Quantum Mechanics III
HW 9

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Due: Mar. 28

7.1 (a) Write down the density operator of the electromagnetic field at temperature T and chemical potential $\mu = 0$.

$$\rho = \frac{1}{\mathcal{Z}} e^{-\beta(\hat{H}-\mu\hat{N})}\Big|_{\mu=0} = \frac{e^{-\beta\hat{H}}}{\mathcal{Z}}$$

where

$$\mathcal{Z} = \text{Tr } e^{-\beta(\hat{H}-\mu\hat{N})}\Big|_{\mu=0} = \text{Tr } e^{-\beta\hat{H}}.$$

The Hamiltonian of the electromagnetic field, given in a basis of the Fock space characterized by free photons with mode energy $\hbar\omega_n$, is

$$\hat{H} = \sum_n \hbar\omega_n a_n^\dagger a_n.$$

Here n denotes a general index of the photon mode; it could, for example, stand for a momentum index $\mathbf{k}$ and polarization vector λ. This defines the density operator given above.

(b) Show that the grand partition function is

$$\mathcal{Z} = \prod_n \frac{1}{1 - e^{-\beta\hbar\omega_n}},$$

where the product runs over all photon modes.

$$\mathcal{Z} = \text{Tr}\left(e^{-\beta\sum_n \hbar\omega_n a_n^\dagger a_n}\right)$$

To trace over all possible photon modes, we may first sum over a fixed particle number N and then sum over all possible permutations of the occupation numbers n_i of single mode states i

$$\begin{aligned}
\mathcal{Z} &= \sum_N \sum_{\{\{n_i\}:\sum_i n_i = N\}} e^{-\sum_i \beta\hbar\omega_i n_i} \\
&= \sum_{\{n_i\}} e^{-\sum_i \beta\hbar\omega_i n_i} \\
&= \sum_{\{n_i\}} \left(\prod_i e^{-\beta\hbar\omega_i n_i}\right) \\
&= \prod_i \left(\sum_{n_i} e^{-\beta\hbar\omega_i n_i}\right)
\end{aligned}$$

$$= \prod_i \frac{1}{1 - e^{-\beta\hbar\omega_i}}$$

Summing over all possible sets $\{\{n_i\} : \sum_i n_i = N\}$ and then summing over N is equivalent to carrying out a sum over all possible sets of $\{n_i\}$, unconstrained. In addition, as we sum over all sets $\{n_i\}$, the term $\sum_{\{n_i\}} \prod_i$ can be rearranged to a product of a sum, analogous to factorization.

7.2 As we have discussed, in atom-field interactions two forms of the interaction Hamiltonian are in common use. Let us denote these by

$$H_{\mathbf{d}\cdot\mathbf{E}} = -q\mathbf{r}\cdot\mathbf{E}(t), \quad H_{\mathbf{p}\cdot\mathbf{A}} = -\frac{q}{m}\mathbf{p}\cdot\mathbf{A}(t).$$

The term quadratic in $\mathbf{A}$ is immaterial in the present context, as it does not involve the quantum variables $\mathbf{r}$ or $\mathbf{p}$ and can be removed with a trivial unitary transformation.

(a) By studying the commutator $[x, H_A]$ show that the matrix elements of position between the eigenstates $|n\rangle$ of the atomic Hamiltonian H_A satisfy $\langle m|\mathbf{p}|n\rangle = im\omega_{mn}\langle m|\mathbf{r}|n\rangle$, where $\omega_{nm} = (E_m - E_n)/\hbar$ is the frequency difference between the states $|m\rangle$ and $|n\rangle$.

(b) Suppose the atom is driven by electromagnetic fields such that $\mathbf{A}(t)$ tends to zero smoothly with $t \to \pm\infty$. Consider transitions from some initial ($t = -\infty$) state of the atom $|n\rangle$ to the other states using first-order time dependent perturbation theory. Show that the transition probabilities after the fields have turned back to zero ($t = \infty$), are the same for the two choices of the interaction Hamiltonian.

(a) Given the atomic Hamiltonian

$$H_A = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r})$$

and its commutator with position

$$[\mathbf{r}, H_A] = \frac{1}{2m}[\mathbf{r}, \mathbf{p}^2] = \frac{\mathbf{p}}{m}[\mathbf{r}, \mathbf{p}] = i\hbar\frac{\mathbf{p}}{m},$$

take the commutator between the expectation of eigenstates $|m\rangle$ and $|n\rangle$ of H_A

$$\begin{aligned}\langle m|[H_A, \mathbf{r}]|n\rangle &= \langle m|H_A\mathbf{r} - \mathbf{r}H_A|n\rangle \\ &= \hbar\omega_{mn}\langle m|\mathbf{r}|n\rangle \\ &= -\frac{i\hbar}{m}\langle m|\mathbf{p}|n\rangle .\end{aligned}$$

