Final Exam
Graduate Quantum I
Physics 6572

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Due Friday, December 7, 2012 at 5:00pm
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This is an open-book exam. You may use any texts, software packages, or Internet resources that don't involve communication with other people. No consultation, of course, with others. Questions about the exercises should be addressed to Sethna, who will likely provide needed clarifications or corrections to the entire class.

F.1 **Your name.** (Administration) ③

(a) *(5 points.) Make sure your name is on the upper right-hand corner of each page of your exam writeup. Number the pages, so we can make sure we haven't lost any.*

(b) *(5 points.) On the front page of your exam, please write and sign a brief statement saying that "I have not used, obtained, or provided unauthorized assistance on this exam." (If you inadvertently do use, obtain, or provide assistance on this exam, contact Sethna for retroactive authorization and adjudication.)*

(c) *(0 points.) If you find uncomfortably useful resources for doing any of the exercises (such as a worked-out version on the Web), please clearly acknowledge the source. No points will be deducted from your solution, but we'd like to know.*

F.2 **F-electrons and graphene.** (Quantum) ③

In this exercise, we shall explore how seven degenerate f-electron states of an atom split under a weak perturbation which breaks the rotational symmetry.

Atoms often sit atop surfaces with weak interactions without strong bonding; we describe them as *adsorbed*. Consider a light atom[1] in an electronic f-state (i.e., with $\ell = 3$), adsorbed on a monolayer of graphene (Fig. 1). Assume the atom is positioned above a point of hexagonal symmetry, so the symmetry group for the atom is broken from $SO(3)$ to C_{6v}.

How do we know this? Why is the symmetry group not just C_6? Why is our system not symmetric under D_{6h}, the symmetry group of graphene?

(a) *(20 points) What symmetry is exhibited by our adsorbed atom that is not in C_6? What symmetry in D_{6h} is not a symmetry of our adsorbed atom?*

The character of a spin-ℓ representation for SO(3) for a rotation by angle θ is $\chi^{(\ell)}(\theta) = \sin[(\ell + \frac{1}{2})\theta]/\sin[\frac{1}{2}\theta]$. (Check this for the $\ell = 1$ representation, where you know $\chi^{(1)}$ in terms of $\cos[\theta]$. You'll need to use L'Hôpital's rule to evaluate $\chi^{(\ell)}(0)$.)

[1] The atom is light so that we may ignore the spins of the electrons. A heavy atom would have significant spin-orbit interactions.

C_{6v}	E	C_2	$2C_3$	$2C_6$	$3\sigma_v$	$3\sigma'_v$
A_1	1	1	1	1	1	1
A_2	1	1	1	1	-1	-1
B_2	1	-1	1	-1	1	-1
B_1	1	-1	1	-1	-1	1
E_2	2	2	-1	-1	0	0
E_1	2	-2	-1	1	0	0

Table 1: Character table for C_{6v}

Six of the symmetry operations in C_{6v} (conjugacy classes σ_v and σ'_v) are reflections – in $O(3)$ but not in $SO(3)$. The characters for representations of $O(3)$ are not so commonly studied. Let's figure them out for the special case of reflections.

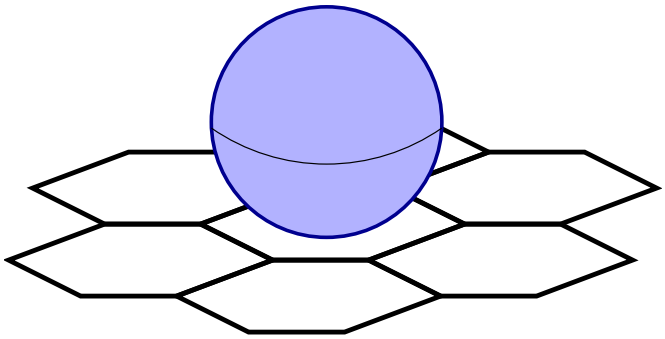

Fig. 1 ***Atom adsorbed on graphene.***

Every reflection $\Sigma(\hat{n})$ in $O(3)$ takes the mirror plane into itself, and the perpendicular $\hat{n}$ of the mirror plane to $-\hat{n}$. Thus $\Sigma(\hat{y})$ is a reflection in the $x-z$ mirror plane. Let $R_{\hat{n}}$ be a rotation that takes the coordinate axis $\hat{y}$ to $\hat{n}$.

