive} \rangle$. Instead of a cat, the environment is a crystal. We'll start by discussing the effects of the positions of the atoms in the crystal when a quantum transition occurs. The positions of the atoms have their quantum wavefunction too: their quantum excitations are called *phonons*. In the Mössbauer effect we'll find that the quantum overlap between the two phonon wavefunctions is not zero (despite the huge number of degrees of freedom). Bizarre and useful quantum effects result! We'll see that quantum tunneling of atoms in insulating solids usually also has non-zero quantum overlap, but that for one-dimensional chains and for tunneling of atoms from one surface to another the quantum overlap can go to zero.

We'll also consider metals, where it is the wavefunction for the conduction electrons which acts as the environment for the quantum defect. Here we find that it's quite normal for the overlap of the quantum states to be zero, no matter how delicate the coupling to the quantum transition. We'll give a brief, qualitative discussion of several experimental systems: quantum dots, the Kondo effect, and the X-ray edge effect.

Schrödinger's cat inspires us to focus on the quantum overlaps of the environment under different histories, and it provides an intellectual link between zero overlap and the collapse of the wavefunction. We'll find in each case that the interaction of the quantum system with the environment produces qualitative changes in behavior. From the quantum suppression of recoil and thermal motion in the Mössbauer

effect to the power laws and scaling in the X-ray edge effect, the environment is closely tied into the quantum behavior.

2 Phonons: Mössbauer, Overlaps, and Instantons

2.1 The Mössbauer Effect

Let's take our nuclear decay and embed it into a solid. Instead of α radiation, let's have the nucleus emit a gamma ray. (Figure 3). This has a big advantage, in that the gamma ray, like X-rays, can penetrate feet of matter without leaving a trace, while the α particle leaves a trail behind it as it leaves the solid. (The trail would kill the interference effects.)

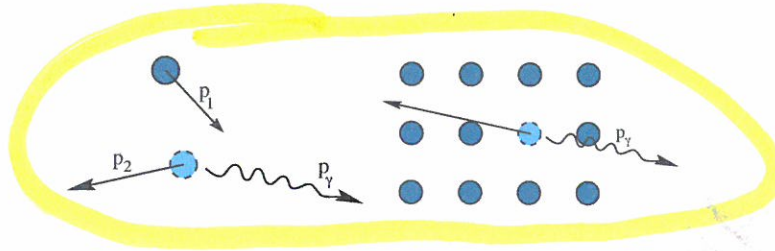


Figure 3: (Left) Nuclear γ decay in a (finite-temperature) gas. Notice that the gamma ray photon of frequency ω has momentum $p_\gamma = \hbar\omega/c\hat{k}$, so by conservation of momentum the atom changes from its original thermal momentum p_1 to $p_2 = p_1 - p_\gamma$. (Right) Nuclear γ decay in a solid (at zero temperature). The decaying atom is left with a large recoil velocity.

How does the quantum decay affect the atoms in the crystal? When the γ particle leaves the nucleus, the atom recoils (figure 3). The quantum mechanics of how this recoil changes the quantum wavefunction

of the atoms will tell us about the energy and properties of the emitted gamma ray.

At this point, we have to do some calculations. Let's assume the gamma ray is emitted in the x direction from atom of mass m at position zero, and has frequency Ω . The recoil velocity of the atom is then

$$\dot{x}_0 = -p_\gamma/m = -\hbar\Omega/mc. \quad (7)$$

We need to change variables to phonon coordinates: a configuration of N atoms with lattice sites X_n and displaced positions $x_n = X_n + u_n$ is the same as a superposition of sound waves of amplitudes q_k , with

$$q_k = \sum_n^N u_n e^{ik \cdot X_n} / \sqrt{N}. \quad (8)$$

By doing this, the interaction energy between the atoms becomes very simple: each sound wave is independent and has a frequency ω_k . (If you don't like complex coordinates, you can do this with sines and cosines, but it's messier.) We'll need to know two things [7]: for long wavelengths ω_k is given by the speed of sound

$$\omega_k \sim c |k| \text{ as } k \rightarrow 0 \quad (9)$$

and for N atoms there are N different k vectors, arranged with uniform density $V/8\pi^3$ around zero.¹

If we start the atoms at zero temperature, then after the decay only atom zero will be moving. Using (7) for \dot{x}_0 and setting $x_n \equiv 0$ otherwise, we find

$$\dot{q}_k = \sum_n^N \dot{x}_n e^{ikn} / \sqrt{N} = \overset{= \dot{x}_0 / \sqrt{N} =}{-\frac{p_\gamma}{\sqrt{Nm}}}, \quad (10)$$

