4.6: Quantum Dynamics- Three Pictures

So far in this chapter, I shied away from the discussion of the system's dynamics, implying that the bra- and ket-vectors were just their "snapshots" at a certain instant t. Now we are sufficiently prepared to examine their evolution in time. One of the most beautiful features of quantum mechanics is that this evolution may be described using either of three alternative "pictures", giving exactly the same final results for the expectation values of all observables.

From the standpoint of our wave-mechanics experience, the Schrödinger picture is the most natural one. In this picture, the operators corresponding to time-independent observables (e.g., to the Hamiltonian function H of an isolated system) are also constant in time, while the bra- and ket-vectors evolve in time as

$$\left\langle\alpha(t)\right|=\left\langle\alpha\left(t_0\right)\right|\hat{u}^{\dagger}\left(t, t_0\right), \quad\left|\alpha(t)\right\rangle=\hat{u}\left(t, t_0\right)\left|\alpha\left(t_0\right)\right\rangle . \tag{4.6.1}$$

Here $\hat{u}\left(t, t_0\right)$ is the time-evolution operator, which obeys the following differential equation:

$$i \hbar \frac{\partial}{\partial t} \hat{u}=\hat{H} \hat{u} \tag{4.6.2}$$

where $\hat{H}$ is the Hamiltonian operator of the system - which is always Hermitian: $\hat{H}^{\dagger}=\hat{H}$, and t_0 is the initial moment of time. (Note that Eqs. (157) remain valid even if the Hamiltonian depends on time explicitly.) Differentiating the second of Eqs. (157a) over time t, and then using Eq. (157b) twice, we can merge these two relations into a single equation, without explicit use of the time-evolution operator:

$$i \hbar \frac{\partial}{\partial t}|\alpha(t)\rangle=\hat{H}|\alpha(t)\rangle \tag{4.6.3}$$

which is frequently more convenient. (However, for some purposes the notion of the time-evolution operator, together with Eq. (157b), are useful - as we will see in a minute.) While Eq. (158) is a very natural generalization of the wave-mechanical equation (1.25), and is also frequently called the Schrödinger equation, [30] it still should be considered as a new, more general postulate, which finds its final justification (as it is usual in physics) in the agreement of its corollaries with experiment - more exactly, in the absence of a single credible contradiction to an experiment.Starting the discussion of Eq. (158), let us first consider the case of a time-independent Hamiltonian, whose eigenstates a_n and eigenvalues E_n obey Eq. (68) for this operator: [31]

$$\hat{H}\left|a_n\right\rangle=E_n\left|a_n\right\rangle, \tag{4.6.4}$$

and hence are also time-independent. (Similarly to the wavefunctions ψ_n defined by Eq. (1.60), a_n are called the stationary states of the system.) Let us use Eqs. (158)-(159) to calculate the law of time evolution of the expansion coefficients α_n (i.e. the probability amplitudes) defined by Eq. (118), in a stationary state basis, using Eq. (158):

$$\dot{\alpha}_n(t)=\frac{d}{d t}\left\langle a_n \mid \alpha(t)\right\rangle=\left\langle a_n\left|\frac{d}{d t}\right| \alpha(t)\right\rangle=\left\langle a_n\left|\frac{1}{i \hbar} \hat{H}\right| \alpha(t)\right\rangle=\frac{E_n}{i \hbar}\left\langle a_n \mid \alpha(t)\right\rangle=-\frac{i}{\hbar} E_n \alpha_n . \tag{4.6.5}$$

This is the same simple equation as Eq. (1.61), and its integration, with the initial moment t_0 taken for 0 , yields a similar result — cf. Eq. (1.62), just with the initial time t_0 rather than 0 :

$$\alpha_n(t)=\alpha_n\left(t_0\right) \exp \left\{-\frac{i}{\hbar} E_n t\right\} . \tag{4.6.6}$$

