the equations of motion we found that the commutation relation and the hermiticity conditions continue to hold at all times t. This is nontrivial but it is not a coincidence. As we will soon see, the quantum mechanical time evolution of all systems[7] preserves the commutation relations and hermiticity. The preservation of the commutation relations is of course the preservation of the Poisson bracket. And we have in classical and quantum mechanics that the Poisson brackets between the positions and momenta are preserved by the dynamics through the Hamilton equation: $d/dt\ \{\hat{x},\hat{p}\} = \{\{\hat{x},\hat{p}\},\hat{H}\} = \{1,\hat{H}\} = 0$. We can also turn the logic around. Assume we know nothing about Hamiltonians and about the dynamics of quantum systems. Except, we may want to assume that, whatever the time evolution is, it must preserve the Poisson algebra structure, i.e., we require that the Poisson brackets be conserved in time. The structure of the Poisson algebra then demands (we don't show this explicitly here) that the time evolution must be generated through an equation of the type of the Hamilton equation, by some generator which we may call H, and which we may then as well call the Hamiltonian.

3.4.5 Example: Solving the equations of motion for a harmonic oscillator with matrix-valued functions

The vibrational degree of freedom of a diatomic molecule such as HF, CO or HCl can be described as a harmonic oscillator (as long as the oscillations are small). Now let x stand for the deviation from the equilibrium distance between the two nuclei. This distance oscillates harmonically and is described by this effective Hamiltonian of the form of a harmonic oscillator:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 \tag{3.50}$$

The term "Effective Hamiltonian" expresses the fact that this Hamiltonian is not really the exact Hamiltonian but that it is a good approximation to the Hamiltonian in the regime of low energies (i.e., of small oscillations) that we are considering here. By the way, how do we know that the true Hamiltonian is not simply a harmonic oscillator? Easy: we know from experiments that diatomic molecules will, for example, split apart at sufficiently high temperatures, i.e., that they do not have infinite binding energy. A harmonic oscillator potential, however, just keeps going up faster with distance and therefore if you tried to pull apart the two particles in the diatomic molecule, they would just get pulled together more and more strongly. Diatomic molecules could never be split if they were truly harmonically bound.

So then if we know that the true potential is not harmonic, how do we know that a harmonic potential is a good approximation at low energies? That's because

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[7] With the possible exception of systems that involve black hole horizons or other gravitational horizons or singularities.

any potential $V(x)$ is normally well described by a smooth function $V(x)$ with a minimum at, say x_0, around which we can Taylor expand the potential: $V(x) = V(x_0) + V'(x_0)(x - x_0) + \frac{1}{2}V''(x_0)(x - x_0)^2 + ...$ Here, $V'(x_0) = 0$ because x_0 is assumed to be the minimum and therefore in the regime of small oscillations, where x is close to x_0, any potential starts out quadratic, i.e., as a harmonic oscillator.

Now let us remember that the matrix-valued functions $\hat{x}(t)$ and $\hat{p}(t)$ that we want to solve the harmonic oscillator problem Eq.3.50 have to obey three conditions, as always in quantum theory. First, the matrix-valued functions $\hat{x}(t)$ and $\hat{p}(t)$ must obey the equations of motion of the harmonic oscillator given in Eq.3.50. Second, they must be hermitean, $\hat{x}(t) = \hat{x}^\dagger(t)$ and $\hat{p}(t) = \hat{p}^\dagger(t)$. Third, they must obey the canonical commutation relation $[\hat{x}(t), \hat{p}(t)] = i\hbar 1$ (where 1 is now to be represented by the identity matrix).

