Moderne Theoretische Physik I
Grundlagen der Quantenmechanik

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Exercise Sheet 12

Prof. Jörg Schmalian
Iksu Jang, Grgur Palle
Karlsruher Institut für Technologie (KIT)
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The problems whose solutions you need to upload are designated with stars.

$\star$ Problem 1 $\star$ Anharmonic oscillator

Consider an anharmonic oscillator of the form

$$H = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 + \alpha\hat{x}^4 \tag{1}$$

where the third term can be considered as a perturbation $\alpha x_0^4 \ll \hbar\omega$. Here $x_0 = \sqrt{\frac{\hbar}{m\omega}}$ is the characteristic length scale of the simple harmonic oscillator. For $\alpha = 0$, the problem is exactly solvable, where the energies of the states $\{|n\rangle\}$ for $n \in N_0$ are given by $E_n^{(0)} = \hbar\omega(n + \frac{1}{2})$. It was shown that ascending and descending operators

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left[\hat{x} + \frac{i}{m\omega}\hat{p}\right], \tag{2}$$

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left[\hat{x} - \frac{i}{m\omega}\hat{p}\right] \tag{3}$$

whose effect on states is given by

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \tag{4}$$

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{5}$$

The first correction to the state energy is

$$E_n^{(1)} = \alpha\langle n|\hat{x}^4|n\rangle. \tag{6}$$

1. Calculate the matrix element $\langle n|\hat{x}^2|n'\rangle$. Show that $n' = n, n \pm 2$ must hold to have non-zero value.
2. Compute $E_n^{(1)}$ to first order in α. (Hint: The identity operator is given by $\hat{1} = \sum_n |n\rangle\langle n|$.)
3. Derive an expression for $n = n_{max}$ for which the perturbation theory is no longer valid. One possible criterion is

$$E_{n_{max}}^{(0)} \approx E_{n_{max}}^{(1)} \tag{7}$$

⋆ Problem 2 ⋆ Schmidt decomposition and reduced density matrices

Consider a bipartite quantum system built from a direct product Hilbert space of the two parts, $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. Let $|a_i\rangle_A$ with $i = 1, 2, \cdots n$ label a complete orthonormal basis of states in Hilbert space A, and likewise for Hilbert space B: $|b_j\rangle_B$, with $j = 1, 2, \cdots N \geq n$. The most general quantum state in the full Hilbert space can be expressed as,

$$|\Phi\rangle = \sum_{n=1}^{n} \sum_{j=1}^{N} c_{ij} |a_i\rangle_A \otimes |b_j\rangle_B, \tag{8}$$

with complex coefficients, c_{ij}.

A theorem proven on the wikipedia page, https://en.wikipedia.org/wiki/Schmidt_decomposition, states that there always exist orthonormal sets, $|\psi_i\rangle_A$, $|\phi_j\rangle_B$ with $i, j = 1, 2, \cdots n$ such that the general state $|\Phi\rangle$ can be re-expressed in a Schmidt-decomposed form:

$$|\Phi\rangle = \sum_{i}^{n} v_i |\psi_i\rangle_A \otimes |\phi_i\rangle_B \tag{9}$$

with the normalization condition, $\sum_{i=1}^{n} |v_i|^2 = 1$.

1. Using this Schmidt form, obtain expressions for the reduced density matrices,

$$\hat{\rho}_A = Tr_B |\Phi\rangle\langle\Phi|, \quad \hat{\rho}_B = Tr_A |\Phi\rangle\langle\Phi| \tag{10}$$

   Demonstrate that the reduced density matrices are Hermitian with eigenvalues $\lambda_i = |v_i|^2$, $i = 1, 2, \cdots n$, and associated eigenvectors, $|\psi_i\rangle_A$, $|\phi_i\rangle_B$. Thus, the Schmidt-decomposition for any state $|\Phi\rangle$ can be obtained by computing and then diagonalizing the reduced density matrices.

2. Now consider, as an example, two spin-$\frac{1}{2}$ particles, labelled A and B, in a (normalized) pure state,

$$|\Phi\rangle = \frac{1}{\sqrt{2}} |\downarrow\rangle_A \otimes |\downarrow\rangle_B + \frac{1}{2} |\uparrow\rangle_A \otimes (|\uparrow\rangle_B + |\downarrow\rangle_B). \tag{11}$$

   Obtain the Schmidt-decomposition of this state by computing and diagonalizing the two reduced density matrices and show that the expression of $|\Phi\rangle$ obtained from Eq. (9) is same to the Eq. (11).

Problem 3 Stark effect

Consider a hydrogen atom in the ground state $n = 1$ in a homogeneous electric field $\mathbf{E} = E\hat{e}_z$. The field can be considered as a perturbation. The Hamiltonian is given by

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{12}$$

where $\hat{H}_0$ represents the unperturbed hydrogen atom and $\hat{V} = -eE\hat{z}$ corresponds to the perturbation term. Calculate the energy correction of the ground state in leading order.

1. Show that the energy correction vanishes to first order $E_1^{(1)} = 0$. Use the parity operator $\hat{P}$ for this. (Hint: The eigenstates of the hydrogen atom transform as $\hat{P}|nlm\rangle = (-1)^l |nlm\rangle$ and $\hat{P}\hat{z}\hat{P}^\dagger = -\hat{z}$. In addition, $\hat{P}^\dagger \hat{P} = \hat{1}$.)

2. Show that the matrix elements $\langle 100|\hat{z}|nml\rangle$ are finite only for $l = 1$ and $m = 0$. (Hint: z can be expressed using spherical harmonics. Also use their orthogonality.)

3. Calculate the second order energy correction $E_1^{(2)}$ where only states with $n = 2$ need to be considered. States with higher excitation energies $n \geq 3$ can be neglected.