Thus

$$im\omega_{mn}\langle m|\mathbf{r}|n\rangle = \langle m|\mathbf{p}|n\rangle .$$

(b) To first order, the probability of transition from initial state $|n\rangle$ to state $|m\rangle$ is given by the time dependent coefficient $c_m(t)$ (more specifically the modulus square)

$$c_m^1(t) = \frac{-i}{\hbar}\int_{-\infty}^{\infty} dt\ \langle m|H_{int}|n\rangle\, e^{i\omega_{mn}t}.$$

We evaluate with both forms of the interaction Hamiltonian

$$c_m^1(t) = \frac{-i}{\hbar}\int_{-\infty}^{\infty} dt\ \langle m|H_{int}|n\rangle\, e^{i\omega_{mn}t}$$

$$
\begin{aligned}
&= \frac{iq}{\hbar}\int dt\ \langle m|\mathbf{r}\cdot\mathbf{E}(t)|n\rangle\, e^{i\omega_{mn}t} \\
&= \frac{iq}{\hbar}\int dt\ \langle m|\mathbf{r}|n\rangle\cdot\mathbf{E}(t) e^{i\omega_{mn}t} \\
&= -\frac{iq}{\hbar}\int dt\ \langle m|\mathbf{r}|n\rangle\cdot\frac{\partial\mathbf{A}(t)}{\partial t} e^{i\omega_{mn}t} \\
&= -\frac{q}{\hbar m\omega_{mn}}\int dt\ \langle m|\mathbf{p}|n\rangle\cdot\frac{\partial\mathbf{A}(t)}{\partial t} e^{i\omega_{mn}t} \\
&= \frac{i\omega_{mn}q}{\hbar m\omega_{mn}}\int dt\ \langle m|\mathbf{p}|n\rangle\cdot\mathbf{A}(t) e^{i\omega_{mn}t} \\
&= \frac{iq}{\hbar m}\int dt\ \langle m|\mathbf{p}\cdot\mathbf{A}(t)|n\rangle\, e^{i\omega_{mn}t}
\end{aligned}
$$

where in the sixth line, we integrate by parts with a vanishing surface term

$$\langle m|\mathbf{p}|n\rangle\cdot\mathbf{A}(t)e^{i\omega_{mn}t}|_{-\infty}^{\infty} = 0.$$

We see our result for $c_m^1(t)$ is the same for either interacting Hamiltonian.

7.3 Study a transition in an atom where the lower state has the angular momentum $J = 0$ and the upper state the angular momentum $J' = 1$. Using the Wigner-Eckart theorem, show that the dipole matrix elements between the state $J = 0$, $m = 0$ and $J' = 1$, $m' = 0$ may be chosen to be a real vector that points along the quantization (z) axis.

The dipole matrix elements between states $|jm\rangle$ that we seek are

$$\langle 00|\mathbf{d}|10\rangle = q\,\langle 00|\mathbf{r}|10\rangle\,.$$

Meanwhile, according the Wigner-Eckart theorem

$$\langle 00|T_q^{(k)}|10\rangle = \langle 10; kq|00\rangle\,\langle 0||T^{(k)}||1\rangle$$

where $T^(k)_q$ is an irreducible spherical tensor of rank k, $\langle 10; kq|00\rangle$ is a Clebsch-Gordon coefficient, and $\langle 0||T^{(k)}||1\rangle$ is proportionality factor independent of the geometric features. To compute the dipole elements, we may form a rank 1 spherical tensor, with a representation along quantization axis z

$$z = T_0^1, \qquad y = \frac{i(T_{-1}^1 + T_1^1)}{\sqrt{2}}, \qquad x = \frac{T_{-1}^1 - T_1^1}{\sqrt{2}}.$$

Putting the theorem to use, we then have (using a shorthand for the Clebsch-Gordon coefficients)

$$\langle 00|\mathbf{d}_x|10\rangle = \frac{q}{\sqrt{2}}\,\langle 0||T^{(1)}||1\rangle\,(C^{00}_{1(-1)10} - C^{00}_{1110}) = \frac{q}{\sqrt{2}}\,\langle 0||T^{(1)}||1\rangle\,(0-0) = 0$$

$$\langle 00|\mathbf{d}_y|10\rangle = i\frac{q}{\sqrt{2}}\,\langle 0||T^{(1)}||1\rangle\,(C^{00}_{1(-1)10} + C^{00}_{1110}) = i\frac{q}{\sqrt{2}}\,\langle 0||T^{(1)}||1\rangle\,(0+0) = 0$$

$$\langle 00|\mathbf{d}_z|10\rangle = q\,\langle 0||T^{(1)}||1\rangle\,C^{00}_{1010}$$

Treating each matrix element as a vector component, we may represent $\langle 00|\mathbf{d}|01\rangle$ as a real vector $\mathbf{a}$ of which only one component is nonzero, the component along the quantization axis. Note that the common factor of the double bar matrix element (reduced matrix) is set through normalization.