EXAM QUANTUM THEORY January 17, 2008
(Course Dr. P.J.H. Denteneer, Fall 2007) 10.00 - 13.00h

Write NAME, INITIALS and STUDENT NUMBER on every sheet you hand in. Start each problem on a new page. The problems below can earn you the following number of grade points: (1) 20, (2) 20, (3) 30, (4) 20.

1) Consider a spin $\frac{1}{2}$ object and define $\hat{\sigma}_\alpha \equiv \cos\alpha\,\hat{\sigma}_x + \sin\alpha\,\hat{\sigma}_y$. We study a physical system in a *mixture* state, constructed from the $\hat{\sigma}_z$-eigenstate $|\sigma_z = -1\rangle$ and the $\hat{\sigma}_\alpha$-eigenstate $|\sigma_\alpha = 1\rangle$ with weights $\frac{1}{4}$ and $\frac{3}{4}$, respectively.

   (a) Write down the state **operator** $\hat{\rho}$ that describes the mixture.

   (b) Show that:
   $$\hat{\rho} = \tfrac{1}{2}\,\hat{1} - \tfrac{1}{8}\left(\hat{\sigma}_z - 3\,\hat{\sigma}_\alpha\right)$$

   (c) Write down the matrix $\rho_{\sigma,\sigma'}$ in the σ_z–representation. Show explicitly using this matrix that the state operator indeed describes a mixture?

   (d) Compute the expectation values $\langle\sigma_x\rangle$, $\langle\sigma_y\rangle$, $\langle\sigma_z\rangle$ and $\langle\sigma_\alpha\rangle$ in the mixture state.

2) Consider a harmonic oscillator with Hamiltonian $\hat{H}$:
$$\hat{H} = \tfrac{1}{2}\left(\hat{P}^2 + \hat{Q}^2\right)\hbar\omega = \left(\hat{N} + \tfrac{1}{2}\right)\hbar\omega,$$
$$\hat{N} \equiv \hat{a}^\dagger\hat{a} \quad , \quad \hat{a} \equiv \frac{1}{\sqrt{2}}\left(\hat{Q} + i\hat{P}\right)$$

The commutator of position operator $\hat{Q}$ and momentum operator $\hat{P}$ is given by: $\left[\hat{Q}, \hat{P}\right] = i\,\hat{1}$. Let $|n\rangle$ denote the orthonormal set of eigenstates of $\hat{N}$: $\hat{N}|n\rangle = n\,|n\rangle$ $(n = 0, 1, 2, \ldots)$. The operation of the lowering operator $\hat{a}$ on these states is given by: $\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle$.

   (a) Let $|q\rangle$ denote the eigenstates of the position operator $\hat{Q}$ (with real eigenvalues $q \in (-\infty, \infty)$). The wave function of state $|n\rangle$ in the position representation is then given by: $\varphi_n(q) = \langle q|n\rangle$. Write down the relation between the states $|q\rangle$ and the states $|n\rangle$ in terms of the wave function $\varphi_n(q)$.

   (b) Let $|\chi(t)\rangle$ denote a (time-dependent) state vector, which at time $t = 0$ is given in terms of two eigenstates of $\hat{N}$: $|\chi(0)\rangle = \frac{1}{\sqrt{2}}\left(|2\rangle + i\,|3\rangle\right)$. Calculate $|\chi(t)\rangle$.

   (c) Calculate the expectation value in state $|\chi(t)\rangle$ of the operator $\hat{P}$.

   (d) Calculate the dispersion $\Delta_\chi P$.

P.T.O.

3) As an application of the *Second Quantization* formalism we study the following *electron-phonon Hamiltonian* for electrons in a crystal interacting with phonons, i.e. lattice vibrations:

$$H = H_0 + H_1 \quad ,$$

$$H_0 = \sum_{\vec{q}} \hbar\omega_{\vec{q}}\, \hat{b}^\dagger_{\vec{q}} \hat{b}_{\vec{q}} + \sum_{\vec{k}} \varepsilon_{\vec{k}}\, \hat{a}^\dagger_{\vec{k}}\, \hat{a}_{\vec{k}} \quad ,$$

$$H_1 = \sum_{\vec{k},\vec{q}} M_{\vec{q}}\, \hat{a}^\dagger_{\vec{k}+\vec{q}}\, \hat{a}_{\vec{k}} \left(\hat{b}_{\vec{q}} + \hat{b}^\dagger_{-\vec{q}}\right) \quad ,$$

where H_0 contains parts for independent harmonic oscillators (describing the phonons; wave vectors $\vec{q}$, frequencies $\omega_{\vec{q}}$, creation operators $\hat{b}^\dagger_{\vec{q}}$) and independent electrons (wave vectors $\vec{k}$, energies $\varepsilon_{\vec{k}}$, creation operators $\hat{a}^\dagger_{\vec{k}}$). H_1 is the interaction term with $M_{\vec{q}}$ the electron-phonon coupling, which we assume to be weak; the interaction term can therefore be seen as a perturbation. Note that the spin-index is suppressed for the electrons, i.e. we don't write it, although we keep in mind that electrons do have spin; for our convenience this convention is maintained in the following.

(a) Give the fundamental algebraic relations for the phonon operators $\hat{b}_{\vec{q}}$ and $\hat{b}^\dagger_{\vec{q}}$, and for the electron operators $\hat{a}_{\vec{k}}$ and $\hat{a}^\dagger_{\vec{k}}$.

