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Advanced Quantum Theory

Exercise Sheet 6

Problem 10

Let $(\mathcal{H}, \langle \cdot | \cdot \rangle)$ be the Hilbert space. and let $f: \mathbb{R} \to \mathbb{C}$ with $f(0) = 0$ and some good differentiability properties ;)

We define: $H_0 : \mathcal{H} \to \mathcal{H}$ linear, self-adjoint operator

$$H_0 := \hbar\omega \left(a^+ a + \tfrac{1}{2}\right) \quad \text{with} \quad a := \sqrt{\frac{m\omega}{2\hbar}} \left(X + \frac{i}{m\omega} P\right)$$

for some constants $m, \omega \in (0, \infty)$.

Then H_0 is the Hamiltonian of the harmonic oscillator, thus giving us a discrete orthonormal basis of eigen states $\{ |n\rangle \mid n \in \mathbb{N}_0 \}$.

For all times $t \in \mathbb{R}$, we define the time-dependent Hamiltonian through

$$H(t) := H_S(t) := \underbrace{\hbar\omega \left(a^+ a + \tfrac{1}{2}\right)}_{= H_0} + \underbrace{f(t)\, a + f^*(t)\, a^+}_{=: H_{1,S}(t)}$$

Currently, everything is formulated in the Schrödinger picture.
For the formulation of the Interaction picture one has to put the implicit time-dependence caused by H_0 into the operators. The explicit time-dependence of $H_{1,S}(t)$ will be handled by the interaction states.

(1) For any operator $A(t) = A_S(t)$ in the Schrödinger picture the corresponding operator in the interaction picture is given by

$$A_I(t) = e^{\frac{i}{\hbar} H_0 t} A_S(t)\, e^{-\frac{i}{\hbar} H_0 t}$$

$$\Rightarrow \quad H_{0,I}(t) = e^{\frac{i}{\hbar} H_0 t} H_0\, e^{-\frac{i}{\hbar} H_0 t} = H_0\, e^{\frac{i}{\hbar} H_0 t} e^{-\frac{i}{\hbar} H_0 t} = H_0$$

$$\Rightarrow \quad H_I(t) = H_0 + H_{1,I}(t), \quad H_I(0) = H_0$$

Theofore the annihilation operators in the interaction picture are given by

$$a_I(t) = e^{\frac{i}{\hbar} H_0 t}\, a\, e^{-\frac{i}{\hbar} H_0 t}, \qquad a_I^+(t) = e^{\frac{i}{\hbar} H_0 t}\, a^+\, e^{-\frac{i}{\hbar} H_0 t}$$

(2) The interaction-picture state is given for all $t \in \mathbb{R}$:

$$|n,t\rangle_I = e^{\frac{i}{\hbar}H_0 t}\,|n,t\rangle_S \qquad \text{with} \quad |n,0\rangle_S := |n\rangle$$

Therefore, we can derive the following time-evolution equation:

and $i\hbar\,\partial_t |n,t\rangle_S = H_S(t)\,|n,t\rangle_S$

($|n,t\rangle_S$ is state in Schrödinger picture)

$\Rightarrow |n,0\rangle_I = |n,0\rangle_S = |n\rangle$

$$i\hbar\,\partial_t |n,t\rangle_I = H_{1,I}(t)\,|n,t\rangle_I$$

with $H_I(t) = e^{\frac{i}{\hbar}H_0 t}\,H_S(t)\,e^{-\frac{i}{\hbar}H_0 t} = H_0 + H_{1,I}(t)$

$$\Rightarrow \quad -i\hbar\,{}_I\langle n,t| = {}_I\langle n,t|\,H_{1,I}(t)$$

(3) We use the Taylor-Expansion to approximate the matrix elements:

$${}_I\langle m,\delta t|\,H_I(\delta t)\,|n,\delta t\rangle_I = \underbrace{{}_I\langle m,0|\,H_I(0)\,|n,0\rangle_I} + \delta t\cdot D\left[{}_I\langle m,\cdot|\,H_I(\cdot)\,|n,\cdot\rangle_I\right](0) + \mathcal{O}(\delta t^2)$$

