

## 5. gyakorlat (okt. 8)

### 1. Time-evolution pictures:

#### (a) Schrödinger-picture:

Wave functions are time-evolved by the Hamiltonian

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle \quad (1)$$

$$|\psi(t)\rangle = U(t, 0) |\psi(0)\rangle = U(t, 0) |\psi(0)\rangle = e^{-\frac{i}{\hbar} H t} |\psi(0)\rangle \quad (2)$$

where the time-evolution operator takes a simple form of  $\mathcal{T}e^{-\frac{i}{\hbar} \int_0^t dt' H(t')}$  in case of time-independent Hamiltonians.

#### (b) Heisenberg-picture:

Wave-function remains in its initial state and instead operators are "rotated"/time-evolved according to

$$|\psi^H(t)\rangle = U^\dagger(t, 0) |\psi(0)\rangle = |\psi(0)\rangle \quad (3)$$

$$A^H(t) = U^\dagger(t, 0) A U(t, 0) \quad (4)$$

$$\frac{dA^H(t)}{dt} = \frac{i}{\hbar} [H^H(t), A^H(t)] + \frac{\partial A^H(t)}{\partial t} \quad (5)$$

One can easily verify that so the time evolution of matrix elements of operators are unchanged!

$$\begin{aligned} \frac{d\langle A^H(t) \rangle}{dt} &= \langle \psi(t) | \frac{i}{\hbar} [H, A] + \partial_t A | \psi(t) \rangle = \langle \psi(0) | U^\dagger(t, 0) \frac{i}{\hbar} [H, A] U(t, 0) + \partial_t A^H(t) | \psi(0) \rangle \\ &= \langle \psi(0) | \frac{i}{\hbar} [H^H(t), A^H(t)] + \partial_t A^H(t) | \psi(0) \rangle \end{aligned} \quad (6)$$

#### (c) Interaction/Dirac-picture:

Now wave-functions are time-evolved only by the potential part of the Hamiltonian  $H(t) = H_0 + V(t)$ , while operators evolve in time with respect to the free Hamiltonian,  $H_0$  with the time-evolution operator,  $U(t, 0) = e^{-\frac{i}{\hbar} H_0 t}$ :

$$|\psi^D(t)\rangle = U^\dagger(t, 0) |\psi(0)\rangle \quad (7)$$

$$A^D(t) = U^\dagger(0, t) A U(t, 0) \quad (8)$$

$$i\hbar \frac{\partial}{\partial t} |\psi^D(t)\rangle = V^D(t) |\psi^D(t)\rangle \quad (9)$$

Similarly matrix-elements' time-evolution again remains unchanged in the Dirac-picture, as it should!

#### (d) Time-dependent perturbation theory:

Let us first approximate the time-ordered exponential up to first order in the perturbation operator in Dirac-picture, in  $V^D(t)$  and compute the wave- function up to first order in Dirac picture again:

$$U^D(t, 0) = \mathcal{T}e^{-\frac{i}{\hbar} \int_0^t dt' H(t')} \approx I - \frac{i}{\hbar} \int_0^t dt' V^D(t') = I - \frac{i}{\hbar} \int_0^t dt' e^{\frac{i}{\hbar} H_0 t'} V(t') e^{-\frac{i}{\hbar} H_0 t'} \quad (10)$$

$$|\psi^{D(1)}(t)\rangle = |\varphi\rangle - \frac{i}{\hbar} \int_0^t dt' e^{\frac{i}{\hbar} H_0 t'} V(t') e^{-\frac{i}{\hbar} H_0 t'} |\varphi\rangle \quad (11)$$

Now let us transform back to Schrödinger picture:

$$|\psi^{S(1)}(t)\rangle = e^{-\frac{i}{\hbar}H_0t}|\psi^{D(1)}(t)\rangle = e^{-\frac{i}{\hbar}H_0t}|\varphi\rangle - \frac{i}{\hbar}e^{-\frac{i}{\hbar}H_0t}\int_0^t dt' e^{\frac{i}{\hbar}H_0t'}V(t')e^{-\frac{i}{\hbar}H_0t'}|\varphi\rangle \quad (12)$$