¹We're oversimplifying here: there are three different modes, and the speed of sound depends on both mode and direction...

$$H = \sum \frac{p_n^2}{2m} + V(x) \approx \sum \frac{p_n^2}{2m} + \frac{1}{2} \omega^2 x^2$$

↙ quadratic

$$= \sum_k \left(\frac{p_k^2}{2m} + \frac{1}{2} m \omega_k^2 q_k^2 \right)$$

Wave equation: $\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$

① Solution $u(x,t) = f(x-ct)$

Plane wave normal mode:

$$g_k \cdot e^{ikx_n}, \text{ energy } E_k = \hbar \omega_k$$

↑
quantum

② $u_n(x,t) = e^{-i \frac{E_k}{\hbar} t} g_k \cdot e^{ikx_n}$

$$= g_k \cdot e^{i(kx_n - \omega_k t)} = g_k \cdot e^{ik(x_n - \frac{\omega_k}{k} t)}$$

③ $= f(x-ct)$ with $\boxed{\omega_k = ck}$

so all phonon modes moving in the x direction will be equally excited, each by a tiny amount which vanishes as $N \rightarrow \infty$.

At zero temperature, the solid is described by the wavefunction

$$\Psi_i(q_{k1}, \dots, q_{kN}) = \psi_i(q_{k1})\psi_i(q_{k2})\dots \quad (11)$$

which factors into a product of ground-state harmonic-oscillator wavefunctions involving one mode q_k at a time:

$$\psi_i(q_k) = (m\omega_k/\pi\hbar)^{1/4} e^{-m\omega_k q_k^2/2\hbar} \quad (12)$$

After the decay, the velocity of mode k is $\dot{q}_k = -\frac{p_\gamma}{\sqrt{Nm}}$ (from 10). Emission of electromagnetic radiation happens essentially instantaneously, so the atoms don't move substantially during the decay: $|\psi_f(q_k)|^2 = |\psi_i(q_k)|^2$. The change in velocity multiplies the wavefunction of each mode by a phase:

$$\psi_f(q_k) = e^{-ip_\gamma q_k/\sqrt{N}\hbar} \psi_i(q_k). \quad (13)$$

so

$$\Psi_f(q_{k1}, \dots, q_{kN}) = \psi_f(q_{k1})\psi_f(q_{k2})\dots \quad (14)$$

(This is standard: you can see that it works by noticing that the velocity \dot{q}_k times $|\psi_f(q_k)|^2$ equals the current density $i\hbar/2m(\psi\nabla\psi^* - \psi^*\nabla\psi)$.)

Now, the total energy emitted by the nucleus is pretty nearly fixed: if the decay leaves the phonons in an excited state, the energy (and hence the frequency) of the gamma ray is shifted down. Mössbauer discovered [1, 2], despite the recoil, that there is a large probability for the lattice to be left in the same state it started in! The probability that the wave-function Ψ_f is in the ground state is (as usual) given by the overlap

$$|\langle\Psi_i|\Psi_f\rangle|^2 = \prod_{k=k1}^{kN} |\langle\psi_i(q_k)|\psi_f(q_k)\rangle|^2. \quad (15)$$

No recoil! No doppler!

Probability of n -phonons
 $= \langle \psi_i^{(i)} | \psi_f \rangle$

We compute the overlap for each mode by completing the square:

$$\begin{aligned}
 \langle \psi_i | \psi_f \rangle &= \int e^{-i(p_\gamma / \sqrt{N\hbar})q_k} (m\omega_k / \pi\hbar)^{1/2} e^{-m\omega_k q_k^2 / \hbar} dq_k \\
 &= \int (m\omega_k / \pi\hbar)^{1/2} e^{-m\omega_k (q_k - ip_\gamma / 2m\omega_k \sqrt{N})^2 / \hbar} dq_k \\
 &\quad \times \exp(-p_\gamma^2 / 4mN\hbar\omega_k) \\
 &= \exp\left(\frac{-p_\gamma^2}{4mN\hbar\omega_k}\right),
 \end{aligned} \tag{16}$$

so

$$|\langle \Psi_f | \Psi_i \rangle|^2 = \prod_{k=k_1}^{k_N} \exp\left(\frac{-p_\gamma^2}{2mN\hbar\omega_k}\right) = \exp\left(-\sum_{k=k_1}^{k_N} \frac{p_\gamma^2}{2mN\hbar\omega_k}\right). \tag{17}$$

