List of exercises #4 - 7600037

1. Consider a one-particle quantum mechanical system with a Hilbert space spanned by three orthonormal states $|n\rangle$, with $n = 1, 2, 3$. Three non-interacting particles occcupy these states. Determine how many distinct physical states there are if these particles are (neglect their spin):

   (a) three identical fermions,

   (b) three identical bosons,

   (c) two identical fermions and one boson,

   (d) two identical bosons and one fermion,

   (e) three distinct fermions, and

   (f) three distinct bosons.

2. Same as the previous problem, but for 3 identical spin-1/2 particles. In each case, classify the corresponding orbital states with respect to all possible permutations.

3. The purpose of this problem is to derive the algebra for the bosonic and fermionic creation and annihilation operators. It is interesting to follow the different derivations in many books such as those of Feynman, *Statistical Mechanics*, Landau & Lifshitz, *Quantum Mechanics* vol. III, Ballentine, *Quantum Mechanics*, and Merzbacher, Quantum Mechanics. Here, we will follow the latter one.
   Let $\{|\phi_i\rangle\}$ and $\{|\varphi_i\rangle\}$ be two orthonormal one-particle basis of the Hilbert space. We define the corresponding creation operators ($a_i^\dagger$ and $b_i^\dagger$) such that $a_j^\dagger|0\rangle = |\phi_j\rangle = |0, \dots, n_j = 1, 0, \dots\rangle$ and $b_j^\dagger|0\rangle = |\varphi_j\rangle = |0, \dots, \tilde{n}_j = 1, 0, \dots\rangle$, where $|0\rangle$ is the vacuum state. Likewise, the destruction operators are such that $a_j|\phi_k\rangle = \delta_{j,k}|0\rangle$, and $b_j|\varphi_k\rangle = \delta_{j,k}|0\rangle$.

   (a) Prove that the probability of the particle having the quantum number ϕ_i, $|\langle\phi_i|\psi\rangle|^2 = |\langle 0|\, a_i\, |\psi\rangle|^2$, where $|\psi\rangle$ is a generic one-particle state, is equal to the expectation value $\left\langle \psi \left| a_i^\dagger a_i \right| \psi \right\rangle$.

   (b) Show that

   $$a_i^\dagger = \sum_k \langle\varphi_k|\phi_i\rangle\, b_k^\dagger, \text{ and } a_i = \sum_k \langle\varphi_k|\phi_i\rangle^*\, b_k.$$

   In the following we will assume that this transformation is valid for the states will an arbitrary number of particles (not only for the 0 and 1-particle subspaces as defined). This is the principle of unitary symmetry (which is not obeyed by the anyonic particles).

   (c) Assuming that $a_i^\dagger a_j^\dagger|\psi\rangle = \zeta a_j^\dagger a_i^\dagger|\psi\rangle$, where $|\psi\rangle$ is an N-particle generic state, show that ζ can only be ± 1. And thus, that $\left[a_i^\dagger, a_j^\dagger\right]_\zeta = [a_i, a_j]_\zeta = 0$, where $[A, B]_\zeta = AB - \zeta BA$. (*Hint*: Perform the unitary transformation of the previous item and show that $b_i^\dagger b_j^\dagger = \zeta b_j^\dagger b_i^\dagger$ for any i and j.)

   (d) Argue that $\zeta = -1$ corresponds to fermionic particles.

   (e) Applying the same reasoning to $a_i a_j^\dagger|\psi\rangle = \mu a_j^\dagger a_i|\psi\rangle$, show that $a_i a_j^\dagger - \mu a_j^\dagger a_i = A$, where A is a constant. Show that $A = 1$.

