Problem Set 14: Cats
Graduate Quantum I
Physics 6572
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Due Monday Dec. 1
(Takehome Final due 5:00 Dec. 12) Last correction at August 21, 2014, 7:58 pm

Potentially useful reading
Weinberg, section 3.7 (interpretations of quantum mechanics)
Sethna, *Mössbauer, the X-ray Edge, and Macroscopic Quantum Effects*, half-done draft manuscript from years ago.

14.1 **Quantum dissipation from phonons.** (Quantum) ②

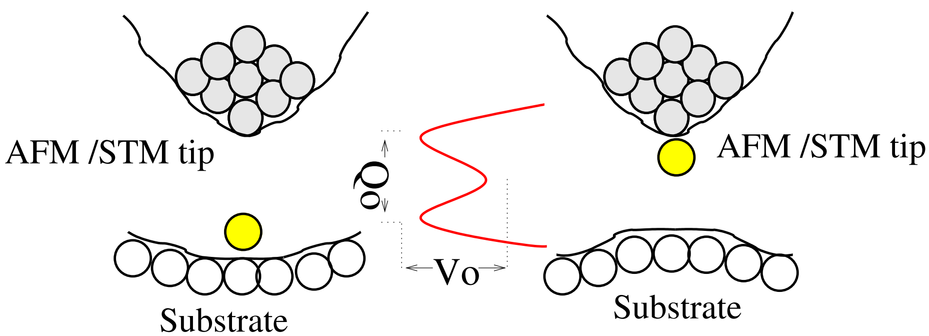

Fig. 1 Atomic tunneling from a tip. Any *internal* transition among the atoms in an insulator can only exert a force impulse (if it emits momentum, say into an emitted photon), or a force dipole (if the atomic configuration rearranges); these lead to non-zero phonon overlap integrals only partially suppressing the transition. But a quantum transition that changes the net force between two macroscopic objects (here a surface and a STM tip) can lead to a change in the net force (a force monopole). We ignore here the surface, modeling the force as exerted directly into the center of an insulating elastic medium.[1]See "Atomic Tunneling from a STM/AFM Tip: Dissipative Quantum Effects from Phonons" Ard A. Louis and James P. Sethna, *Phys. Rev. Lett.* **74**, 1363 (1995), and "Dissipative tunneling and orthogonality catastrophe in molecular transistors", S. Braig and K. Flensberg, *Phys. Rev. B* **70**, 085317 (2004).

Electrons cause overlap catastrophes (X-ray edge effects, the Kondo problem, macroscopic quantum tunneling); a quantum transition of a subsystem coupled to an electron bath ordinarily must emit an infinite number of electron-hole excitations because the bath states before and after the transition have zero overlap. This is often called an *infrared* catastrophe (because it is low-energy electrons and holes that cause the zero overlap), or an *orthogonality* catastrophe (even though the two bath states aren't just orthogonal, they are in different Hilbert spaces). Phonons typically do not produce overlap catastrophes (Debye–Waller, Frank–Condon, Mössbauer). This difference is usually attributed to the fact that there are many more low-energy electron-hole pairs (a constant density of states) than there are low-energy phonons ($\omega_k \sim ck$, where c is the speed of sound and the wave-vector density goes as $(V/2\pi)^3 \mathrm{d}^3k$).

However, the coupling strength to the low energy phonons has to be considered as well. Consider a small system undergoing a quantum transition which exerts a net force at $x = 0$ onto an insulating crystal:

$$\mathcal{H} = \sum_k p_k^2/2m + 1/2\, m\omega_k^2 q_k^2 + F \cdot u_0. \tag{1}$$

Let us imagine a kind of scalar elasticity, to avoid dealing with the three phonon branches (two transverse and one longitudinal); we thus naively write the displacement of the atom at lattice site x_n as $u_n = (1/\sqrt{N}) \sum_k q_k \exp(-\mathrm{i}kx_n)$ (with N the number of atoms), so $q_k = (1/\sqrt{N}) \sum_n u_n \exp(\mathrm{i}kx_n)$.

