Problem Set 4: Bell & Harmonic Oscillators
Graduate Quantum I
Physics 6572
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Potentially useful reading

Weinberg sections 2.5 (Harmonic oscillator), 12.2 (Bell)
Sakurai and Napolitano sections 2.3, 2.5 (Harmonic oscillator), 2.7 (Aharonov-Bohm,
Schumacher & Westmoreland sections 5.4 (Exponentials of matrices), 6.5, 6.6 (Bell), 13.1, 13.2 (Harmonic oscillator),

4.1 **Exponentials of matrices.** (Math) ③

In quantum mechanics, one often takes exponentials of operators. The exponential of a matrix $\exp(M)$ can be computed using several different equivalent relations.

First, one can compute it as a power series:

$$\exp(M) = \sum_{n=0}^{\infty} M^n/n! \tag{1}$$

Let's take the exponential $\exp(-\mathrm{i}\phi\sigma_2/2)$, where $\sigma_2 = \left(\begin{smallmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{smallmatrix}\right)$ is the second Pauli matrix (also known as σ_y). This is the definition of how spin ½ particles transform under rotations.

(a) Note that $\sigma_2^2 = 1$. Separate the infinite series into even and odd terms, and express $\exp(-\mathrm{i}\phi\sigma_2/2)$ *as a linear combination of the identity matrix $\mathbb{1}$ and the matrix σ_2. In your answer, note that a 360° rotation is not equal to the identity, but to minus the identity!*

Secondly, one can compute it as an infinite product of infinitesimal transformations:

$$\exp(M) = \lim_{n\to\infty} \exp(M/n)^n = \lim_{n\to\infty} (\mathbb{1} + M/n)^n. \tag{2}$$

This will be the basic trick we use to generate the path-integral formulation of quantum mechanics. It is also the way we generate symmetry operations (like rotations) from infinitesimal generators (like angular momentum).[1] For example, in two dimensions the angular momentum operator is $J = \mathrm{i}\hbar \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$.

(b) Show that a 2×2 rotation matrix by an angle θ/n, in the limit $n \to \infty$, can be written as $\mathbb{1} + (C\theta/n)J$. What is the constant C? Argue, without calculation, that the product in eqn 2 must generate the finite-angle rotations.

[1] Continuous groups like the rotations are called *Lie groups*. The corresponding infinitesimal generators, and their commutation relations, are called the *Lie algebra* for the group.

Finally, many matrices which arise in quantum mechanics (symmetric matrices, Hermitian matrices, and the more general category of *normal matrices*) can be diagonalized by a unitary change of basis: $D = \left(\begin{smallmatrix} \lambda_1 & 0 & \cdots \\ 0 & \lambda_2 & \cdots \\ 0 & 0 & \cdots \end{smallmatrix}\right) = U^\dagger M U$, with $U^\dagger = (U^T)^* = U^{-1}$. Thus $M^n = (UDU^\dagger)^n = UD(U^\dagger U)D \cdots DU^\dagger = UD^nU^\dagger$. For these matrices, we can compute the exponential of a matrix by doing a coordinate change to the basis that diagonalizes it:

$$\exp(M) = \sum_{n=0}^{\infty} M^n/n! = \sum_{n=0}^{\infty} UD^nU^\dagger/n! = U\left(\sum_{n=0}^{\infty} D^n/n!\right)U^\dagger = U\left(\begin{smallmatrix} e^{\lambda_1} & 0 & \cdots \\ 0 & e^{\lambda_2} & \cdots \\ 0 & 0 & \cdots \end{smallmatrix}\right)U^\dagger \quad (3)$$

Let's apply this to the time evolution operator $\exp(-iHt/\hbar)$ for the Hamiltonian we studied in the Eigen exercise (3.1): $H = \left(\begin{smallmatrix} 0 & -4 \\ -4 & 6 \end{smallmatrix}\right)$.

(c) Apply the relation eqn 3 to calculate the 2×2 *time evolution operator* $\exp(-iHt/\hbar)$ *for our Hamiltonian. Apply the resulting time evolution operator to the state* $\psi(0) = \left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)$ *to calculate* $\psi(t)$*. Also write the time evolved state as* $\sum_n \exp(-iE_nt/\hbar)|n\rangle\langle n|\psi\rangle$*, where* $|n\rangle$ *are the eigenstates of* H*. Do the two methods agree?*

4.2 **Light Proton Atomic Size.** (Dimensional Analysis) ③

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

In solving the hydrogen atom in your undergraduate quantum course, you may have noted that in going from the 6-dimensional electron-proton system into the three-dimensional center-of-mass coordinates, the effective mass gets shifted to a *reduced mass* $m_{\text{red}} = \mu = 1/(1/m_e + 1/m_{\text{nucleus}})$, and is otherwise the hydrogen potential with a fixed (infinite-mass) nucleus. Let us assume that the atomic sizes and the excitation energies are determined solely by this mass shift.