   (f) In order to compute μ, we introduce the total number operator $\hat{N}$ which counts the total number of particles of a generic state of the Fock space

   $$\hat{N}|n_1, n_2, \dots\rangle = \left(\sum_{i=1}^{\infty} n_i\right)|n_1, n_2, \dots\rangle \text{ and } \hat{N}|n_1, n_2, \dots\rangle = \left(\sum_{i=1}^{\infty} \tilde{n}_i\right)|\tilde{n}_1, \tilde{n}_2, \dots\rangle.$$

   For this reason, this operator must be proportional to the identity operator. Show that

   $$\sum_i a_i^\dagger a_i = \sum_i b_i^\dagger b_i,$$

and, for that reason,

$$\hat{N} = \sum_i \hat{n}_i, \text{ with } \hat{n}_i = \alpha a_i^\dagger a_i + \beta a_i a_i^\dagger + \gamma = \alpha' a_i^\dagger a_i + \gamma'.$$

Finally, show that $\alpha' = 1$ and $\gamma' = 0$.

(g) Using the definition that $\hat{n}_i \left|\ldots, n_i, \ldots\right\rangle \propto \left|\ldots, n_i, \ldots\right\rangle$ and that $a_i \left|\ldots, n_i, \ldots\right\rangle \propto \left|\ldots, n_i - 1, \ldots\right\rangle$, show that $[\hat{n}_i, a_j] = \left[\hat{n}_i, a_j^\dagger\right] = 0$ for $i \neq j$.

(h) Likewise, show that $[\hat{n}_i, a_i] = -a_i$ and $\left[\hat{n}_i, a_i^\dagger\right] = a_i^\dagger$.

(i) Finally, show that $\mu\zeta = 1$, and therefore, $\mu = \zeta$.

(j) Write the identity operator $\mathbb{I} = \sum_k \left|\phi_k\right\rangle \left\langle\phi_k\right|$ in the second quantization representation. Is your result expected? Explain.

4. The purpose of this problem is to understand the exchange interaction: the mechanism that gives stability to the Hydrogen molecule and the covalent bond, among other things such as magnetism. (Use first quantization.)

(a) Write the complete Hamiltonian H of the Hydrogen molecule.

(b) In the limit the two protons are faraway from each other, $R \gg a_0$, with a_0 being the Bohr radius, write $H = H_0 + H_1$ with H_0 and H_1 being the nonperturbed Hamiltonian and its pertubation, respectively. Justify your choice of H_0 and H_1.

(c) Now, use the limit in which the protons are much heavier than the electrons. What is the physical meaning of this limit? Moreover, consider the protons being classical particles (thus, R becomes a parameter in the problem) and treat the electrons as indistinguishable spin-1/2 quantum particles. Write the simplified H_0 and H_1.

(d) Write down the ground-state wavefunctions of H_0 (do not forget the spin and the normalization). What is the degeneracy of the ground state? Discuss the permutation properties of the ground-state wavefunctions. Make a sketch of these wavefunctions in the plane $r_1 \times r_2$, where r_i is the distance of the i-th electron to the first proton (which you can conviniently set as the orign).

(e) In first order of perturbation theory, compute the correction to the ground-state energy ΔE due to H_1, and analyze how the degeneracy is lifted. (Do not compute the integrals. Just analyze how they can lift the degeneracy.)

(f) Which is the new ground state? Discuss its symmetry properties and the role of the parameter R. (As the integrals in (e) were not computed, you cannot decide for which one. Thus, discuss all the possible outcomes. Alternatively, you can give a physical insight in order to guess if the integral is positive or negative)

   i. (Optional) Compute the integrals. (All of them, but one, can be computed analytically. Perform the remaining one numerically.)

(g) What is the condition that ΔE must satisfy in order to guarantee the stability of the Hydrogen molecule?

(h) Notice that the degeneracy of the ground state is lifited in a way that the new spectrum can be represented by the effective hamiltonian $H_{\text{eff}} = \text{const} + J\mathbf{S}_1 \cdot \mathbf{S}_2$, where $\mathbf{S}_i$ is the spin operator of the i-th electron. Give the expression for the exchange coupling J. (Do not compute any integral.)