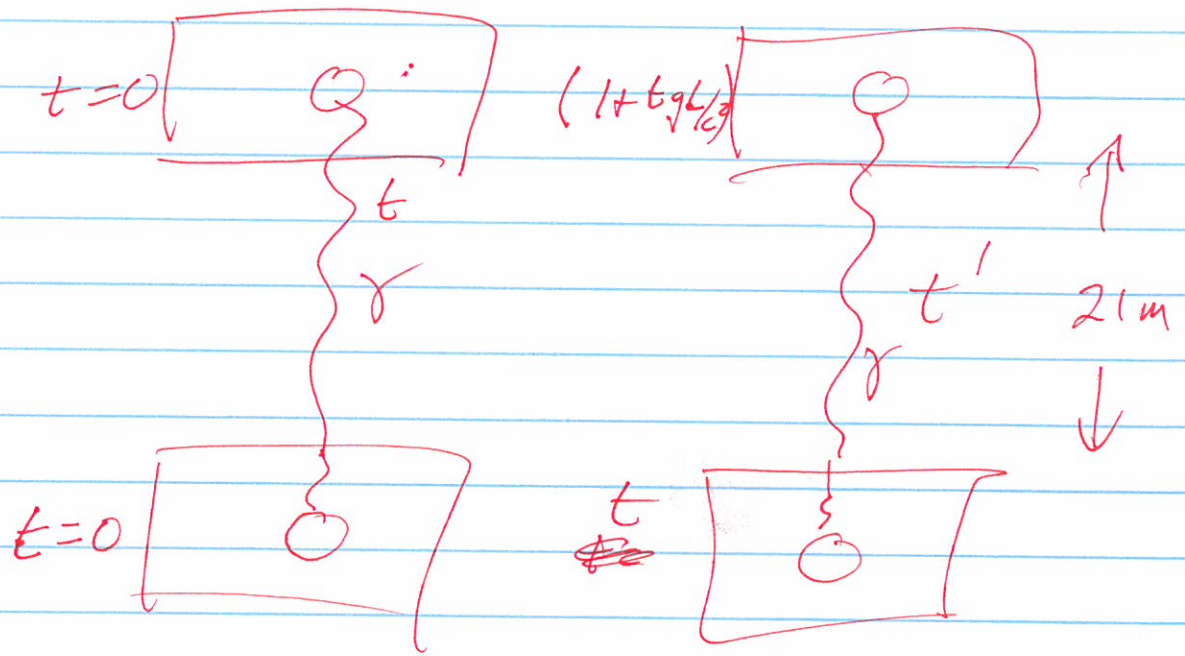
Notice that each of the N modes contributes a term of size $1/N$ to the exponent: if all of the frequencies ω_k were the same, the suppression would be just the exponent of a constant ($-p_\gamma^2 / 2m\hbar\omega$) and hence definitely not zero.² The only danger is in the low frequency modes: only for long-wavelength phonons (small k) where the frequency $\omega \sim c|k|$ is small do the terms in the sum get big.

To see if the long-wavelength phonons can make the overlap go to zero, we replace \sum_k with $(V/8\pi^3) \int_k d^3k$ using the uniform density of k points described above [7].

$$|\langle \Psi_f | \Psi_i \rangle|^2 \sim \exp\left(-\frac{V}{8\pi^3} \int \frac{p_\gamma^2}{2m\hbar\omega_k} d^3k\right) \tag{18}$$

Since $\int 1/\omega_k d^3k = \int 4\pi k^2 / c|k| d|k| \sim \int k dk$ converges at small k , the integral is not divergent and the overlap is not zero.

²After all, only one atom has shifted velocity: the N phonon modes each own only a piece $1/N$ of the suppression. Indeed, while it's easiest to do the calculation using phonon modes, working back into the original coordinates is illuminating. One can show [2] that the suppression is exactly $\exp(-\langle x^2 \rangle / (\lambda/2\pi)^2)$, where $\langle x^2 \rangle$ is the zero-point motion of the decaying atom and λ is the wavelength of the gamma ray. If the "source" of the electromagnetic wave is spread out over a size large compared to its wavelength, it's not a surprise that the amplitude goes down.



Interfere?

In part I, the big question was noticing that the overlap of the dead and live cat wavefunctions was zero, leading to the philosophically controversial problem of quantum measurement. Here we find the overlap of the environment before and after the decay is not zero. This has quite startling consequences.