What is the reduced mass for the hydrogen atom in the parallel world of light protons, compared to the electron mass? How much larger will the atom be? How much will the binding energy of the atom change? (You may approximate $M_p \sim \infty$ *when appropriate.)* (Units hint: $[\hbar] = ML^2/T$, $[ke^2] = Energy * L = ML^3/T^2$, and $[m_e] = M$. Here $k = 1$ in CGS units, and $k = 1/(4\pi\epsilon_0)$ in SI units.)

4.3 **δ-function bound states.** (Sakurai Exercise 2.24) ◯

Consider a particle in one dimension bound to a fixed center by a δ-function potential of the form

$$V(x) = -\nu_0\delta(x), \qquad (\nu_0 \text{ real and positive}).$$

Find the wave function and the binding energy of the ground states. Are there excited bound states?

4.4 **Baker-Campbell-Hausdorff identity.** (Expanded upon from Gottfried & Yan exercise 2.13.) ③

For operators A and B, we know $e^{A+B} \neq e^A e^B$ unless A and B commute, so $C = [A, B] = 0$. The BCH theorem tells us that, for any two linear operators A and B, that

$$e^A e^B = \exp(A + B + \tfrac{1}{2}[A, B] + \tfrac{1}{12}([A, [A, B] - [B, [A, B]]) \dots) \tag{4}$$

where ... alludes to multiple commutators of even higher order.

We start with the special case where A and B do not commute with each other but which both commute with $[A, B]$. In that case, they satisfy

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]} \tag{5}$$

(a) *Examine the power series of both sides. Show that they agree at low orders.*

(b) *To prove this, first show that* $[B, e^{xA}] = e^{xA}[B, A]x$, *where* x *is a scalar (a number, which commutes with everything). Next, define* $G(x) = e^{xA}e^{xB}$ *and show that*

$$\frac{dG}{dx} = (A + B + [A, B]x)G. \tag{6}$$

Integrate this to obtain the desired result.

(c) *Let* K *and* P *be two non-commuting operators (e.g., the kinetic and potential energy parts of the Hamiltonian* $H = K + P$*). Let* ϵ *be small (e.g.,* $i dt/\hbar$ *in a small time-step* $U(dt) = \exp(-iH dt/\hbar)$*). Show that*

$$e^{\epsilon(K+P)} = e^{\epsilon K} e^{\epsilon P} + O(\epsilon^2) \tag{7}$$

by explicitly expanding out the power series. What order is the error in the approximation

$$e^{\epsilon(K+P)} \approx e^{\epsilon K/2} e^{\epsilon P} e^{\epsilon K/2}? \tag{8}$$

(Hint: We have a good reason to do the extra work of adding the third step.)

4.5 **Coherent States.** (Adapted from Sakurai problem 2.19) ③

A coherent state of a one-dimensional simple harmonic oscillator is defined to be an eigenstate of the (non-Hermitian) annihilation operator a:

$$a|\lambda\rangle = \lambda|\lambda\rangle,$$

where λ is, in general, a complex number.

(a) *Prove that*

$$|\lambda\rangle = e^{-|\lambda|^2/2} e^{\lambda a^\dagger}|0\rangle$$

is a normalized coherent state.

(b) *Prove the minimum uncertainty relation for such a state ($\Delta x \Delta p = \hbar/2$ where Δx and Δp are the root-mean-square fluctuations in position and momentum.)*

(c) *Write $|\lambda\rangle$ as*

$$|\lambda\rangle = \sum_{n=0}^{\infty} f(n)|n\rangle.$$

Show that the distribution of $|f(n)|^2$ with respect to n is of the Poisson form. Find the most probable value of n, and hence of E.

(d) *Show that a coherent state can also be obtained by applying the translation (finite-displacement) operator $e^{-ipl/\hbar}$ (where p is the momentum operator and l is the displacement distance) to the ground state.* (See also Gottfried 1966, 262-264).

4.6 **Bell.**[2] (Quantum,Qbit) ③

Consider the following cooperative game played by Alice and Bob: Alice receives a bit x and Bob receives a bit y, with both bits uniformly random and independent. The players win if Alice outputs a bit a and Bob outputs a bit b, such that[3]

$$(a + b = xy) \mod 2. \tag{9}$$

They can agree on a strategy in advance of receiving x and y, but no subsequent communication between them is allowed.