(b) To gain insight in the effect of the phonons on the electrons in a crystal, one may perform a *similarity* transformation:

$$\tilde{H} = e^{-S}\, H\, e^{S} \quad ,$$

with e^S an unitary transformation. Show that if we can find S such that:

$$H_1 + [H_0, S] = 0 \quad ,$$

and take it that S is of the same order as H_1, then the transformed Hamiltonian $\tilde{H}$ can be written as H_0 plus terms that are second order or higher in the perturbation. Compute the second order term. Note that you don't need the explicit forms of H_0 and H_1 for this part.

(c) We propose that S can be of the form:

$$S = \sum_{\vec{k},\vec{q}} \left(A\, \hat{b}^\dagger_{-\vec{q}} + B\, \hat{b}_{\vec{q}}\right) M_{\vec{q}}\, \hat{a}^\dagger_{\vec{k}+\vec{q}}\, \hat{a}_{\vec{k}} \quad .$$

Compute A and B such that the condition in (b) is fulfilled.

(d) Write down the result for S and give an interpretation of the denominators in the coefficients A and B.

(e) Show that the second order term in $\tilde{H}$, which is proportional to $|M_{\vec{q}}|^2$, will have terms where the operator part is of the form:

$$\hat{a}^\dagger_{\vec{k}+\vec{q}}\, \hat{a}_{\vec{k}}\, \hat{a}^\dagger_{\vec{k}'-\vec{q}}\, \hat{a}_{\vec{k}'} \quad .$$

(f) Compute the pre-factors of the terms treated under (e), assuming $\omega_{\vec{q}} = \omega_{-\vec{q}}$. From this result, what can you say about the effect of phonons on the electrons in a crystal?

4) We consider a particle with mass m in one spatial dimension on which no forces act. The Lagrangian L is then given by:

$$L(\dot{x}, x) = \tfrac{1}{2} m \dot{x}^2 \quad ,$$

where x denotes position and the dot above x means differentiation with respect to time. The action $\mathcal{S}[x(t)]$ in terms of the Lagrangian is generally given by:

$$\mathcal{S}[x(t)] = \int_{t_A}^{t_B} \mathrm{d}t \, L(\dot{x}, x) \quad .$$

Therefore the classical action $\mathcal{S}_{\mathrm{cl}}$ for such a particle that at time t_A is at position x_A and at (later) time t_B at position x_B is given by:

$$\mathcal{S}_{\mathrm{cl}} = \frac{m\,(x_B - x_A)^2}{2\,(t_B - t_A)} \quad .$$

Using the above result the quantummechanical *propagator* for a free particle can be derived through a path integral. The propagator is given by:

$$< x_B, t_B | x_A, t_A >= \int_{x_A}^{x_B} \mathfrak{D}[x(t)] e^{i\mathcal{S}[x(t)]/\hbar} .$$

To calculate the path integral we first split up the integration path $x(t)$ in the classical path $\bar{x}(t)$ and a deviation $y(t)$: $x(t) = \bar{x}(t) + y(t)$.

(a) Show that the propagator can be written as:

$$< x_B, t_B | x_A, t_A >= e^{\frac{i}{\hbar}\mathcal{S}_{\mathrm{cl}}} \int_0^0 \mathfrak{D}[y(t)] \exp\left\{ \frac{i}{\hbar} \int_{t_A}^{t_B} \mathrm{d}t \, L(\dot{y}, y) \right\} .$$

To evaluate the path integral over $y(t)$ the interval $[t_A, t_B]$ is split up in N small intervals Δt. We remind the reader that for general L the action can then be written as (identify x_A with x_0 and x_B with x_N):

$$\mathcal{S}[x(t)] = \lim_{N\to\infty, \Delta t \to 0} \Delta t \sum_{j=1}^{N} \left[\frac{m}{2} \left(\frac{x_j - x_{j-1}}{\Delta t} \right)^2 - V(x_{j-1}) \right] .$$

Also remember that the measure for path integration is defined as:

$$\int_{x_A}^{x_B} \mathfrak{D}[x(t)] = \lim_{N\to\infty} \int_{-\infty}^{+\infty} \mathrm{d}x_1 \cdots \int_{-\infty}^{+\infty} \mathrm{d}x_{N-1} \left(\frac{m}{2\pi i \hbar \Delta t} \right)^{\frac{N}{2}} .$$

(b) Evaluate the path integral and write down the full expression for the propagator of a free particle in terms of x_A, x_B, t_A, and t_B. You will probably need the following identity:

$$\int_{-\infty}^{+\infty} \mathrm{d}x_1 \cdots \int_{-\infty}^{+\infty} \mathrm{d}x_{N-1} \exp\left\{ i \sum_{j=1}^{N} (x_j - x_{j-1})^2 \right\} = \left(\frac{(i\pi)^{N-1}}{N} \right)^{\frac{1}{2}} e^{i(x_N - x_0)^2/N} .$$

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(c) Give an analysis of how the (properly generalized) result of (b) can be used to describe the *double-slit interference experiment*. Use a set-up in which the particle source is at the origin $\mathcal{O}$, the two slits are at $x = L$ and heights $z = \pm z_0$, and the screen on which the interference pattern is detected is at $x = 2L$. Your analysis should include an expression involving free-particle propagators for the probability to detect a particle on the screen at arbitrary height z (calculation of this expression is not required).