In order to illustrate how this result works, let us consider the dynamics of a spin- $1/2$ in a timeindependent, uniform external magnetic field $\mathscr{R}$. To construct the system's Hamiltonian, we may apply the correspondence principle to the classical expression for the energy of a magnetic moment $\mathbf{m}$ in the external magnetic field $\mathscr{R}, 32$

$$U=-\mathbf{m} \cdot \mathscr{R} . \tag{4.6.7}$$

In quantum mechanics, the operator corresponding to the moment $\mathbf{m}$ is given by Eq. (115) (suggested by W. Pauli), so that the spin-field interaction is described by the so-called Pauli Hamiltonian, which may be, due to Eqs. (116)-(117), represented in several equivalent forms:

$$\hat{H}=-\hat{\mathbf{m}} \cdot \mathscr{B} \equiv-\gamma \hat{\mathbf{S}} \cdot \mathscr{B} \equiv-\gamma \frac{\hbar}{2} \hat{\boldsymbol{\sigma}} \cdot \mathscr{B} . \tag{4.6.8}$$

If the z-axis is aligned with the field's direction, this expression is reduced to

$$\hat{H}=-\gamma\mathscr{B}\hat{S}_z\equiv-\gamma\mathscr{B}\frac{\hbar}{2}\hat{\sigma}_z. \tag{4.6.9}$$

According to Eq. (117), in the z-basis of the spin states $\uparrow$ and $\downarrow$, the matrix of the operator (163b) is

$$\mathrm{H}=-\frac{\hbar\mathscr{B}}{2}\sigma_z\equiv\frac{\hbar\Omega}{2}\sigma_z,\qquad \text{where }\Omega\equiv-\gamma\mathscr{B}. \tag{4.6.10}$$

The constant Ω so defined coincides with the classical frequency of the precession, about the z-axis, of an axially-symmetric rigid body (the so-called symmetric top), with an angular momentum $\mathbf{S}$ and the magnetic moment $\mathbf{m}=\gamma\mathbf{S}$, induced by the external torque $\tau=\mathbf{m}\times\mathscr{B}^{33}$ (For an electron, with its negative gyromagnetic ratio $\gamma_{\mathrm{e}}=-g_{\mathrm{e}}e/2m_{\mathrm{e}}$, neglecting the tiny difference of the g_{e}-factor from 2 , we get

$$\Omega=\frac{e}{m_{\mathrm{e}}}\mathscr{B}, \tag{4.6.11}$$

so that according to Eq. (3.48), the frequency Ω coincides with the electron's cyclotron frequency ω_{c}.)

In order to apply the general Eq. (161) to this case, we need to find the eigenstates a_n and eigenenergies E_n of our Hamiltonian. However, with our (smart :-) choice of the z-axis, the Hamiltonian matrix is already diagonal:

$$\mathrm{H}=\frac{\hbar\Omega}{2}\sigma_z\equiv\frac{\hbar\Omega}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}, \tag{4.6.12}$$

meaning that the states $\uparrow$ and $\downarrow$ are the eigenstates of this system, with the eigenenergies, respectively,

Spin -1⁄2 in magnetic field: eigenenergies

$$E_{\uparrow}=+\frac{\hbar\Omega}{2}\text{ and }E_{\downarrow}=-\frac{\hbar\Omega}{2}. \tag{4.6.13}$$

Note that their difference,

corresponds to the classical energy $2|m\mathscr{B}|$ of flipping a magnetic dipole with the moment's magnitude $m=\hbar/2$, oriented along the direction of the field $\mathscr{B}$. Note also that if the product $\gamma\mathscr{B}$ is positive, then Ω is negative, so that $E_{\uparrow}$ is negative, while $E_{\downarrow}$ is positive. This is in the agreement with the classical picture of a magnetic dipole $\mathbf{m}$ having negative potential energy when it is aligned with the external magnetic field $\mathscr{B}$ - see Eq. (162) again.

So, for the time evolution of the probability amplitudes of these states, Eq. (161) immediately yields the following expressions:

allowing a ready calculation of the time evolution of the expectation values of any observable. In particular, we can calculate the expectation value of S_z as a function of time by applying Eq. (130) to the (arbitrary) time moment t :

$$\langle S_z\rangle(t)=\frac{\hbar}{2}\left[\alpha_{\uparrow}(t)\alpha_{\uparrow}^*(t)-\alpha_{\downarrow}(t)\alpha_{\downarrow}^*(t)\right]=\frac{\hbar}{2}\left[\alpha_{\uparrow}(0)\alpha_{\uparrow}^*(0)-\alpha_{\downarrow}(0)\alpha_{\downarrow}^*(0)\right]=\langle S_z\rangle(0). \tag{4.6.14}$$