(a) *Give a deterministic strategy by which Alice and Bob can win this game with 3/4 probability.*

(b) *Show that no deterministic strategy lets them win with more than 3/4 probability. (Note that Alice has four possible deterministic strategies*[4] *$[0, 1, x, \sim x]$, and Bob has four $[0, 1, y, \sim y]$, so theres a total of 16 possible joint deterministic strategies.)*

(c) *Show that no probabilistic strategy lets them win with more than 3/4 probability. (In a probabilistic strategy, Alice plays her possible strategies with some fixed probabilities $p_0, p_1, p_x, p_{\sim x}$, and similarly Bob plays his with probabilities $q_0, q_1, q_y, q_{\sim y}$.)*

The upper bound of <= 75% of the time that Alice and Bob can win this game provides, in modern terms, an instance of the Bell inequality, where their prior cooperation encompasses the use of any local hidden variable.

[2]This exercise was developed by Paul Ginsparg, based on an example by Bell '64 with simplifications by Clauser, Horne, Shimony, & Holt ('69).

[3]The notation $n \mod 2$ means n modulo two; it is zero if n is even and one if n is odd.

[4]The notation $\sim x$ means 'not x'; it is zero if x is one and one if x is zero.

Let's see how they can beat this bound of 3/4, by measuring respective halves of an entangled state, thus quantum mechanically violating the Bell inequality.[5]

Suppose Alice and Bob share the entangled state $\frac{1}{\sqrt{2}}(|\uparrow\rangle_\ell|\uparrow\rangle_r + |\downarrow\rangle_\ell|\downarrow\rangle_r)$, with Alice holding the left Qbit and Bob holding the right Qbit. Suppose they use the following strategy: if $x = 1$, Alice applies the unitary matrix $R_{\pi/6} = \begin{pmatrix} \cos\frac{\pi}{6} & -\sin\frac{\pi}{6} \\ \sin\frac{\pi}{6} & \cos\frac{\pi}{6} \end{pmatrix}$ to her Qbit, otherwise doesn't, then measures in the standard basis and outputs the result as a. If $y = 1$, Bob applies the unitary matrix $R_{-\pi/6} = \begin{pmatrix} \cos\frac{\pi}{6} & \sin\frac{\pi}{6} \\ -\sin\frac{\pi}{6} & \cos\frac{\pi}{6} \end{pmatrix}$ to his Qbit, otherwise doesn't, then measures in the standard basis and outputs the result as b. (Note that if the Qbits were encoded in photon polarization states, this would be equivalent to Alice and Bob rotating measurement devices by $\pi/6$ in inverse directions before measuring.)

(d) *Using this strategy: (i) Show that if $x = y = 0$, then Alice and Bob win the game with probability 1.*
(ii) Show that if $x = 1$ and $y = 0$ (or vice versa), then Alice and Bob win with probability 3/4.
(iii) Show that if $x = y = 1$, then Alice and Bob win with probability 3/4.
(iv) Combining parts (i)–(iii), conclude that Alice and Bob win with greater overall probability than would be possible in a classical universe.

This proves an instance of the CHSH/Bell Inequality, establishing that "spooky action at a distance" cannot be removed from quantum mechanics. Alice and Bob's ability to win the above game more than 3/4 of the time using quantum entanglement was experimentally confirmed in the 1980s (A. Aspect et al.).[6]

(e) *(Bonus) Consider a slightly different strategy, in which before measuring her half of the entangled pair Alice does nothing or applies $R_{\pi/4}$, according to whether x is 0 or 1, and Bob applies $R_{\pi/8}$ or $R_{-\pi/8}$, according to whether y is 0 or 1. Show that this strategy does even better than the one analyzed in a–c, with an overall probability of winning equal to $\cos^2 \pi/8 = (1 + \sqrt{1/2})/2 \approx .854$.*
(Extra bonus) Show this latter strategy is optimal within the general class of strategies in which before measuring Alice applies R_{α_0} or R_{α_1}, according to whether x is 0 or 1, and Bob applies R_{β_0} or R_{β_1}, according to whether y is 0 or 1.

[5] Remember the GHZ state, where three people have to get a+b+c mod 2 = x or y or z. Again one can achieve only 75% success classically, but they can win *every* time sharing the right quantum state.