(b) *(20 points) Using $R_{\hat{n}}$, show that all reflections in $O(3)$ are conjugate to $\Sigma(\hat{y})$.*

Since the trace is invariant under rotations, and conjugacy in $SO(3)$ is a rotation, and the character is a trace, this means that all reflections will have the same character under representations of $O(3)$. Consider the angular momentum ℓ representation of $O(3)$ generated by the rotations of the spherical harmonics $Y_\ell^m(\theta,\phi)$. Remember that θ is the angle from the $\hat{z}$ axis, and ϕ is measured from the $\hat{x}$ axis.

(c) *(20 points) How does Y_ℓ^m transform under the reflection $\Sigma(\hat{y})$ in the $x-z$ plane? In the $(2\ell+1)$-dimensional space of Y_ℓ^m for fixed ℓ, what are the elements of the $(2\ell+1)\times(2\ell+1)$ matrix $D_{mm'}$ representing $\Sigma(\hat{y})$? Show that the trace $\chi^{(\ell)}(\Sigma(\hat{y}))=1$, and hence that the character for all reflections is one in all (integer) representations of $O(3)$, independent of ℓ.*

Table 1 gives the character table for C_{6v}.

(d) *(40 points) When the f-electron eigenstates are split by the hexagonal crystal field*

from the graphene, what irreducible representations and degeneracies will be represented? (Hint: Use the orthogonality of the representations to decompose the $\ell = 3$ representation. Also, check that the total number of states equals the number of f-states.) For example, your answer might be "Two non-degenerate eigenstates with reps A_1 and B_2, and three doublet eigenstates, two with reps E_2 and one with rep E_1.")

F.3 **Juggling buckyballs.** (Path Integrals) ③

Paul McEuen in Physics and Jiwoong Park in Chemistry here discovered in 2000 that buckyballs (C_{60} molecules) bounce inside their transistors.[2] Here use path integrals to discuss how buckyballs evolve under juggling. (We'll focus on juggling one buckyball, by throwing it straight up into the air and waiting for it to fall down.) The Lagrangian for the buckyball is

$$\mathcal{L} = \tfrac{1}{2}m\dot{y}^2 - mgy. \tag{1}$$

(a) *(10 points) In classical mechanics, if the buckyball starts and ends at $y = 0$ and travels for a time $2\Delta t$, how high y_{peak} must its trajectory reach at the midpoint?* (Hint: Nothing tricky yet.)

Feynman tells us that the propagator for a particle starting at $(y = y_i, t = t_i)$ and ending at $(y = y_f, t = t_f)$ is a path integral over all trajectories $y(t)$:

$$\langle y_f, t_f | y_i, t_i \rangle = \iiint_{y_i,t_i}^{y_f,t_f} \mathcal{D}[y(t)] \exp\left(\mathrm{i}/\hbar S[y(t)]\right) = \iiint_{y_i,t_i}^{y_f,t_f} \mathcal{D}[y(t)] \exp\left(\mathrm{i}/\hbar \int \mathcal{L}\mathrm{d}t\right) \tag{2}$$

where the three integral signs represent a suitably normalized integral over all paths $y(t)$. We, like Feynman, will make a discrete 'trapezoidal rule' approximation to the propagator. As a rough example, we'll do two segments and only one intermediate point y_2:

$$S[y(t)] \approx \left[\tfrac{1}{2}m\left(\frac{y_3 - y_2}{\Delta t}\right)^2 - \tfrac{1}{2}mg(y_1 + y_2) - \tfrac{1}{2}mg(y_2 + y_3) + \tfrac{1}{2}m\left(\frac{y_2 - y_1}{\Delta t}\right)^2\right]\Delta t. \tag{3}$$

(b) *(20 points) What intermediate point y_2^* minimizes the trapezoidal action (eqn 3), for general y_1 and y_3? For $y_1 = y_3 = 0$, how does this compare to the peak of the trajectory in part (a)? What is the action $S^* = S[y_2^*]$ for this minimum action trajectory?* (Note: we're doing an approximation; the heights need not be the same. Hint: Check units of S^*. Also, does it have the right sign?)