(i) Notice that $J\mathbf{S}_1 \cdot \mathbf{S}_2$ is a magnetic type interaction (two dipoles interacting). However, the Hamiltonian H is purely electric. Discuss which physical principle (or principles) is (are) involved in order to give an effective magnetic interaction from "purely" electric interactions.

5. Consider a system of two distinct bosonic particles (type A and B) in which only one mode of each is present:

$$H = \epsilon_{\text{A}} a^\dagger a + \epsilon_{\text{B}} b^\dagger b + V a^\dagger b + V^* b^\dagger a.$$

(a) Show that $c \equiv ua - vb$ and $d \equiv v^* a + u^* b$, with $|u|^2 + |v|^2 = 1$ are bosonic operators.

(b) Show that when $\epsilon_{\text{A}} = \epsilon_{\text{B}}$ and $V = V^*$, the choice $u = v = 1/\sqrt{2}$ decouples the system of bosonic particles C and D.

(c) Determine u and v that diagonalizes the system in the general case. Find the Eigenenergies and Eigenvectors of the system.

6. Consider a system of two spin-1/2 identical fermionic particles that can occupy three different states of energies E_i, $i = 1, 2, 3$. The matrix elements allowing the transitions between these states are M_{ij}.
   (a) Write down the system Hamiltonian in terms of the criation and annihilation operators.
   (b) Determine the equation that gives the Eigenenergies of the sytem.
   (c) Diagonalize the system for the particular case $E_i = E$ and $M_{ij} = M$, and the spins of the particles are the same.

7. The Grand partition function is given by the trace

$$Z_{\mathrm{G}} = \mathrm{tr}\, e^{-\beta(H-\mu N)}, \text{ where } H = \sum_i \epsilon_i a_i^\dagger a_i \text{ and } N = \sum_i a_i^\dagger a_i,$$

   and the constants β and μ are the inverse of temperature and the chemical potential, respectively. In the following compute the required quantities for both cases of identical bosonic and fermionic particles.
   (a) Compute Z_{G}. (*Hint*: Use the trace in the Fock space: $\mathrm{tr}\, O = \sum_{n_i \ldots n_\infty} \langle n_1 \ldots n_\infty |O| n_1 \ldots n_\infty \rangle$, and recall that in the Grand-canonical ensamble the number of particles is not fixed.)
   (b) Compute the average occupation number $\langle n_i \rangle$, such that $\mathcal{N} = \sum_i \langle n_i \rangle$. (*Hint*: Recall the thermodynamic Grand-potential $\Omega(T, V, \mu) = \beta^{-1} \ln Z_{\mathrm{G}}$, and that $\mathcal{N} = -\left(\frac{\partial \Omega}{\partial \mu}\right)_{T,V}$.)
   (c) Show that the fractional deviation from the mean occupation number

$$\frac{\left\langle (n_i - \langle n_i \rangle)^2 \right\rangle}{\langle n_i \rangle^2} = e^{\beta(\epsilon_i - \mu)} = \frac{1}{\langle n_i \rangle} + \zeta,$$

   with the $\zeta = \pm 1$ for bosons and fermions, respectively.

8. Consider the simplified Hubbard model which consists of a simple molecule made of 2 sites and 2 electrons descibed by

$$H = -t \sum_\sigma \left(c_{1,\sigma}^\dagger c_{2,\sigma} + c_{2,\sigma}^\dagger c_{1,\sigma} \right) + U \left(n_{1,\uparrow} n_{1,\downarrow} + n_{2,\uparrow} n_{2,\downarrow} \right),$$

   with $\sigma = \uparrow$ or $\downarrow$, $c_{i,\sigma}$ ($c_{i,\sigma}^\dagger$) being the anihillation (creation) operator of electrons at site i with spin projection σ at the z-axis, $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$, and $t > 0$ and $U > 0$ being constants.
   (a) Write the spin operators $\mathbf{S}_1$ and $\mathbf{S}_2$ in terms of the operators $c_{i,\sigma}$ and $c_{i,\sigma}^\dagger$.
   (b) Give a physical interpretation (orign) of each term in the Hamiltonian H.
   (c) Write the matrix H in the basis $\{i, \sigma; j, \tau\}$, where i,j denotes the sites the electrons occupy and σ,τ denotes their spin projection.
   (d) Diagonalize the matrix H. What is the ground state?
   (e) Interpret and discuss your results in the limits $U \gg t$ and $U \ll t$.