Substituting for u_0 in the Hamiltonian and completing the square, find the displacement Δ_k of each harmonic oscillator. (Physically, the force F adds a small linear term to the phonon mode with wavevector k, whose minimum becomes displaced by some amount Δ_k.) Let $|F\rangle$ be the ground state of the harmonic oscillators under the force F. Write the formula for the likelihood $\langle F|0\rangle$ that the phonons will all end in their ground states, as a product over k of the phonon overlap integral $\exp(-\Delta_k^2/8\sigma_k^2)$ *(with $\sigma_k = \sqrt{\hbar/2m\omega_k}$ the zero-point motion in that mode). Converting the product to the exponential of a sum, and the sum to an integral $\sum_k \sim (V/(2\pi)^3 \int \mathrm{d}^3\mathbf{k}$, do we observe an overlap catastrophe?*

Note that you've calculated the probability of a zero-phonon transition – the likelihood that the quantum transition can happen without emitting any phonons is zero. But the same argument shows that there is zero probability of emitting one phonon, or any finite number of phonons. The only allowed transitions emit an infinite number of low-energy phonons. The initial and final ground states are in 'different Hilbert spaces' – no finite number of excitations can connect them.

14.2 **Decoherence.**[2] (Density Matrices) ③

In this exercise, we will explore the effects of decoherence on a quantum system using density matrices and the Bloch sphere. We will study the dynamics of spin-1/2 particles in a magnetic field, with and without decoherence. We will work in the z-spin basis, and denote the spins pointing parallel to and anti-parallel to the z-direction by $|{\uparrow_z}\rangle$ and $|{\downarrow_z}\rangle$. The spins are subjected to a magnetic field $\vec{B} = B\hat{x}$ in the x-direction. Convince yourself that the Hamiltonian modeling this is $\mathcal{H} = -\mu_0 B(|{\uparrow_x}\rangle\langle{\uparrow_x}| - |{\downarrow_x}\rangle\langle{\downarrow_x}|)$.

(a) *Write this Hamiltonian in the z-spin basis.*

[2] Developed in collaboration with Bhuvanesh Sundar.

(b) *Suppose the initial wavefunction is $|\psi(t=0)\rangle = |{\uparrow_z}\rangle$. Solve the Schrödinger equation to find $|\psi(t)\rangle$. Do you observe that the spin oscillates between $|{\uparrow_z}\rangle$ and $|{\downarrow_z}\rangle$? What is the frequency ω of the oscillation?*

Recall from problem 11.1 that any 2×2 density matrix can be written as $\rho = \frac{1}{2}(\mathbb{1}+\vec{n}\cdot\vec{\sigma})$. The vector $\vec{n}$ is called the *Bloch vector*, and always has norm $|\vec{n}| \leq 1$, forming the solid *Bloch sphere*. (Remember $\sigma_x = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$, $\sigma_y = \left(\begin{smallmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{smallmatrix}\right)$, and $\sigma_z = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$.)

(c) *Calculate $\rho(t)$ for $|\psi(t)\rangle$ from your calculation in part (b), in terms of ω. Calculate $\vec{n}(t)$, and use the double angle formulas to simplify your answer. Geometrically, what is the trajectory of $\vec{n}(t)$? Show that this agrees with your solution*[3] *to exercise 11.1, $\mathrm{d}\vec{n}/\mathrm{d}t \propto -\vec{B}\times\vec{n}$.*

(d) *Show that the eigenvalues of a general 2×2 density matrix $\rho = \frac{1}{2}(\mathbb{1} + \vec{n}\cdot\vec{\sigma})$ are $\frac{1}{2}(1 \pm |\vec{n}|)$. What is the entropy $S = -k_B \mathrm{Tr}(\rho \log \rho)$ of a general density matrix in terms of $\vec{n}$?* (Hint: use the basis in which ρ is diagonal, and your eigenvalues.) *Show that the zero-entropy pure states are those on the surface $|\vec{n}| = 1$ of the Bloch sphere.* (Hint: $x \log x$ is negative for $0 < x < 1$, and equal to 0 at the end points $x = 0$ and $x = 1$.) *Does your solution $\vec{n}(t)$ from part (c) stay a zero entropy pure state, as it should?*

Decoherence arises in a system due to interaction with a large environment. Essentially, the universe is constantly looking at our system, and as a result of interaction with the rest of the universe, our spins get entangled with the universe. Since we observe only the spins and do not observe the infinitely many degrees of freedom in the rest of the universe, it appears to us that the spins lose information about any coherences they may have developed.

(e) *How does a general density matrix $\rho = \left(\begin{smallmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{smallmatrix}\right)$ written in the z basis change when its s_z component is measured? Show that the effect of a measurement in the z-basis is to project $\vec{n}$ onto the z-axis.*

For the remainder of the exercise, we consider the evolution under the specific hamiltonian $\mathcal{H}$ you studied in parts (a) through (c). We shall model decoherence as a measurement being done on the spins with small probability Γ per unit time. In a small time interval δt, the spin is measured in the z-basis with a probability $\Gamma\delta t$, and not measured with a probability $1 - \Gamma\delta t$, and then the system evolves for a time δt.

