Problem Set 6: Path Integrals
Graduate Quantum I
Physics 6572

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Due Friday Oct. 3
Note: Prelim Tues Sept 30, 7:30-9:30pm, Rock 115
Last correction at October 1, 2014, 4:23 pm

Potentially useful reading

Sakurai and Napolitano, 2.6 (path integrals)
Weinberg section 9.6 (path integrals, Greens functions)
Feynman and Hibbs chapters 1 & 2 (Path integrals in detail)

6.1 **Light Proton Tunneling.** (Dimensional Analysis) ③

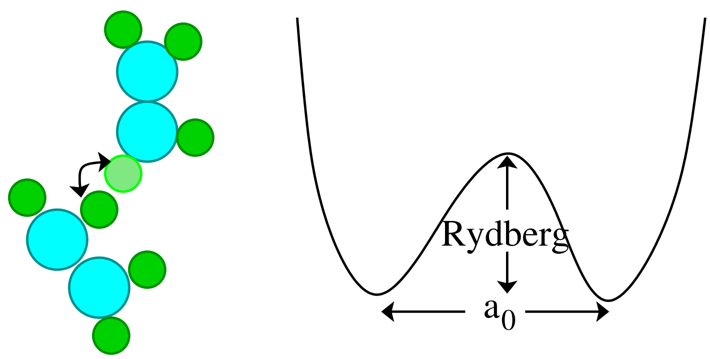

Fig. 1 Atom tunneling. A hydrogen atom tunnels a distance a_0, breaking a bond of strength E_{bind} equal to its ionization energy.

In this exercise, we continue to examine a parallel world where the proton and neutron masses are equal to the electron mass, instead of ∼2000 times larger.

With everything two thousand times lighter, will atomic tunneling become important? Let's make a rough estimate of the tunneling suppression (given by the approximate WKB formula $\exp(-\sqrt{2MV}Q/\hbar)$).

Imagine an atom hopping between two positions, breaking and reforming a chemical bond in the process – an electronic energy barrier, and an electronic-scale distance. The distance will be some fraction of a Bohr radius a_0 and the barrier energy will be some fraction of a Rydberg, but the the atomic mass would be some multiple of the proton mass.

In our world, what would the suppression factor be for an hydrogen atom of mass $\sim M_p$ *tunneling through a barrier of height* V *of one Rydberg* $= \hbar^2/(2m_e a_0^2)$*, and width* Q *equal* *to the Bohr radius a_0? How would this change in the parallel world where $M_p \to m_e$? (Simplify your answer as much as possible.)* (Use the real-world[1] a_0 and Rydberg for the parallel world, not your answers from a previous exercise. Also please use the simple formula above: don't do the integral. Your answer should involve only two of the fundamental constants.)

6.2 **Propagators to Path Integrals.** (PathIntegrals) ③

In class, we calculated the propagator for free particles, which Sakurai also calculates (eqn 2.6.16):

$$K(x', t; x_0, t_0) = \sqrt{\frac{m}{2\pi i\hbar(t - t_0)}} \exp\left[\frac{im(x' - x_0)^2}{2\hbar(t - t_0)}\right]. \tag{1}$$

Sakurai also gives the propagator for the simple harmonic oscillator (eqn 2.6.18):

$$\begin{aligned} K(x', t; x_0, t_0) &= \sqrt{\frac{m\omega}{2\pi i\hbar \sin[\omega(t - t_0)]}} \\ &\times \exp\left[\left\{\frac{im\omega}{2\hbar \sin[\omega(t - t_0)]}\right\}\right. \\ &\left.\Big[(x'^2 + x_0^2)\cos[\omega(t - t_0)] - 2x'x_0\Big]\right]. \end{aligned} \tag{2}$$

In deriving the path integral, Feynman approximates the short-time propagator in a potential $V(x)$ using the 'trapezoidal' rule:

$$\begin{aligned} &K(x_0{+}\Delta x, t_0 + \Delta t; x_0, t_0) \\ &= N_{\Delta t} \exp\left[\frac{i\Delta t}{\hbar}\left\{\tfrac{1}{2}m(\Delta x/\Delta t)^2 - V(x_0)\right\}\right], \end{aligned} \tag{3}$$

where the expression in the curly brackets is the straight-line approximation to the Lagrangian $\frac{1}{2}m\dot{x}^2 - V(x)$. We're going to check Feynman's approximation: is it correct to first order in Δt for the free particle and the simple harmonic osillator? For simplicity, let's ignore the prefactors (coming from the normalizations), and focus on the terms inside the exponentials.

Taking $t = t_0 + \Delta t$ and $x' = x_0 + \dot{x}\Delta t$, expand to first order in Δt the terms in the exponential for the free particle propagator (eqn 1) and the simple harmonic oscillator (eqn 2). Do they agree with Feynman's formula? (Hint: For the simple harmonic oscillator, the first term is proportional to $1/\Delta t$, so you'll need to keep the second term to second order in Δt.)

[1] The reduced mass effects you found in the earlier exercise will be much less important for larger atoms and molecules, so we shall not include them here.

6.3 **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

$$\mathcal{L} = \tfrac{1}{2} m\dot{y}^2 - mgy. \tag{4}$$

(a) *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 $y(t)$:

$$\langle y_f|U(t_f - t_i)|y_i\rangle = \iiint_{y_i,t_i}^{y_f,t_f} \mathcal{D}[y(t)] \exp\left(\mathrm{i}/\hbar S[y(t)]\right) = \iiint_{y_i,t_i}^{y_f,t_f} \mathcal{D}[y(t)] \exp\left(\mathrm{i}/\hbar \int \mathcal{L}\mathrm{d}t\right) \tag{5}$$

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:

$$S[y(t)] \approx \left[\tfrac{1}{2} m \left(\frac{y_3 - y_2}{\Delta t}\right)^2 - \tfrac{1}{2} mg(y_1 + y_2) - \tfrac{1}{2} mg(y_2 + y_3) + \tfrac{1}{2} m \left(\frac{y_2 - y_1}{\Delta t}\right)^2\right] \Delta t. \tag{6}$$

(b) *What intermediate point y_2^* minimizes the trapezoidal action (eqn 6), for general y_1 and y_3? For the symmetric path $y_1 = y_3 = 0$, how does this compare to the peak of the trajectory in part (a)? What is the action $S^* = S[y_2^*]$ for this symmetric 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) *What is our one-point trapezoidal approximation to the propagator*

$$\langle y = 0|U(2\Delta t)|y = 0\rangle? \tag{7}$$

(Request: Please write your answer factoring out the contribution from the minimum action part S^*. Hints: Don't forget the 'weight factor' 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, $\langle y_f|U(0)|y_i\rangle = \delta(y_f - y_i)$ has units of inverse length. Also, $\int_{-\infty}^{\infty} \mathrm{d}x \exp(-\mathrm{i}Ax^2) = \sqrt{\pi/\mathrm{i}A}$.)

[2] See "Nanomechanical oscillations in a single-C60 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).