Now the first problem would seem easy to solve: we know that the equations of motion are solved any linear combination of $\sin(\omega t)$ and $\cos(\omega t)$. But these are just number-valued functions and cannot by themselves obey the commutation relations! On the other hand, we do have matrices a and $a^\dagger$ that are beautifully noncommutative. But they are constant in time and therefore cannot alone describe the dynamics given by the equations of motion. This suggests that we try to construct the solution by combining the a and $a^\dagger$ matrices with the sine and cosine solutions. Let's try this ansatz[8]

$$\hat{x}(t) = \xi(t)a + \xi^*(t)a^\dagger, \tag{3.51}$$

and let us choose $\xi(t)$ to be a linear combination of the sine and cosine solutions to the equations of motion:

$$\xi(t) := r\sin(\omega t) + s\cos(\omega t) \tag{3.52}$$

Here, for now, r and s can be any complex numbers. By the way, whenever one makes an ansatz of this kind (and one often does, especially in quantum field theory), then $\xi(t)$ is called a mode function. The task now is to find out if we can find coefficients r and s such that the matrix-valued function $\hat{x}(t)$ and the corresponding $\hat{p}(t) = m\dot{\hat{x}}(t)$ obey the equations of motion, are hermitean and obey the canonical commutation relation.

Exercise 3.15 *Show that for any arbitrary choice of complex numbers r, s, the matrix-valued functions $\hat{x}(t)$ and $\hat{p}(t)$ defined through Eqs.3.51,3.52 obey the equations of motion at all time.*

Exercise 3.16 *Show that, again for any arbitrary choice of complex numbers r, s, the matrix-valued functions $\hat{x}(t)$ and $\hat{p}(t)$ defined through Eqs.3.51,3.52 obey the hermiticity conditions at all time.*

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[8] An ansatz is an educated guess.

Exercise 3.17 *Find the equation that the complex numbers* r, s *have to obey so that the matrix-valued functions* $\hat{x}(t)$ *and* $\hat{p}(t)$ *defined through Eqs.3.51,3.52 obey the canonical commutation relations at all time. This equation for* r, s *is called the Wronskian condition and it has many solutions. Give an example of a pair of complex numbers* r, s *that obey the Wronskian condition and write down* $\hat{x}(t)$ *explicitly with these values for* r, s *filled in.*

Since there are many pairs r, s that obey the Wronskian condition, our ansatz given by Eqs.3.51,3.52 allows us to generate many solutions! We knew that there are always many linear representations of $\hat{x}(t)$ and $\hat{p}(t)$ in quantum theory (and that they are all physically equivalent because they are all related by changes of bases). Here, with our ansatz we have found already infinitely many of these representations of $\hat{x}(t)$ and $\hat{p}(t)$ for the harmonic oscillator. Actually, among the representations that we just found, some representations are particularly convenient and most of the time one uses one of those. These choices of r, s turn out to be convenient because the matrix-representation of the Hamiltonian $\hat{H}(t)$ is much simpler for clever choices of r, s than for other choices.

Exercise 3.18 *Use Eqs.3.51,3.52 to express the Hamiltonian in terms of functions and the operators* $a, a^\dagger$. *There should be terms proportional to* a^2, *to* $(a^\dagger)^2, aa^\dagger$ *and* $a^\dagger a$.

Exercise 3.19 *It turns out that it is possible to choose the coefficients* r *and* s *so that the terms in the Hamiltonian which are proportional to* a^2 *and* $(a^\dagger)^2$ *drop out. Find the condition which the equation that* r *and* s *have to obey for this to happen. Choose a pair of complex numbers* r, s *such that the Hamiltonian simplifies this way, and of course such that the Wronskian condition is obeyed. Write down* $\hat{H}(t)$ *as an explicit matrix for this choice of* r, s. *It should be a diagonal matrix.*

Remark: Notice that this convenient choice of r, s depends on the parameters m and ω of the harmonic oscillator. This means that each harmonic oscillator has its own optimal choices of parameters r, s. Making such wise choices of the parameters r, s is particularly useful in quantum field theory where each wavevector (and therefore frequency ω) of a quantum field has its own harmonic oscillator degree of freedom, and should therefore best have its own convenient choice of r, s that diagonalizes its Hamiltonian.

3.4.6 From matrix-valued functions to number predictions

Let us assume now that we have solved a quantum mechanical problem in the sense that we have found explicit matrix-valued functions $\hat{x}_i^{(r)}(t)$ and $\hat{p}_j^{(j)}(t)$ which obey the canonical commutation relations, the hermiticity conditions, and the equations of motion. For example, the quantum mechanical problem of the free particle in one dimension is solved by the matrix-valued functions given in Eqs.3.48,3.49.