(f) *What is $\vec{n}(t+\delta t)$ in terms of $\vec{n}(t)$, including first the possibility of observation and then the time evolution from $\mathcal{H}$? Write a differential equation for the components of $\vec{n}(t)$ by taking $\delta t \to 0$.*

(g) *Show that n_z obeys the second-order differential equation for a damped harmonic oscillator, $\mathrm{d}^2 n_z/\mathrm{d}t^2 + \eta \mathrm{d}n_z/\mathrm{d}t + \omega_0^2 n_z = 0$. What are η and ω_0 in terms of Γ and ω?*

(h) *What is the long-time limit for $\vec{n}$? For ρ? For the entropy?*

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[3] That exercise had funny units, but the form of the equation and the sign should agree.

14.3 **Solving Schrödinger: WKB, resonances, and lifetimes.** (Computation) ③

We study the problem of quantum tunneling through a barrier. We shall use a potential in the form of a cubic polynomial.[4]

$$V(y) = \tfrac{1}{2} m\omega^2 (y^2 - y^3/Q). \tag{2}$$

You should observe that this potential has frequency ω for small oscillations in the well, and has a turning point at $y = Q$. (The *turning point* is where the potential energy goes to zero again.)

Remember that the instanton formula for the tunneling decay rate is of the form

$$\Gamma_0 \exp(-S_0/\hbar) = \Gamma_0 \exp\left(-2\int_0^Q \sqrt{2mV(q)}\mathrm{d}q/\hbar\right) \tag{3}$$

where Γ_0 is a prefactor of order ω that we will estimate numerically. Note the factor of two in the exponent compared to the symmetric double well tunnel splitting: the instanton bounce for decay out of a metastable well crosses the barrier *twice*.[5] Remember that $a_0 = \sqrt{\hbar/(2m\omega)}$ is the root-mean-square width of the ground state wavefunction in the well in the harmonic approximation.

(a) *If we set $Q = n_0 a_0$, calculate the barrier height $V_{\max}$ and the instanton action $S_0/\hbar$.* Simplify your answer: it should only depend on n_0. (Hint: If you aren't using a symbolic manipulation package like Mathematica, you can do the integral for $S_0/\hbar$ numerically, by changing variables and pulling out all the factors of m, $\hbar$, ω, n_0, etc.)

How tall and wide a barrier can one tunnel through in a reasonable time? It depends on what's considered reasonable. For our simulation, we shall simulate 1000 periods of the oscillation $P = 2\pi/\omega$. In an experiment with a few molecules, one can wait for a few seconds. In a radioactive decay experiment, where 10^{23} potential decays can be monitored, one can measure lifetimes of billions of years. For this calculation, pretend that the true decay rate is given by eqn 3 with $\Gamma_0 = \omega = 10^{12}/\text{sec}$.

(b) *How big can n_0 be to get a lifetime of $1000P$? Of one second? Of a billion years? How big is $V_{\max}$ and Q, in units of Rydbergs and Bohr radii?* (Hint: There are approximately $\pi \times 10^7$ seconds in a year. The Bohr radius is $\hbar/(\alpha m_e c)$ and the Rydberg is $m_e c^2 \alpha^2/2$, where the fine structure constant $\alpha = e^2/\hbar c \approx 1/137.036$.)

It may be remarkable how little the barrier changes to make such a large difference in the tunneling.

[4] The cubic potential is not only convenient for analytic calculations, it also approximates a generic potential when the barrier is low. (More precisely, it approximates a *generic* potential near the *saddle-node* transition when the barrier vanishes.) We saw in exercise (6.1) that tunneling of atoms is very slow unless the barrier is low and narrow compared to the typical scales of one Rydberg and one Bohr radius.

[5] In the symmetric well, ψ leaks through the barrier. In the decay from the metastable well, probability $\psi^*\psi$ must escape, leading to two suppression factors. This rough argument can be made precise in simple two-level models.

We set $Q = 5a_0$ (hence $n_0 = 5$) to get a reasonable tunneling rate. We set m to be the mass of a hydrogen atom and $\omega = 10^{12}$/sec. Our WKB formula is asymptotically exact in the limit when the barrier height is many times the energy splitting $\hbar\omega$ in the well.