Thus the expectation value of the spin component parallel to the applied magnetic field remains constant in time, regardless of the initial state of the system. However, this is not true for the components perpendicular to the field. For example, Eq. (132), applied to the moment t, gives

$$\langle S_x\rangle(t)=\frac{\hbar}{2}\left[\alpha_{\uparrow}(t)\alpha_{\downarrow}^*(t)+\alpha_{\downarrow}(t)\alpha_{\uparrow}^*(t)\right]=\frac{\hbar}{2}\left[\alpha_{\uparrow}(0)\alpha_{\downarrow}^*(0)e^{-i\Omega t}+\alpha_{\downarrow}(0)\alpha_{\uparrow}^*(0)e^{+i\Omega t}\right]. \tag{4.6.15}$$

Clearly, this expression describes sinusoidal oscillations with frequency (164). The amplitude and the phase of these oscillations depend on initial conditions. Indeed, solving Eqs. (132)-(133) for the probability amplitude products, we get the following relations:

$$\hbar\alpha_{\downarrow}(t)\alpha_{\uparrow}^*(t)=\langle S_x\rangle(t)+i\langle S_y\rangle(t),\quad \hbar\alpha_{\uparrow}(t)\alpha_{\downarrow}^*(t)=\langle S_x\rangle(t)-i\langle S_y\rangle(t), \tag{4.6.16}$$

valid for any time t. Plugging their values for $t=0$ into Eq. (171), we get

$$\begin{aligned}\langle S_x\rangle(t)&=\frac{1}{2}[\langle S_x\rangle(0)+i\langle S_y\rangle(0)]e^{+i\Omega t}+\frac{1}{2}[\langle S_x\rangle(0)-i\langle S_y\rangle(0)]e^{-i\Omega t}\\&\equiv\langle S_x\rangle(0)\cos\Omega t-\langle S_y\rangle(0)\sin\Omega t\end{aligned}$$

An absolutely similar calculation using Eq. (133) gives

$$\langle S_y\rangle(t)=\langle S_y\rangle(0)\cos\Omega t+\langle S_x\rangle(0)\sin\Omega t. \tag{4.6.17}$$

These formulas show, for example, that if at moment $t=0$ the spin's state was $\uparrow$, i.e. $\langle S_x\rangle(0)=\langle S_y\rangle(0)=0$, then the oscillation amplitudes of the both "lateral" components of the spin vanish. On the other hand, if the spin was initially in the state $\rightarrow$, i.e. had the definite, largest possible value of S_x, equal to $\hbar/2$ (in classics, we would say "the spin- $1/2$ was oriented in the x-direction"), then both expectation values $\langle S_x\rangle$ and $\langle S_y\rangle$ oscillate in time [34] with this amplitude, and with the phase shift $\pi/2$ between them.

So, the quantum-mechanical results for the expectation values of the Cartesian components of spin- $1/2$ are indistinguishable from the classical results for the precession, with the frequency $\Omega=-\gamma\mathscr{B}$,[35] of a symmetric top with the angular momentum of magnitude $S=\hbar/2$, about the field's direction (our axis z), under the effect of an external torque $\tau=\mathbf{m}\times\mathscr{B}$ exerted by the field $\mathscr{B}$ on the magnetic moment $\mathbf{m}=\gamma\mathbf{S}$. Note, however, that the classical language does not describe the large quantum-mechanical uncertainties of the components, obeying Eqs. (156), which are absent in the classical picture - at least when it starts from a definite orientation of the angular momentum vector. Also, as we have seen in Sec. 3.5, the component L_z of the angular momentum at the orbital motion of particles is always a multiple of $\hbar$ - see, e.g., Eq. (3.139). As a result, the angular momentum of a spin-1/2 particle, with $S_z=\pm\hbar/2$, cannot be explained by any summation of orbital angular moments of its hypothetical components, i.e. by any internal rotation of the particle about its axis.