(c) *(30 points) What is our one-point trapezoidal approximation to the propagator $\langle y = 0, t = 2\Delta t \,|\, y = 0, t = 0\rangle$?* (Request: Please write your answer factoring out the contribution from the minimum action part S^*. Hints: Don't forget the 'weight factor'

[2] See "Nanomechanical oscillations in a single-C_60 transistor", by Hongkun Park, Jiwoong Park, Andrew K.L. Lim, Erik H. Anderson, A. Paul Alivisatos, and Paul L. McEuen, *Nature* **407**, 57-60 (2000).

from Sakurai. You can check that you've included the right number of weight factors by checking the units of your propagator: at $t_f = t_i$, for example, $\langle y_f, t_i | y_i, t_i \rangle = \delta(y_f - y_i)$ has units of inverse length. Also, $\int_{-\infty}^{\infty} \mathrm{d}x \exp(-\mathrm{i}Ax^2) = \sqrt{\pi/\mathrm{i}A}$.)

F.4 **Resonances: α-decay.** (Quantum) ③

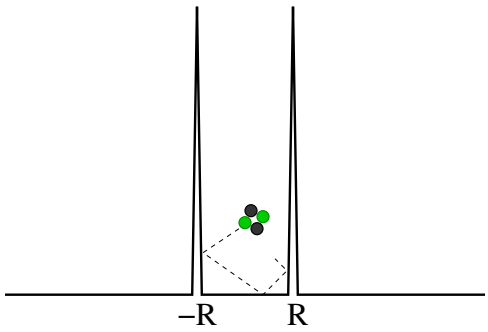

Fig. 2 ***One-dimensional nuclear potential.***

In this exercise, we solve a one-dimensional model of radioactive α-decay, where a nucleus ejects a particle formed by two protons and two neutrons (a Helium-4 nucleus).

We assume that the strong force minus the Coulomb repulsion provides a constant potential for the α particle inside a nucleus of radius R, which for simplicity we shall assume is zero. At the edge of the nucleus in the real world, the (short-range) strong interaction drops rapidly to zero, but the Coulomb repulsion decays slowly with distance, leading to a tunneling barrier. We model this barrier with a δ-function of strength $U > 0$[3] (see Fig. 2). Outside the nucleus, the potential is zero:

$$\begin{aligned} V(x) &= 0 && (|x| < R) \\ V(x) &= U\delta(x \pm R) && (x = \mp R) \\ V(x) &= 0 && (R < |x| < \infty) \end{aligned}$$

(The attractive case $U < 0$ is a model for hydrogen, and is discussed for example in Wikipedia's *Double Delta Potential* article, http://en.wikipedia.org/wiki/Delta_potential#Double_Delta_Potential.)

Parts (a)-(d) of this exercise solve analytically for the energy eigenstates, but getting them correct is important for the later parts.[4]

Our Hamiltonian has a symmetry which allows us to choose energy eigenstates that are even (ψ_E) or odd (ϕ_E).

[3] In one-dimensional quantum mechanics, the first derivative of the wave-function jumps where the potential has a δ-function. Find details in a textbook or on the Web.

[4] Feel free to check your answers by solving Schrödinger's equation numerically, approximating $\delta(x - R) = (1/\sqrt{2\pi\sigma^2}) \exp(-x^2/(2\sigma^2))$ for σ as small as is numerically convenient.

(a) *(10 points) What symmetry of the Hamiltonian is this? Given an energy eigenstate $\zeta_E(x)$ with mixed symmetry (in particular, ζ_E is not odd), construct an even eigenstate of the same energy (ignoring the overall normalization).*

In this exercise, we will be interested in the family of states ψ_E which can be non-zero at $x = 0$.