(c) *What is the ratio of the barrier height $V_{\max}$ to $\hbar\omega$? Is $V_{\max}$ at least larger than the zero point energy $\frac{1}{2}\hbar\omega$?*

We'll use a grid of length $L = 80a_0$ with $N_p = 200$ points. As the wavefunction leaks out of the well, we need it to disappear before it reflects back into the well. There are several ways of doing this, mathematically and numerically. We shall do it by adding a negative imaginary part to the potential energy V_{damp}:

$$U(t) = \mathrm{e}^{-\mathrm{i}(H - \mathrm{i}V_{\text{damp}}[x])t/\hbar} = \mathrm{e}^{-V_{\text{damp}}[x]t/\hbar - \mathrm{i}Ht/\hbar} \tag{4}$$

This imaginary part depletes the wavefunction exponentially with a rate $V_{\text{damp}}[x]/\hbar$ wherever it is non-zero. We shall make V_{damp} zero near the well and the barrier, starting linearly at $|y| > x_D = L/10 = 8a_0 = 1.6Q$ with slope $-2\hbar\omega/L$ Plot the real and imaginary parts of $V(x)$, and check them against Fig. 2.

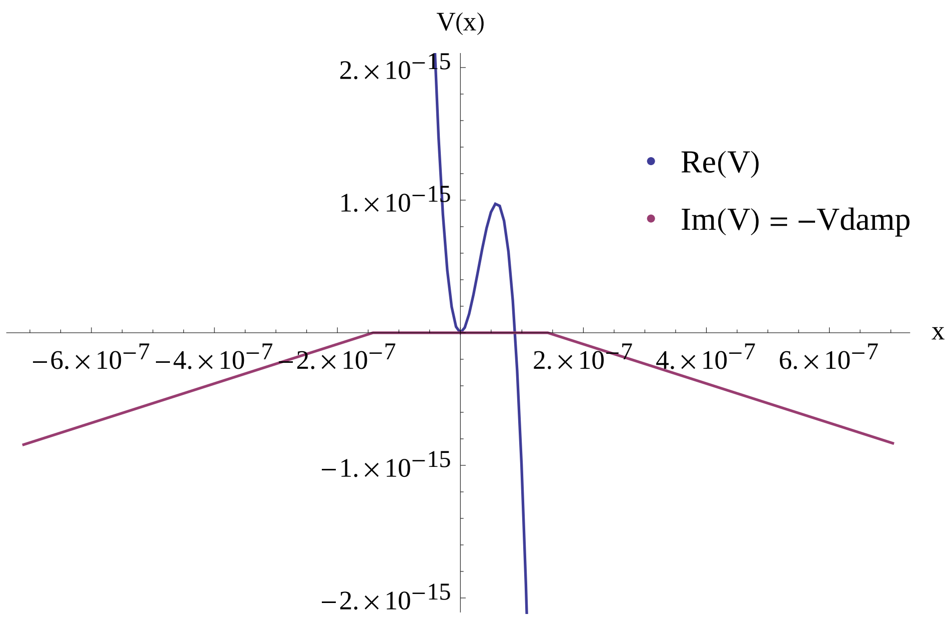

Fig. 2 Real and imaginary part of $V(x)$.

Letting the time step $\mathrm{d}t = P/50 = 2\pi/(50\omega)$, make an array $U_{\text{pot}}(dt/2)$ as usual, but incorporating both the real and imaginary parts of the potential energy. Make the array $U_{\text{kin}}(dt)$ as usual, and start the wavefunction in the harmonic-oscillator ground state in the well. Using our operator-splitting Fourier method based on the Baker-Campbell-Hausdorff formula (Exercise 5.6), iterate to $1000P = 50000\mathrm{d}t$. (This should take a good fraction of a minute.)

(d) *On a single plot, show* $|\psi(x,t)|^2$ *versus* x *for* $t = 0$, $200P$, *and* $800P$. *Does it appear to be exponentially decaying?*

(e) *Write a routine to integrate* $P(t) = \int |\psi(x,t)|^2 \mathrm{d}x$ *over the system, to see what fraction of the probability has not escaped the well and been eaten by the imaginary potential. Fit your answer, for* $t > 40P$, *to determine the exponential decay rate* Γ. *Use this to measure the prefactor* Γ_0 *that would make eqn 3 correct. What is the ratio of* Γ_0 *to our rough estimate* ω*?*