Now let us choose  $|\varphi\rangle \equiv |k\rangle$  some eigenstate of  $H_0 = \sum_n \varepsilon_n |n\rangle\langle n|$  with  $\varepsilon_n$  being the eigenenergies and  $|n\rangle$  the eigenstates and with this we have  $e^{\pm\frac{i}{\hbar}H_0t} = \sum_n e^{\pm\frac{i}{\hbar}\varepsilon_n t}|n\rangle\langle n|$ , inserting the identity, as  $I = \sum_n |n\rangle\langle n|$

$$\begin{aligned} |\psi^{S(1)}(t)\rangle &= e^{-\frac{i}{\hbar}H_0t}|k\rangle - \frac{i}{\hbar}\sum_n e^{-\frac{i}{\hbar}H_0t}\int_0^t dt' e^{\frac{i}{\hbar}H_0t'}|n\rangle\langle n|V(t')e^{-\frac{i}{\hbar}H_0t'}|k\rangle \\ &= e^{-\frac{i}{\hbar}\varepsilon_k t}|k\rangle - \frac{i}{\hbar}\sum_n e^{-i\varepsilon_n t}|n\rangle\int_0^t dt' e^{\frac{i}{\hbar}\omega_{nk}t'}V_{nk}(t') \end{aligned} \quad (13)$$

with  $\omega_{nk} = \frac{\varepsilon_n - \varepsilon_k}{\hbar}$  and  $V_{nk}(t) = \langle n|V(t)|k\rangle$ . From this one can immediately read out the expansion coefficients:

$$|\psi^{S(1)}(t)\rangle = \sum_n c_n^{(1)}(t)e^{-\frac{i}{\hbar}\varepsilon_n t}|n\rangle \quad (14)$$

with the coefficients given thus by:

$$c_k^{(1)}(t) = 1 - \frac{i}{\hbar}\int_0^t dt' V_{kk}(t') \quad (15)$$

$$c_{n\neq k}^{(1)}(t) = -\frac{i}{\hbar}\int_0^t dt' e^{i\omega_{nk}t'}V_{nk}(t') \quad (16)$$

2. **Determine the mean displacement,  $\langle\psi(t)|x|\psi(t)\rangle$ , in case of a free particle moving in constant electric field using the Heisenberg picture description in case of an initial Gaussian wave-packet:**

$$H = \frac{p^2}{2m} - \mathcal{E}qx, \quad i\hbar\partial_t\psi = H\psi \quad (17)$$

Wave packet in electric field,  $\psi(0, x) = \frac{1}{\sqrt{x_0\sqrt{\pi}}}e^{-\frac{x^2}{2x_0^2}}$ . Knowing the solution of the eigenvalue equation  $H\varphi_n = E_n\varphi_n$  we can expand the wave-function started from the initial wave packet as:

$$\psi(t) = \sum_n c_n e^{-\frac{i}{\hbar}E_n t}\varphi_n, \quad c_n = \langle\varphi_n|\psi(0)\rangle \quad (18)$$

Let us introduce the length scale  $x_0 = \left(\frac{\hbar^2}{2m\mathcal{E}q}\right)^{\frac{1}{3}}$  with which we can write the Schrödinger equation as

$$\frac{d^2\psi}{d\xi^2} - \xi\psi = 0 \quad (19)$$

with  $\xi = \frac{x}{x_0} + \frac{E}{x_0\mathcal{E}q}$ . The solutions of this equation are the Airy functions,  $\psi = \text{Ai}\left(\frac{x}{x_0} + \frac{E}{x_0\mathcal{E}q}\right)$ . These solutions form a continuous basis, with continuously many eigenvalues, as there is no potential gap just a potential with constant slope, with infinitely many possible eigenenergies, or with other words no periodic orbits classically. So the time-dependent solution is given by the integral, i.e.: the summation over the continuously many energy eigenstates, reads

$$\psi(t, x) = \int_{-\infty}^{\infty} dE c(E)e^{-\frac{i}{\hbar}Et}\text{Ai}\left(\frac{x}{x_0} + \frac{E}{x_0\mathcal{E}q}\right) \quad (20)$$

with the expansion coefficients defined as:

$$c(E) = \int_{-\infty}^{\infty} dx \operatorname{Ai} \left( \frac{x}{x_0} + \frac{E}{x_0 \mathcal{E}q} \right) \frac{1}{\sqrt{x_0 \sqrt{\pi}}} e^{-\frac{x^2}{2x_0^2}} \quad (21)$$

Now we see that in terms of these complicated wave functions we can tell, in theory, in terms of horribly complicated integrals the average displacement,  $\langle \psi(t) | x | \psi(t) \rangle$ . Nevertheless we come around the problem by the Heisenberg time-evolution picture, considering the operators rather than the wave functions evolving in time, that is it is satisfactory only to consider the initial wave-packet and calculate the time-evolved/transformed operator with the time-evolution operator:

$$x(t) = e^{\frac{i}{\hbar} H t} x e^{-\frac{i}{\hbar} H t} \quad (22)$$

the expectation value of which in the initial state gives the same result as the "usual" coordinate operator with the time-evolved states, which in an operator language reads as  $|\psi(t)\rangle = e^{-\frac{i}{\hbar} H t} |\psi(0)\rangle$

$$\langle \psi(0) | e^{\frac{i}{\hbar} H t} x | e^{-\frac{i}{\hbar} H t} \psi(0) \rangle = \langle \psi(0) | e^{\frac{i}{\hbar} H t} x e^{-\frac{i}{\hbar} H t} | \psi(0) \rangle \quad (23)$$