After this illustration, let us return to the discussion of the general Schrödinger equation (157b) and prove the following fascinating fact: it is possible to write the general solution of this operator equation. In the easiest case when the Hamiltonian is time-independent, this solution is an exact analog of Eq. (161),

$$\hat{u}(t,t_0)=\hat{u}(t_0,t_0)\exp\left\{-\frac{i}{\hbar}\hat{H}(t-t_0)\right\}=\exp\left\{-\frac{i}{\hbar}\hat{H}(t-t_0)\right\}. \tag{4.6.18}$$

To start its proof we should, first of all, understand what a function (in this particular case, the exponent) of an operator means. In the operator (and matrix) algebra, such nonlinear functions are defined by their Taylor expansions; in particular, Eq. (175) means that

$$\begin{aligned}\hat{u}(t,t_0)&=\hat{I}+\sum_{k=1}^{\infty}\frac{1}{k!}\left[-\frac{i}{\hbar}\hat{H}(t-t_0)\right]^k\\&\equiv\hat{I}+\frac{1}{1!}\left(-\frac{i}{\hbar}\right)\hat{H}(t-t_0)+\frac{1}{2!}\left(-\frac{i}{\hbar}\right)^2\hat{H}^2(t-t_0)^2+\frac{1}{3!}\left(-\frac{i}{\hbar}\right)^3\hat{H}^3(t-t_0)^3+\ldots\end{aligned}$$

where $\hat{H}^2\equiv\hat{H}\hat{H},\hat{H}^3\equiv\hat{H}\hat{H}\hat{H}$, etc. Working with such series of operator products is not as hard as one could imagine, due to their regular structure. For example, let us differentiate both sides of Eq. (176) over t, at constant t_0, at the last stage using this equality again - backward:

$$\begin{aligned}\frac{\partial}{\partial t}\hat{u}(t,t_0)&=\hat{0}+\frac{1}{1!}\left(-\frac{i}{\hbar}\right)\hat{H}+\frac{1}{2!}\left(-\frac{i}{\hbar}\right)^2\hat{H}^2 2(t-t_0)+\frac{1}{3!}\left(-\frac{i}{\hbar}\right)^2\hat{H}^3 3(t-t_0)^2+\ldots\\&\equiv\left(-\frac{i}{\hbar}\right)\hat{H}\left[\hat{I}+\frac{1}{1!}\left(-\frac{i}{\hbar}\right)\hat{H}(t-t_0)+\frac{1}{2!}\left(-\frac{i}{\hbar}\right)^2\hat{H}^2(t-t_0)^2\right]+\ldots\equiv-\frac{i}{\hbar}\hat{H}\hat{u}(t,t_0),\end{aligned}$$

so that the differential equation (158) is indeed satisfied. On the other hand, Eq. (175) also satisfies the initial condition

$$\hat{u}(t_0,t_0)=\hat{u}^{\dagger}(t_0,t_0)=\hat{I} \tag{4.6.19}$$

that immediately follows from the definition (157a) of the evolution operator. Thus, Eq. (175) indeed gives the (unique) solution for the time evolution operator - in the Schrödinger picture.

Now let us allow the operator $\hat{H}$ to be a function of time, but with the condition that its "values" (in fact, operators) at different instants commute with each other:

$$\left|\hat{H}(t'),\hat{H}(t'')\right|=0,\quad \text{for any } t',t''. \tag{4.6.20}$$

(An important non-trivial example of such a Hamiltonian is the time-dependent part of the Hamiltonian of a particle, due to the effect of a classical, time-dependent, but position-independent force $\mathbf{F}(t)$,

$$\hat{H}_F = -\mathbf{F}(t) \cdot \hat{\mathbf{r}}. \tag{4.6.21}$$

Indeed, the radius vector's operator $\hat{\mathbf{r}}$ does not depend explicitly on time and hence commutes with itself, as well as with the c-numbers $\mathbf{F}(t')$ and $\mathbf{F}(t'')$.) In this case, it is sufficient to replace, in all the above formulas, the product $\hat{H}(t-t_0)$ with the corresponding integral over time; in particular, Eq. (175) is generalized as

$$\hat{u}(t, t_0) = \exp\left\{-\frac{i}{\hbar}\int_{t_0}^{t} \hat{H}(t')\, dt'\right\}. \tag{4.6.22}$$

This replacement means that the first form of Eq. (176) should be replaced with

$$\hat{u}(t, t_0) = \hat{I} + \sum_{k=1}^{\infty} \frac{1}{k!}\left(-\frac{i}{\hbar}\right)^k \left(\int_{t_0}^{t} \hat{H}(t')\, dt'\right)^k \tag{4.6.23}$$

$$\equiv \hat{I} + \sum_{k=1}^{\infty} \frac{1}{k!}\left(-\frac{i}{\hbar}\right)^k \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \ldots \int_{t_0}^{t} dt_k \hat{H}(t_1)\, \hat{H}(t_2) \ldots \hat{H}(t_k). \tag{4.6.24}$$

The proof that Eq. (182) satisfies Eq. (158) is absolutely similar to the one carried out above.