[6] Ordinarily, an illustration of these inequalities would appear in the physics literature not as a game but as a hypothetical experiment. The game formulation is more natural for computer scientists, who like to think about different parties optimizing their performance in various abstract settings. As mentioned, for physicists the notion of a classical strategy is the notion of a hidden variable theory, and the quantum strategy involves setting up an experiment whose statistical results could not be predicted by a hidden variable theory.

This will demonstrate that no local hidden variable theory can reproduce all predictions of quantum mechanics for entangled states of two particles.

4.7 **Harmonic oscillators and symbolic manipulation.** (Computation) ③

In this exercise, we shall use *symbolic manipulation* environments (*Mathematica* or *SymPy*) to explore the raising and lowering operators a and $a^\dagger$. We'll use them to generate the position-space eigenstates $\psi_n(x)$, along with their associated Hermite polynomials. We'll distinguish between *analytical* calculations (paper and pencil) and *symbolic* calculations (using the symbolic manipulation package on the computer).

Remember that the Hamiltonian for a simple harmonic oscillator[7] is

$$H = p^2/2m + \tfrac{1}{2}m\omega^2 x^2. \tag{10}$$

with

$$p = -\mathrm{i}\hbar\frac{\partial}{\partial x} \tag{11}$$

The ground state probability distribution is a Gaussian of width $a_0 = \sqrt{\hbar/2m\omega}$, so

$$\psi_0(x) = (m\omega/\pi\hbar)^{1/4}\mathrm{e}^{-m\omega x^2/(2\hbar)}. \tag{12}$$

For plots, we'll take constants from McEuen's bouncing buckyballs (Park et al., "Nanomechanical oscillations in a single-C_{60} transistor", *Nature* **407**, 57 (2000)). Thus $m \approx 60 * 12$amu, with an amu $= 1.66054$e-24 gm, $\hbar \approx 1.0545716 \times 10^{-27}$ erg sec, and $\omega = 1.2$THz.

(a) *Do a symbolic integration to check if ψ_0 is properly normalized. Plot ψ_0 from $-4a_0$ to $4a_0$ using McEuen's constants. How do the zero-point fluctuations for McEuen's buckyball compare to the size of an atom?*

(b) *Define an operator $H(\psi)$ that symbolically takes a function $\psi(x) = |\psi\rangle$ and returns another function $H|\psi\rangle$. Symbolically calculate the ground state energy $E_0 = H(\psi_0)/\psi_0$.* (Hint: it should be independent of x.)

Remember that the ladder operators are written in terms of the position and momentum:

$$a = \sqrt{m\omega/2\hbar}(x + \mathrm{i}p/m\omega) \tag{13}$$
$$a^\dagger = \sqrt{m\omega/2\hbar}(x - \mathrm{i}p/m\omega) \tag{14}$$

Remember the number operator $N = a^\dagger a$.

(c) *Using the commutation relation $[x, p] = \mathrm{i}\hbar$, analytically (paper and pencil) show that $(N + \tfrac{1}{2})\hbar\omega = H$, $[a, a^\dagger] = 1$, $[N, a^\dagger] = a^\dagger$, and $[N, a] = -a$.*

(d) *Using the commutation relations from above, analytically show that $H(a^\dagger)^n\psi_0 = (n + \tfrac{1}{2})\hbar\omega(a^\dagger)^n\psi_0$, so $\psi_n \propto (a^\dagger)^n\psi_0$.*

[7] The spring constant $K = m\omega^2$; this gives $\omega = \sqrt{K/m}$, which may be more familiar.

(e) *As in parts (b), symbolically define the operator p from eqn 11. Using it, define the operator* $a^\dagger(\psi)$. *Symbolically calculate* $E_1 = H\left(a^\dagger\psi_0\right)\right)/a^\dagger\psi_0$. *Is it normalized?*

(f) *Symbolically, is* $a^\dagger a^\dagger \psi_0$ *normalized? Calculate symbolically the norm of higher powers of* $(a^\dagger)^n\psi_0$ *until you figure out what we need to divide it by to normalize it.*

(g) *Analytically calculate the norm of* $(a^\dagger)^n\psi_0$, *using the commutation relations of part (c). Does it agree with your conclusion of part (f)?*

(h) *Symbolically define* ψ_n *recursively in terms of* ψ_{n-1}, *using the proper normalization from parts (f) and (g). Evaluate it symbolically for* $n = 1, 2, 3, 4$.

(i) *Using McEuen's buckyball constants, plot* $\psi_n(x)$ *for* $n = 1, 2, 3, 4$ *for* $-5a_0 < x < 5a_0$.