Homework 2

Due: 11:59 PM, Tuesday, September 8. Submit your homework via Canvas.

15 points **Problem 1 (Ethylene):** The ethylene molecule C_2H_4 is sketched in Figure 1. In its molecular ground state, the atoms all lie (on average) in a two-dimensional plane. On very long time scales, we can envision that the electrons bound to carbon atoms, as well as those in the covalent bonds, are in their approximate ground state. We can then model the resulting molecular dynamics as an effective quantum mechanical problem for the nuclei alone. A particularly low energy mode of molecular motion corresponds to torsional motion: the twisting of the two halves of the molecule relative to one another, as shown in Figure 1. The torsional motion can be modeled by an effective one dimensional Hamiltonian

$$H = -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\theta^2} + U\sin^2\theta. \tag{1}$$

Here I represents a moment of inertia for the torsional mode and U represents the potential energy barrier for one of the $-CH_2$ groups to flip.

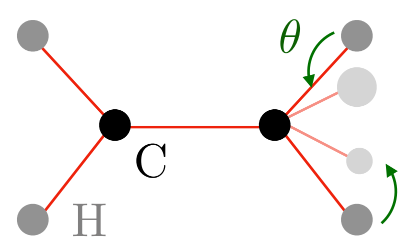

Figure 1: The ethylene molecule C_2H_4. The torsion mode corresponds to the twisting of one $-CH_2$ relative to the other.

(a) Taylor expand the potential near $\theta = 0$, and argue that this model is approximated by a harmonic oscillator. Estimate the smallest eigenvalues of H.

(b) Give a physical argument why H is unchanged if $\theta \to \theta + \pi$.

(c) Give a heuristic estimate for the total number of energy levels which are within the regime of validity of the harmonic oscillator approximation of part (a).

(d) What are the relevant energy, mass and length scales associated with the quantum hydrogen atom (and thus quantum chemistry in general)?[1] Using these scales, make order-of-magnitude estimates of U, the C-H bond length, and ultimately the moment of inertia I. Do *not* worry about factors of 2, only orders of magnitude. Then, estimate the wavelength of light that would be absorbed by this torsional oscillator. Compare to the experimental value: $\lambda \sim 2 \times 10^{-6}$ m.

10 points **Problem 2 (Correlation functions):** It is often useful to define and calculate a correlation function

$$C(t) = \frac{\langle\psi|x(t)x + xx(t)|\psi\rangle}{2} - \langle\psi|x|\psi\rangle\langle\psi|x(t)|\psi\rangle \tag{2}$$

where $x(t) = e^{iHt}xe^{-iHt}$. In a classical statistical ensemble of particles, $C(t)$ measures an extent to which the position of a particle at time $t = 0$, x, correlates with its value $x(t)$ at a later time t. Note that $C(0)$ would simply measure the variance of the position x.

[1] You should be able to simply quote these answers, with no derivation, using the book (or online).

Assume $|\psi\rangle = |0\rangle$ is the ground state of the simple harmonic oscillator in one dimension. Evaluate $C(t)$ and comment on the result.[2] You can work in dimensionless units.

15 points **Problem 3 (Squeezed states):** Consider a particle living in one dimension, controlled by either of the two Hamiltonians

$$H_1 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2, \tag{3a}$$

$$H_2 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 \kappa^4 x^2, \tag{3b}$$

where κ is a positive, dimensionless real number. The operators x, p are the *same* in both H_1 and H_2.

(a) Find creation and annihilation operators $a_{1,2}$ and $a_{1,2}^\dagger$ obeying

$$[a_1, a_1^\dagger] = [a_2, a_2^\dagger] = 1 \tag{4}$$

and

$$H_1 = \hbar\omega\left(a_1^\dagger a_1 + \frac{1}{2}\right), \tag{5a}$$

$$H_2 = \hbar\omega\kappa^2\left(a_2^\dagger a_2 + \frac{1}{2}\right). \tag{5b}$$

(b) Write x and p in terms of both $a_{1,2}$ and $a_{1,2}^\dagger$. Feel free to set $\hbar = m = \omega = 1$, if you like. Show that

$$a_1 + a_1^\dagger = \frac{a_2 + a_2^\dagger}{\kappa}, \tag{6a}$$

$$a_1 - a_1^\dagger = \kappa(a_2 - a_2^\dagger). \tag{6b}$$

Let $|\tilde{n}_{1,2}\rangle$ denote the n^{th} eigenstate of $H_{1,2}$. Suppose that we took the ground state of H_2, $|0_2\rangle$, and wrote it in terms of eigenstates of H_1:

$$|0_2\rangle = \sum_{n=0}^{\infty} c_n |n_1\rangle. \tag{7}$$

(c) To find an expression for c_n, we can use the fact that

$$a_2|0_2\rangle = 0. \tag{8}$$

Combining (8) with the results of part (b), show that

$$\frac{c_{n+2}}{c_n} = -\sqrt{\frac{n+1}{n+2}}\tanh(s). \tag{9}$$

where we have defined $\kappa = \mathrm{e}^s$.[3] Then conclude that

$$c_n = c_0 \begin{cases} 0 & n \text{ odd} \\ \dfrac{(-\tanh s)^{n/2}\sqrt{n!}}{2^{n/2}(\frac{n}{2})!} & n \text{ even} \end{cases}. \tag{10}$$

[2] *Hint:* Recall that $\mathrm{e}^{-\mathrm{i}Ht}|\psi(0)\rangle = |\psi(t)\rangle$ and $\langle\psi(0)|\mathrm{e}^{\mathrm{i}Ht} = \langle\psi(t)|$.