We may now use Eq. (181) to show that the time-evolution operator remains unitary at any moment, even for a time-dependent Hamiltonian, if it satisfies Eq. (179). Indeed, Eq. (181) yields

$$\hat{u}(t, t_0)\, \hat{u}^{\dagger}(t, t_0) = \exp\left\{-\frac{i}{\hbar}\int_{t_0}^{t} \hat{H}(t')\, dt'\right\} \exp\left\{+\frac{i}{\hbar}\int_{t_0}^{t} \hat{H}(t'')\, dt''\right\} \tag{4.6.25}$$

Since each of these exponents may be represented with the Taylor series (182), and, thanks to Eq. (179), different components of these sums may be swapped at will, the expression (183) may be manipulated exactly as the product of c-number exponents, for example rewritten as

$$\hat{u}(t, t_0)\, \hat{u}^{\dagger}(t, t_0) = \exp\left\{-\frac{i}{\hbar}\left[\int_{t_0}^{t} \hat{H}(t')\, dt' - \int_{t_0}^{t} \hat{H}(t'')\, dt''\right]\right\} = \exp\{\hat{0}\} = \hat{I}\,. \tag{4.6.26}$$

This property ensures, in particular, that the system state's normalization does not depend on time:

$$\langle \alpha(t) \mid \alpha(t) \rangle = \left\langle \alpha(t_0) \left| \hat{u}^{\dagger}(t, t_0)\, \hat{u}(t, t_0) \right| \alpha(t_0) \right\rangle = \langle \alpha(t_0) \mid \alpha(t_0) \rangle\,. \tag{4.6.27}$$

The most difficult cases for the explicit solution of Eq. (158) are those where Eq. (179) is violated. [36] It may be proven that in these cases the integral limits in the last form of Eq. (182) should be truncated, giving the so-called Dyson series

$$\hat{u}(t, t_0) = \hat{I} + \sum_{k=1}^{\infty} \frac{1}{k!}\left(-\frac{i}{\hbar}\right)^k \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_k-1} dt_k \hat{H}(t_1)\, \hat{H}(t_2) \ldots \hat{H}(t_k) \tag{4.6.28}$$

Since we would not have time/space to use this relation in our course, I will skip its proof. [37]

Let me now return to the general discussion of quantum dynamics to outline its alternative, Heisenberg picture. For its introduction, let us recall that according to Eq. (125), in quantum mechanics the expectation value of any observable A is a long bracket. Let us explore an even more general form of such bracket:

$$\langle \alpha | \hat{A} | \beta \rangle. \tag{4.6.29}$$

(In some applications, the states α and β may be different.) As was discussed above, in the Schrödinger picture the bra- and ket-vectors of the states evolve in time, while the operators of observables remain time-independent (if they do not explicitly depend on time), so that Eq. (187), applied to a moment t, may be represented as

$$\left\langle \alpha(t) \left| \hat{A}_{\mathrm{S}} \right| \beta(t) \right\rangle, \tag{4.6.30}$$

where the index " S " is added to emphasize the Schrödinger picture. Let us apply the evolution law (157a) to the bra- and ket-vectors in this expression:

$$\left\langle \alpha(t) \left| \hat{A}_{\mathrm{S}} \right| \beta(t) \right\rangle = \left\langle \alpha(t_0) \left| \hat{u}^{\dagger}(t, t_0)\, \hat{A}_{\mathrm{S}} \hat{u}(t, t_0) \right| \beta(t_0) \right\rangle. \tag{4.6.31}$$

This equality means that if we form a long bracket with bra- and ket-vectors of the initial-time states, together with the following time-dependent Heisenberg operator [38]

$$\hat{A}_{\mathrm{H}}(t) \equiv \hat{u}^{\dagger}\left(t, t_0\right) \hat{A}_{\mathrm{S}} \hat{u}\left(t, t_0\right)=\hat{u}^{\dagger}\left(t, t_0\right) \hat{A}_{\mathrm{H}}\left(t_0\right) \hat{u}\left(t, t_0\right), \tag{4.6.32}$$

all experimentally measurable results will remain the same as in the Schrödinger picture:

$$\langle\alpha(t)|\hat{A}| \beta(t)\rangle=\left\langle\alpha\left(t_0\right)\left|\hat{A}_{\mathrm{H}}\left(t, t_0\right)\right| \beta\left(t_0\right)\right\rangle .$$

$$i \hbar \frac{\partial}{\partial t}\begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix}=\frac{\hbar \Omega}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix} \equiv \frac{\hbar \Omega}{2}\begin{pmatrix} u_{11} & u_{12} \\ -u_{21} & -u_{22} \end{pmatrix} .$$