9. Consider the mode expansion of the vector potential (in the Schrödinger representation)

$$\mathbf{A}(\mathbf{r}) = \sqrt{\frac{\hbar}{2\epsilon_0 V}} \sum_{\mathbf{k}} \sum_{\lambda=\pm} \sqrt{\frac{1}{\omega_k}} a_{\mathbf{k},\lambda} e^{i\mathbf{k}\cdot\mathbf{r}} \hat{e}_{\mathbf{k},\lambda} + \text{h.c.},$$

$$\dot{\mathbf{A}}(\mathbf{r}) = -i\sqrt{\frac{\hbar}{2\epsilon_0 V}} \sum_{\mathbf{k}} \sum_{\lambda=\pm} \sqrt{\omega_k} a_{\mathbf{k},\lambda} e^{i\mathbf{k}\cdot\mathbf{r}} \hat{e}_{\mathbf{k},\lambda} + \text{h.c.},$$

   where $a_{\mathbf{k},\lambda}^\dagger$ ($a_{\mathbf{k},\lambda}$) are creation (annihilation) operators of photons the wavevector and polarization of which are respectively $\mathbf{k} = k(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ and λ, $\omega_k = ck$ is their angular frequency, and $\hat{e}_{\mathbf{k},\pm}$ are the polarization vectors

$$\begin{aligned} \hat{e}_{\mathbf{k},1} &= (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta), \\ \hat{e}_{\mathbf{k},2} &= (-\sin\phi, \cos\phi, 0), \\ \hat{e}_{\mathbf{k},\pm} &= \frac{1}{\sqrt{2}} \left(\mp \hat{e}_{\mathbf{k},1} - i \hat{e}_{\mathbf{k},2} \right). \end{aligned}$$

(a) Show that $\nabla \cdot \mathbf{A} = 0$. What is the physical interpretation of this result?

(b) Show that the angular momentum

$$\mathbf{L} = \frac{1}{\mu_0 c^2}\int \mathrm{d}^3 r \mathbf{r} \times (\mathbf{E} \times \mathbf{B}) = \mathbf{L}^{(o)} + \mathbf{L}^{(s)}, \text{ with}$$

$$\mathbf{L}^{(\mathrm{o})} = \frac{1}{\mu_0 c^2}\int \mathrm{d}^3 r \sum_{i=1}^{3} E_i \left(\vec{\ell} A_i\right), \text{ with } \vec{\ell}\psi = \mathbf{r} \times \nabla\psi,$$

$$\mathbf{L}^{(\mathrm{s})} = \frac{1}{\mu_0 c^2}\int \mathrm{d}^3 r \mathbf{E} \times \mathbf{A}.$$

Hint: It is convenient to use techniques of tensor calculus, in particular the Levi-Civita antisymmetrical tensor ε_{ijk}: $\varepsilon_{ijk} = 0$ if $i = j$, or $i = k$, or , $j = k$; $\varepsilon_{ijk} = 1$ if (ijk) equals (123) or any cyclic permutation of these indices, and $\varepsilon_{ijk} = -1$ otherwise. In addition, use the "contract epsilon identy" $\sum_{k=1}^{3} \varepsilon_{ijk}\varepsilon_{klm} = \delta_{i,l}\delta_{j,m} - \delta_{i,m}\delta_{j,l}$. Then show that

$$[\mathbf{r} \times (\mathbf{E} \times \mathbf{B})]_i = \sum_{j,k,l} E_l \left(\varepsilon_{ijk} x_j \frac{\partial}{\partial x_k} A_l\right) - \sum_{j,k,l} \frac{\partial}{\partial x_l}\left(\varepsilon_{ijk} x_j E_l A_k\right) + \sum_{j,k} \varepsilon_{ijk} E_j A_k.$$