[3] *Hint:* Look up hyperbolic trigonometric functions' identities on the Internet!

(d) Use the condition that the wave function is normalized to fix c_0.[4]

(e) The states you have just found are called **squeezed states**. To get some understanding for why squeezed states have practical value, calculate[5] for $i = 1, 2$

$$\Delta x_i = \langle 0_i | x^2 | 0_i \rangle - \langle 0_i | x | 0_i \rangle^2. \tag{11}$$

Conclude that it is possible to generate excited harmonic oscillator states whose position is known better than it is in the ground state! How is this compatible with the Heisenberg uncertainty principle?

In the language of x and p, the result of (e) may not seem very worthwhile. However, squeezed states have enormous practical value in building highly accurate quantum sensors. For example, if we interpret the states $|n_1\rangle$ as states with n quanta of light (photons), then our results hint at the possibility of being able to generate very coherent quantum states of light, whose properties (e.g. phase) are known more accurately than an otherwise coherent state limited only by thermal noise. You would need to construct a slightly more complicated quantum state than in this problem to fully realize this capability, but the essential principles are the same.

10 points **Problem 4 (Casimir force):** Consider a one dimensional cavity $0 < x < L$, with metallic plates on either side. Assume that, as in our three dimensional world, there are electromagnetic waves that propagate at speed c and are confined within the cavity.

(a) Give a heuristic argument, using a simple classical theory of waves (light travels at speed c), that there are oscillations of the electromagnetic waves inside the cavity at frequencies

$$\omega_n = \frac{n\pi c}{L}, \quad (n = 1, 2, 3, \ldots). \tag{12}$$

In the quantum theory, what will happen is that each of the normal modes n above will become a simple quantum harmonic oscillator, of frequency ω_n.[6] So the ground state energy is, naively,

$$E_0 = \frac{\hbar\pi c}{2L} \sum_{n=1}^{\infty} n. \tag{13}$$

Mathematically, (14) makes no sense! One heuristic argument that we can use to make sense of this is to think of the following crude regulator. There exists a very small length scale ℓ, called the Planck scale, below which the conventional physics of space and time is not understood (gravity and quantum mechanics need to be unified). So once the wavelength of the normal modes n approaches ℓ, we cannot trust the simple harmonic oscillator model anymore. We propose to replace the ground state energy with

$$E_0(L, \ell) = \frac{\hbar\pi c}{2L} \sum_{n=1}^{\infty} n \mathrm{e}^{-\ell/\lambda_n}. \tag{14}$$

where λ_n is the wavelength of normal mode n. This regulator will kill terms in the sum above which are very short wavelength compared to the Planck scale.

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[4] *Hint:* $\displaystyle\sum_{n=0}^{\infty} \frac{(2n)!}{n!^2} a^n = \frac{1}{\sqrt{1-4a}}$.

[5] *Hint:* Do not use the results of parts (b) through (d).

[6] The mass of the oscillator is not defined, however. In quantum electrodynamics, the electric and magnetic fields play the role of conjugate position and momentum!

(b) What is λ_n? Show that as $\ell \to 0$,

$$E_0(L,\ell) = \frac{\hbar\pi c}{2L}\left[\frac{4L^2}{\ell^2} - \frac{1}{12} + \cdots\right]. \tag{15}$$

I encourage use of `Mathematica`'s `Sum` and `Series` functions.

Such regulators play a critical role in our modern understanding of quantum field theories and relativistic particle physics. The quantum theory is plagued with numerous divergences which are related to the one above: an inability to understand physics at short distance scales.

(c) The final observation is as follows: our cavity of length L is not isolated, but rather exists as part of a larger universe, which is also filled with electromagnetic waves. Treat the universe as a one-dimensional cavity of size $R \gg L$, with our cavity of length L contained within it, as shown in Figure 2. Conclude that the total energy of the universe is given by

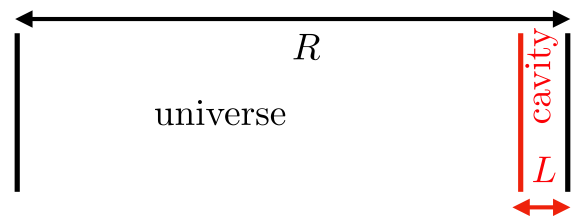

Figure 2: A toy model of the universe of size R and the cavity of size L. For simplicity, take the cavity to be at one end of the universe.

$$E_{\text{tot}} = E_0(L,\ell) + E_0(R-L,\ell) \approx \frac{2\hbar\pi c R}{\ell^2} - \frac{\hbar\pi c}{24L}. \tag{16}$$

(d) The first term of (16) is interpreted as a vacuum energy density that fills the universe, and it cannot be measured experimentally. However, by changing the size L of the cavity, we *can* measure a force

$$F = -\frac{\mathrm{d}E_{\text{tot}}}{\mathrm{d}L} \tag{17}$$

between the two walls of the cavity. Show that this force is independent of the "artificial" cutoff ℓ, which we had not introduced in a microscopically justified way. Hence, this force represents a physical prediction of quantum mechanics. Is the force between plates attractive or repulsive?

The force you have found is the **Casimir force**. It has been seen in experiments. These experiments conclusively show that the non-vanishing ground state energy of the harmonic oscillator is physical.[7]

[7] You might have thought, in particular, that a quantum oscillator should have Hamiltonian

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} - \frac{\hbar\omega}{2}.$$

As $\hbar \to 0$, this Hamiltonian also reduces to the classical harmonic oscillator's Hamiltonian, but this model has ground state energy $E = 0$, and would predict no Casimir force.