$$= \langle m|\,H_0\,|n\rangle = \hbar\omega\left(\langle m|a^\dagger a|n\rangle + \frac{1}{2}\langle m|n\rangle\right)$$

$$= \hbar\omega\left(n+\frac{1}{2}\right)\delta_{mn}$$

The time-evolution of an operator $A_I(t)$ in the interaction picture is given by:

$$i\hbar\,D_t A_I(t) = \left[A_I(t), H_0\right] + i\hbar\,\partial_t A_I(t)$$

$$\Rightarrow i\hbar\,D_t H_I(0) = \underbrace{\left[H_I(0), H_0\right]}_{=0} + i\hbar\,\partial_t H_I(0)$$

$$\Rightarrow \quad D_t H_I(0) = \partial_t H_I(0) = f'(0)\,a_I(0) + f^{*\prime}(0)\,a_I^\dagger(0)$$

$$= f'(0)\,a + f^{*\prime}(0)\,a^\dagger$$

$$D\left[{}_I\langle m,\cdot|\,H_I(\cdot)\,|n,\cdot\rangle_I\right](0) = \left.\begin{array}{l} \partial_t\,{}_I\langle m,t|(0)\;\; H_I(0)\,|n,0\rangle_I \\ +\;{}_I\langle m,0|\;H_I(0)\;\;\partial_t|n,t\rangle_I(0) \end{array}\right\} = 0$$

$$+\;{}_I\langle m,0|\;\;D_t H_I(0)\;\;|n,0\rangle_I$$

$$= \langle m|\left(f'(0)\,a + f^{*\prime}(0)\,a^\dagger\right)|n\rangle = f'(0)\,\langle m|a|n\rangle + f^{*\prime}(0)\,\langle m|a^\dagger|n\rangle$$

$$= f'(0)\,\sqrt{n}\,\delta_{m,n-1} + f^{*\prime}(0)\,\sqrt{n+1}\,\delta_{m,n+1}$$

$$\Rightarrow {}_I\langle m,\delta t|\,H_I(\delta t)\,|n,\delta t\rangle_I = \hbar\omega\left(n+\frac{1}{2}\right)\delta_{mn}$$

$$+\;\delta t\left(f'(0)\,\sqrt{n}\,\delta_{m,n-1} + f^{*\prime}(0)\,\sqrt{n+1}\,\delta_{m,n+1}\right)$$

$$+\;\mathcal{O}(\delta t^2)$$

Problem 11

Let $(\mathcal{H}, \langle \cdot | \cdot \rangle)$ be the Hilbert space. The Hamiltonian is given by

$$H := \frac{p^2}{2m} + V(x) \quad , \quad V(x) := -\frac{m\omega^2}{2} x^2 + \frac{\lambda}{4} x^4$$

with $m, \omega, \lambda \in (0,\infty)$. Additionally, we define for all $k \in (0,\infty)$, $v \in \mathbb{R}$ the following variational test functions.

$$\Psi_{k,v} : \mathbb{R} \longrightarrow \mathbb{C} \quad , \quad \Psi_{k,v}(x) := \sqrt{k}\ \varphi(k(x-v)) \quad \text{with}$$

$$\varphi : \mathbb{R} \longrightarrow \mathbb{R} \quad , \quad \varphi(x) := \frac{1}{\pi^{1/4}} e^{-x^2/2}$$

(1) The energy function is given by:

$$E : (0,\infty) \times \mathbb{R} \longrightarrow \mathbb{R} \quad , \quad E(k,v) := \langle \Psi_{k,v} | H | \Psi_{k,v} \rangle$$

$$\frac{p^2}{2m} = -\frac{\hbar^2}{2m}\Delta \quad , \quad \Delta \Psi_{k,v}(x) \overset{(*)}{=} k^{5/2} \varphi''(k(x-v)) \overset{(**)}{=} k^{5/2}[x^2 - 1]\ \varphi(k(x-v))$$

$$(*) \quad \Delta(f \circ g) = (f \circ g)'' = (f' \circ g \cdot g')' = f'' \circ g \cdot g'^2 + f' \circ g \cdot g''$$