Recall that $\nabla \cdot \mathbf{E} = 0$, $(\mathbf{a} \times \mathbf{b})_i = \sum_{j,k} \varepsilon_{ijk} a_j b_k$ and $(\nabla \times \mathbf{b})_i = \sum_{j,k} \varepsilon_{ijk} \frac{\partial}{\partial x_j} b_k$. Finally, use the boundary conditions that the fields vanish when $r \to \infty$.

(c) Show that

$$\mathbf{L}^{(\mathrm{s})} = \frac{\epsilon_0 i}{\hbar}\int \mathrm{d}^3 r \mathbf{E} \cdot S \cdot \mathbf{A},$$

with S being 3×3 matrices satisfing angular momentum commutation relations and having eigenvalues 0, $\pm\hbar$.

(d) Show and give the physical interpretation of the result

$$\mathbf{L}^{(\mathrm{s})} = \sum_{\mathbf{k}} \hbar \left(a^\dagger_{\mathbf{k},+} a_{\mathbf{k},+} - a^\dagger_{\mathbf{k},-} a_{\mathbf{k},-}\right) \hat{k}.$$

(e) Write $\mathbf{A}$, $\mathbf{E}$ and $\mathbf{B}$ in the Heisenberg representation. (Consider the free-field Hamiltonian $H = \sum_{\mathbf{k},\lambda} \hbar\omega_{k,\lambda} a^\dagger_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda}$, and ignore the zero-point energy.) Compute the commutation relations $[A_i(\mathbf{r},t), A_j(\mathbf{r}',t')]$, $[E_i(\mathbf{r},t), E_j(\mathbf{r}',t')]$, $[A_i(\mathbf{r},t), E_j(\mathbf{r}',t')]$, and $[E_i(\mathbf{r},t), B_j(\mathbf{r}',t')]$? Give a physical consequence of latter one.

(f) Do $\mathbf{E}(\mathbf{r},t)$ and $\mathbf{B}(\mathbf{r},t)$ commute with the *total* photon number operator

$$N(t) = \sum_{\mathbf{k},\lambda} a^\dagger_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda}?$$

Interpret or give a physical consequence of your result.

(g) Consider a coherent state of photons with momentum $\mathbf{p} = \hbar\mathbf{k}$ and helicity λ given by

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} e^{\alpha a^\dagger_{\mathbf{k},\lambda}} |0\rangle,$$

where $|0\rangle$ is the vacuum state and α is a scalar. Compute the time evolution of $\Delta X = \sqrt{\langle X^2\rangle - \langle X\rangle^2}$ and $\Delta P = \sqrt{\langle P^2\rangle - \langle P\rangle^2}$ where $X = \sqrt{\frac{\hbar}{2\omega_k}}\left(a^\dagger_{\mathbf{k},\lambda} + a_{\mathbf{k},\lambda}\right)$ and $P = i\sqrt{\frac{\hbar\omega_k}{2}}\left(a^\dagger_{\mathbf{k},\lambda} - a_{\mathbf{k},\lambda}\right)$ are position and momentum operators of the associated harmonic oscillator, respectively.

(h) Show that the Schrödinger equation $i\hbar\frac{\partial}{\partial t}|\alpha(t)\rangle = H|\alpha(t)\rangle$ has a solution $|\alpha(t)\rangle = |\beta\rangle$, where $\beta = \alpha e^{-i\omega_k t}$. (Ignore the zero-point energy.) Now compute $\langle\alpha(t)|\mathbf{A}|\alpha(t)\rangle$. (Discuss your result relating it with classical electromagnetic waves such as laser.)