Now the only thing to calculate is the transformed coordinate operator, then we only need to calculate a Gaussian integral with this transformed coordinate operator, which can be calculated via the Hausdorff expansion:

$$e^{\frac{i}{\hbar} H t} x e^{-\frac{i}{\hbar} H t} = x + \frac{i}{\hbar} [H, x] t + \left( \frac{i}{\hbar} \right)^2 [H, [H, x]] t^2 / 2 + \dots \quad (24)$$

Now fortunately the series terminates at the quadratic term as  $[H, x] = \frac{\hbar}{i} \frac{p}{m}$ ,  $[H, [H, x]] = \frac{\hbar}{im} [H, p] = \left( \frac{\hbar}{i} \right)^2 \frac{\mathcal{E}q}{m}$ , which is just a number, commuting with  $H$  and making vanish the fourth term!

So now we are in the position to evaluate the emerging integrals:

$$\langle \psi(0) | e^{\frac{i}{\hbar} H t} x e^{-\frac{i}{\hbar} H t} | \psi(0) \rangle = \frac{1}{x_0 \sqrt{\pi}} \int_{-\infty}^{\infty} dx e^{-\frac{x^2}{2x_0^2}} \left( x + \frac{p}{m} t + \frac{\mathcal{E}q}{2m} t^2 \right) e^{-\frac{x^2}{2x_0^2}} = \frac{\mathcal{E}q}{2m} t^2 \quad (25)$$

In fact we were facing a very easy case of Gaussian integrals as both  $\sim x e^{-\frac{x^2}{2x_0^2}}$  and  $\sim e^{-\frac{x^2}{2x_0^2}} \partial_x e^{-\frac{x^2}{2x_0^2}}$  are odd functions integrated over a symmetrical region, yielding zero.

### 3. Determine the ladder operators in Heisenberg picture for the one-dimensional harmonic oscillator and show that in coherent states the $\Delta x \Delta p$ product is a constant!

The Hamiltonian, as usual,  $H = \hbar\omega \left( a^\dagger a + \frac{1}{2} \right)$ , which being time-independent yields the  $e^{-\frac{i}{\hbar} H t}$  time-evolution operator. For this we make use of the usual commutation relations of the ladder operators,  $[a, a^\dagger] = 1 \rightarrow [H, a] = -\hbar\omega a$ ,  $[H, a^\dagger] = \hbar\omega a^\dagger$ , by which we can again conclude that the Hausdorff series goes as:

$$e^{-\frac{i}{\hbar} H t} a e^{\frac{i}{\hbar} H t} = a + \frac{i}{\hbar} (-\hbar\omega) a t + \left( \frac{i}{\hbar} \right)^2 \frac{(-\hbar\omega)^2}{2!} a t^2 + \dots = a e^{-i\omega t} \quad (26)$$

Similarly for  $a^\dagger$ :

$$e^{-\frac{i}{\hbar} H t} a e^{\frac{i}{\hbar} H t} = a^\dagger + \frac{i}{\hbar} (\hbar\omega) a^\dagger t + \left( \frac{i}{\hbar} \right)^2 \frac{(\hbar\omega)^2}{2!} a^\dagger t^2 + \dots = a^\dagger e^{i\omega t} \quad (27)$$

Coherent states: eigenstates of ladder operators:

$$a|\alpha\rangle = \alpha|\alpha\rangle \quad (28)$$

Now let us calculate the variances' time-evolution  $\langle \Delta x \rangle_\alpha^2 = \langle \alpha | x^2(t) | \alpha \rangle - \langle \alpha | x(t) | \alpha \rangle^2$  and  $\langle \Delta p \rangle_\alpha^2 = \langle \alpha | p^2(t) | \alpha \rangle - \langle \alpha | p(t) | \alpha \rangle^2$ , with  $x = \frac{x_0}{\sqrt{2}}(a + a^\dagger) \rightarrow x(t) = \frac{x_0}{\sqrt{2}}(ae^{-i\omega t} + a^\dagger e^{i\omega t})$ ,  $x_0 = \sqrt{\frac{\hbar}{m\omega}}$ ,  $p = i\frac{p_0}{\sqrt{2}}(a^\dagger - a) \rightarrow p(t) = i\frac{p_0}{\sqrt{2}}(a^\dagger e^{i\omega t} - ae^{-i\omega t})$ ,  $p_0 = \sqrt{m\hbar\omega}$