1. The gamma ray is (often) emitted without any energy lost to recoil. Momentum is conserved nonetheless: the momentum is absorbed by the crystal as a whole, whose recoil can be ignored.
2. A more complete calculation shows that the gamma ray can also be emitted without a Doppler shift due to the thermal motion of the decaying atom. Because the atom is trapped in a cage by its neighbors, the thermal velocities average to zero over the half-life of the nucleus. Similar effects are seen for the decay of gas particles trapped in a box [8].
3. The Mössbauer effect is an incredibly monochromatic source of light. A classic example is Fe^{57} , which is formed in an excited state by the decay of Co^{57} . This excited state decays by emitting a gamma-ray with frequency $\nu = E/h = 3.5 \times 10^{18}$ Hz. The half-life of this excited state is $\tau \log 2 = 10^{-7}$ seconds. The line width is determined by τ ; thus fractional frequency shifts as small as $1/\tau\nu \sim 10^{-12}$ can cause the line to stop overlapping. (The full width at half height of this decay has been measured [9] to be 1.13×10^{-12} .) Frauenfelder [2] describes how his lab uses the Doppler effect to remove the resonant absorption, watching the peak vanish as the relative velocity between two pieces of iron increases. Signs in his lab of $\infty = 1.3$ cm/sec vividly illustrate how narrow these lines are.

2.2 The Pound–Rebka experiment [9]

While we haven't made an experiment which gets the decayed nucleus to interfere with a whole one, there are amazing experiments [9] which interfere a nucleus which decays at time t with the same nucleus decaying after a later time t' . The experiments use the gamma ray emitted by the excited state of Fe^{57} described above. The experiment measured the *gravitational red shift* predicted by Einstein [10] in 1911.

Pound and Rebka [9] put two blocks of iron at the top and bottom of a tower, a height $L = 21 \text{ m}$ apart (figure 4). Imagine a nucleus in the top block decaying after a time t , emitting a photon which is absorbed by a nucleus in the bottom block. If no phonons are emitted by either nucleus, there is no trace left after the absorption and emission of the time t of the transition. This means, quantum mechanically, that the amplitudes of the wavefunction for the two nuclei for different decay times t interfere coherently: they must be added together to arrive at the final wavefunction. The contribution from different decay times t will add with different phases, because of the gravitational red shift. Let's say that we're sitting at the bottom of the tower. Einstein says that time at the top of the tower is passing faster, by a rate increase of gL/c^2 , where c is the speed of light and g is the acceleration due to gravity. Thus the nucleus in the top block of iron, which (were it not for gravitation) would have contributed a phase $e^{iEt/\hbar}$, contributes an extra phase $e^{iE(tgL/c^2)/\hbar}$. Since the proportion of decays falls off as $(1/\tau)e^{-t/\tau}$, the final wavefunction and decay probability can be computed³:

$$\begin{aligned}
 \Psi &= \int_0^\infty (1/\tau) e^{-t/\tau} e^{iEt(gL/\hbar c^2)} dt \\
 &= 1/(1 + iEgL/\hbar c^2) \\
 |\Psi|^2 &= 1/(1 + (EgL/\hbar c^2)^2 \tau^2).
 \end{aligned}
 \tag{19}$$

Zero phonon line amplitude \propto

Zero phonon emission prob \propto

Sum over all times

³This isn't quite right: we've ignored the fact that the excited nucleus in the bottom block will decay in turn after a time τ . This increases the width of the line, but the form looks the same.

That is, the absorption probability gets smaller as the height L grows. The incredible sharpness of the Mössbauer line ($\tau E/h = \tau\nu \sim 10^{12}$) allowed them to measure this incredibly small frequency shift ($gL/c^2 \sim 2 \times 10^{-15}$).

2.3 Zero-phonon lines and electronic excitations

Electronic transitions for atoms in insulating solids also can occur without emitting phonons, producing what are called zero-phonon lines [11]. During the transition, the atom typically changes size or alters the bond-lengths with its neighbors, deforming the lattice. Recoil effects are not large at these energies, but the overlap integral of the initial and deformed phonon ground states act to suppress the zero-phonon line, which one can compute [12, 11] in a calculation very similar to 15. An important feature in these systems are vibrational sidebands: absorption from transitions which simultaneously emit or absorb, for example, exactly one phonon.

2.4 Atomic tunneling and the phonon overlap suppression

We've seen that the coupling to the environment can (perversely) lead to the sharpening of the energy emitted in quantum decays. The environment can also have important consequences for quantum transitions that do not emit radiation.

In glasses [14, 15] and doped crystals [16], there are atoms which undergo quantum transitions between two states, forming *tunneling centers*. Lithium doped into KCl, for example, substitutes for one of the potassium ions, but sits off-center: it's so much smaller than potassium that it snuggles into a corner between three of the surrounding six chlorine ions. An isolated lithium defect has six different corners it