(b) *(10 points) For the eigenstates ψ_E which are non-zero at $x = 0$, what is $\psi'_E(0) = (\partial\psi_E/\partial x)|_{x=0}$?*

Next we want to solve for the energy eigenstates. This is best done in three steps. First, we deduce the form of the wavefunction. Note that, away from the δ-function, the wavefunction has wave-vector $k(E) = \sqrt{2mE}/\hbar$; it is convenient to label the wavefunctions by $k(E)$ instead of E.

Using the boundary condition at zero, we write the wavefunction for $|x| < R$ as $\psi_k^{\rm nuc} = A_k \cos(kx)$, with an overall amplitude A_k. For $x > R$, we write the wavefunction as a standing sine wave[5] $\psi_k^{\rm out} = B \sin(kx + \Delta_k)$. Note that there is a continuum of ψ_k eigenstates, so it is proper for us to use the δ-function normalization $\langle\psi_k|\psi_{k'}\rangle = \delta(k-k')$.

(c) *(20 points) Show that $B = 1/\sqrt{\pi}$ for our continuum wavefunction to be properly normalized.* (Hints: Since we're studying only even eigenstates, $k \geq 0$. Also, because the region $|x| < R$ is finite, we can ignore it for the normalization in an infinite box.)

We then impose the conditions induced by the δ-potential at the edge of the nucleus.

(d) *(20 points) Write the condition on A_k and Δ_k given by imposing continuity of $\psi_k(x)$ at $x = R$. Write the conditions on A_k and Δ_k given by the discontinuity of $\psi'_k(x)$ imposed by the δ-function potential (see footnote 3).* For convenience, write your answers from here on in terms of the unitless ratio $\widetilde{U} = 2mRU/\hbar^2$.

We can now solve for the eigenstates of our Hamiltonian that are non-zero at $x = 0$.

(e) *(20 points) Use the conditions of part (d), solve for A_k^2.* (Trick: Arrange the two equations of part (d) to be $\sin(kR + \Delta_k) = \cdots$ and $\cos(kR + \Delta_k) = \cdots$, where $\cdots$ is independent of Δ_k. Sum the squares of the right-hand sides: what must the sum be equal to?)

We now consider the decay of an α-particle injected into this potential at $x = 0$. That is, consider an initial wavefunction $\Psi(x) = \delta(x)$.[6]

(f) *(10 points) What is the probability[7] $P(k)$ of being in eigenstate ψ_k?* (Write your answer abstractly in terms of $\psi_k(x)$. This you can do without solving parts (a-d).)

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[5] For $x < -R$, we use the even symmetry of ψ_E to set $\psi_k = \psi_k^{\rm out}(-x) = B \sin(-kx + \Delta_k)$. Note that we are solving for standing waves in this problem. For other purposes, scattering waves or outgoing waves might be preferable.

[6] This is a nuclear version of tunneling from an STM tip; $P(E) = P(k(E))/(\mathrm{d}k/\mathrm{d}E)$ measures the local density of states for the α particle at the center of the nucleus.

[7] The position eigenstate $\Psi(x) = |x = 0\rangle$ is δ-function normalized, with $\langle x|x'\rangle = \delta(x - x')$. Hence the 'probability' $P(k)$ integrates to infinity, and not to one.

(g) *(20 points) Plot the probabilities $P(k)$ versus kR with $\widetilde{U} = 30$ and for $0 < kR < 10$.*

In the limit $U \to \infty$, the nucleus should approximate a particle in a box of size $2R$. In that limit, the injection of an α-particle can only occur at certain discrete energies – the nuclear eigenstates $\mathcal{E}_m^\infty$ of a free particle in a box of size $2R$.

(h) *(20 points) Compare the peaks you found in part (g) to the wavevectors for the particle-in-a-box states. Why are you missing half of the peaks?*

(i) *(Extra credit, up to 20 points for elegant answers.) Find the density of states $P(E)$ from $P(k)$. Using the FWHM of the peaks, estimate the lifetimes of the first three even resonances of our nucleus (either numerically or analytically). Calculate the integrated probability for being in each of these three resonances. Do they go to the 'particle-in-a-box' values as $U \to \infty$?*