$$\begin{aligned} \langle \alpha | x(t) | \alpha \rangle^2 &= \frac{x_0^2}{2} \langle \alpha | (ae^{-i\omega t} + a^\dagger e^{i\omega t}) | \alpha \rangle^2 = 2x_0^2 \text{Re}(\alpha e^{-i\omega t})^2 \\ \langle \alpha | p(t) | \alpha \rangle^2 &= -\frac{p_0^2}{2} \langle \alpha | (a^\dagger e^{i\omega t} - ae^{-i\omega t}) | \alpha \rangle^2 = 2p_0^2 \text{Im}(\alpha e^{-i\omega t})^2 \\ \langle \alpha | x^2(t) | \alpha \rangle &= \frac{x_0^2}{2} \langle \alpha | 1 + 2a^\dagger a + a^2 e^{-2i\omega t} + (a^\dagger)^2 e^{2i\omega t} | \alpha \rangle = \frac{x_0^2}{2} (1 + 2|\alpha|^2 + 2\text{Re}(\alpha^2 e^{-i2\omega t})) \\ \langle \alpha | p^2(t) | \alpha \rangle &= -\frac{p_0^2}{2} \langle \alpha | -1 - 2a^\dagger a + a^2 e^{-2i\omega t} + (a^\dagger)^2 e^{2i\omega t} | \alpha \rangle = \frac{p_0^2}{2} (1 + 2|\alpha|^2 - 2\text{Re}(\alpha^2 e^{-i2\omega t})) \\ \langle \alpha | \delta x^2(t) | \alpha \rangle &= \langle \alpha | x^2(t) | \alpha \rangle - \langle \alpha | x(t) | \alpha \rangle^2 = \frac{x_0^2}{2} + x_0^2 (|\alpha|^2 + \text{Re}(\alpha^2 e^{-i2\omega t}) - 2\text{Re}(\alpha e^{-i\omega t})^2) \\ &= \frac{x_0^2}{2} + x_0^2 (|\alpha|^2 - \text{Re}(\alpha e^{-i\omega t})^2 - \text{Im}(\alpha e^{-i\omega t})^2) = \frac{x_0^2}{2} - x_0^2 (|\alpha|^2 - |\alpha e^{-i\omega t}|^2) = \frac{x_0^2}{2} \\ \langle \alpha | \delta p^2(t) | \alpha \rangle &= \langle \alpha | p^2(t) | \alpha \rangle - \langle \alpha | p(t) | \alpha \rangle^2 = \frac{p_0^2}{2} + p_0^2 (|\alpha|^2 - \text{Re}(\alpha^2 e^{-i2\omega t}) - 2\text{Im}(\alpha e^{-i\omega t})^2) \\ &= \frac{p_0^2}{2} + p_0^2 (|\alpha|^2 - \text{Im}(\alpha e^{-i\omega t})^2 - \text{Re}(\alpha e^{-i\omega t})^2) = \frac{p_0^2}{2} \end{aligned}$$

From where we can conclude that time-independently the product of the deviations reads as:

$$\langle \Delta x \rangle_\alpha \langle \Delta p \rangle_\alpha = \frac{x_0 p_0}{2} = \frac{\hbar}{2} \quad (29)$$

### Homework:

Consider the Hamiltonian of a particle moving in constant electric field:

$$H = \frac{p^2}{2m} - \mathcal{E}qx \quad (30)$$

Repeat the calculation of the 2. exercise but with a particle starting from a coherent state of a harmonic oscillator:

$$|\psi(0)\rangle = e^{-\frac{|\alpha|^2}{2} + \alpha a^\dagger} |0\rangle \quad (31)$$

with the usual relations,  $x = \frac{x_0}{\sqrt{2}}(a + a^\dagger)$ ,  $x_0 = \sqrt{\frac{\hbar}{m\omega}}$  and  $p = i\frac{p_0}{\sqrt{2}}(a^\dagger - a)$ ,  $p_0 = \sqrt{m\omega\hbar}$ . There are two ways to do that:

- First expand the exponent to get  $\psi(x, 0) = \sqrt{\frac{m\omega}{\hbar\sqrt{\pi}}} e^{-\frac{(x-\langle x \rangle)^2}{2x_0^2} + i\frac{\langle p \rangle x}{\hbar}}$  where  $\langle p \rangle = \sqrt{\frac{m\hbar\omega}{2}} \text{Re}\alpha$  in a coherent state with  $\alpha$  eigenvalue. And with this calculate the above integral (25) with  $x(t) = e^{\frac{i}{\hbar}Ht} x e^{-\frac{i}{\hbar}Ht}$  transformed into Heisenberg picture!
- Or in a more sophisticated way use our knowledge about the ladder operators in Heisenberg picture,  $a(t) = ae^{-i\omega t}$ ,  $a^\dagger(t) = a^\dagger e^{i\omega t}$ .

Hints: Use the Heisenberg picture form of  $x(t)$ , derived in the 2. exercise, and write it in terms of the ladder operators, then calculate the action of  $a$  and  $a^\dagger$  on a coherent state, as dictated by its definition.