$$(**) \quad \varphi'(x) = -\frac{x}{\pi^{1/4}} e^{-x^2/2} \quad , \quad \varphi''(x) = -\frac{1}{\pi^{1/4}} e^{-x^2/2} + \frac{x^2}{\pi^{1/4}} e^{-x^2/2}$$
$$= -\varphi(x) + x^2 \varphi(x)$$

$$\Rightarrow E(k,v) = \int_{\mathbb{R}} \Psi^*_{k,v}(x)\ H\ \Psi_{k,v}(x)\ dx$$
$$= -\frac{\hbar^2}{2m} k^3 \int_{\mathbb{R}} x^2 \varphi^2(k(x-v))\, dx + \frac{\hbar^2}{2m} k^3 \int_{\mathbb{R}} \varphi^2(k(x-v))\, dx$$
$$- \frac{m\omega^2}{2} k \int_{\mathbb{R}} x^2 \varphi^2(k(x-v))\, dx + \frac{\lambda}{4} k \int_{\mathbb{R}} x^4 \varphi^2(k(x-v))\, dx$$
$$= -\frac{\hbar^2}{2m}\frac{k^3}{\sqrt{\pi}} \int_{\mathbb{R}} x^2 e^{-[k(x-v)]^2} dx + \frac{\hbar^2}{2m}\frac{k^3}{\sqrt{\pi}} \int_{\mathbb{R}} e^{-[k(x-v)]^2} dx$$
$$- \frac{m\omega^2}{2}\frac{k}{\sqrt{\pi}} \int_{\mathbb{R}} x^2 e^{-[k(x-v)]^2} dx + \frac{\lambda}{4}\frac{k}{\sqrt{\pi}} \int_{\mathbb{R}} x^4 e^{-[k(x-v)]^2} dx$$

We can choose the same substitution for all integrals: $z(x) := kx$

$$\Rightarrow z'(x) = k \quad , \quad x = \frac{z(x)}{k}$$ (because $k > 0$ the integral bounds do not change)

$$\Rightarrow \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} x^2 e^{-[k(x-v)]^2} dx = \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} \frac{1}{k^3} y^2 e^{-(y-kv)^2} dy = \frac{1}{k^3}\left(\frac{1}{2} + k^2 v^2\right)$$

$$\frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} x^4 e^{-[k(x-v)]^2} dx = \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} \frac{1}{k^5} y^4 e^{-(y-kv)^2} dy = \frac{1}{k^5}\left(\frac{3}{4} + 3k^2v^2 + k^4v^4\right)$$

$$\frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} e^{-[k(x-v)]^2} dx = \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} \frac{1}{k} e^{-(y-kv)^2} dy = \frac{1}{k}$$

$$\Rightarrow E(k,v) = -\frac{\hbar^2}{2m}\left(\frac{1}{2} + k^2v^2 - k^2\right) - \frac{m\omega^2}{2}\frac{1}{k^2}\left(\frac{1}{2} + k^2v^2\right) + \frac{\lambda}{4}\frac{1}{k^4}\left(\frac{3}{4} + 3k^2v^2 + k^4v^4\right)$$

(2) To apply the variational principle we have to find the global minimum of the energy function E. Because E is continuously differentiable we are able to use the necessary condition $\nabla E(k_0, v_0) = 0$ (We assume extremal values do not lie on the boundary)

$$\partial_1 E(k,v) = -\frac{\hbar^2}{2m}\left(2kv^2 - 2k\right)$$

$$- \frac{m\omega^2}{2}\left[\frac{-2}{k^3}\left(\frac{1}{2} + k^2v^2\right) + \frac{1}{k^2}\left(2kv^2\right)\right]$$

$$+ \frac{\lambda}{4}\left[\frac{-4}{k^5}\left(\frac{3}{4} + 3k^2v^2 + k^4v^4\right) + \frac{1}{k^4}\left(6kv^2 + 4k^3v^4\right)\right]$$

$$\partial_2 E(k,v) = -\frac{\hbar^2}{2m}\, 2k^2 v$$

$$- \frac{m\omega^2}{2}\,\frac{1}{k^2}\, 2k^2 v$$

$$+ \frac{\lambda}{4}\,\frac{1}{k^4}\left(6k^2v + 4k^4v^3\right)$$