For full clarity, let us see how does the Heisenberg picture work for the same simple (but very important!) problem of the spin- $1/2$ precession in a z-oriented magnetic field, described (in the z-basis) by the Hamiltonian matrix (164). In that basis, Eq. (157b) for the time-evolution operator becomes

We see that in this simple case the differential equations for different matrix elements of the evolution operator matrix are decoupled, and readily solvable, using the universal initial conditions (178): [39]

$$\mathrm{u}(t, 0)=\begin{pmatrix} e^{-i \Omega t / 2} & 0 \\ 0 & e^{i \Omega t / 2} \end{pmatrix} \equiv \mathrm{I} \cos \frac{\Omega t}{2}-i \sigma_z \sin \frac{\Omega t}{2} . \tag{4.6.33}$$

Now let us use them in Eq. (190) to calculate the Heisenberg-picture operators of spin components - still in the z-basis. Dropping the index " H " for the notation brevity (the Heisenbergpicture operators are clearly marked by their dependence on time anyway), we get

$$\begin{aligned} \mathrm{S}_x(t) & =\mathrm{u}^{\dagger}(t, 0) \mathrm{S}_x(0) \mathrm{u}(t, 0)=\frac{\hbar}{2} \mathrm{u}^{\dagger}(t, 0) \sigma_x \mathrm{u}(t, 0) \\ & =\frac{\hbar}{2}\begin{pmatrix} e^{i \Omega t / 2} & 0 \\ 0 & e^{-i \Omega t / 2} \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} e^{-i \Omega t / 2} & 0 \\ 0 & e^{i \Omega t / 2} \end{pmatrix} \\ & =\frac{\hbar}{2}\begin{pmatrix} 0 & e^{i \Omega t} \\ e^{-i \Omega t} & 0 \end{pmatrix}=\frac{\hbar}{2}\left(\sigma_x \cos \Omega t-\sigma_y \sin \Omega t\right) \equiv \mathrm{S}_x(0) \cos \Omega t-\mathrm{S}_y(0) \sin \Omega t . \end{aligned}$$

Absolutely similar calculations of the other spin components yield

$$\begin{gathered} \mathrm{S}_y(t)=\frac{\hbar}{2}\begin{pmatrix} 0 & -i e^{i \Omega t} \\ i e^{-i \Omega t} & 0 \end{pmatrix}=\frac{\hbar}{2}\left(\sigma_y \cos \Omega t+\sigma_x \sin \Omega t\right) \equiv \mathrm{S}_y(0) \cos \Omega t+\mathrm{S}_x(0) \sin \Omega t, \\ \mathrm{S}_z(t)=\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}=\frac{\hbar}{2} \sigma_z=S_z(0) . \end{gathered}$$

One practical advantage of these formulas is that they describe the system's evolution for arbitrary initial conditions, thus making the analysis of initial state effects very simple. Indeed, since in the Heisenberg picture the expectation values of observables are calculated using Eq. (191) (with $\beta=\alpha$), with time-independent bra- and ket-vectors, such averaging of Eqs. (194)-(196) immediately returns us to Eqs. (170), (173), and (174), which were obtained above in the Schrödinger picture. Moreover, these equations for the Heisenberg operators formally coincide with the classical equations of the torqueinduced precession for c-number variables. (Below we will see that the same exact correspondence is valid for the Heisenberg picture of the orbital motion.)

In order to see that the last fact is by no means a coincidence, let us combine Eqs. (157b) and (190) to form an explicit differential equation of the Heisenberg operator's evolution. For that, let us differentiate Eq. (190) over time:

$$\frac{d}{d t} \hat{A}_{\mathrm{H}}=\frac{\partial \hat{u}^{\dagger}}{\partial t} \hat{A}_{\mathrm{S}} \hat{u}+\hat{u}^{\dagger} \frac{\partial \hat{A}_{\mathrm{S}}}{\partial t} \hat{u}+\hat{u}^{\dagger} \hat{A}_{\mathrm{S}} \frac{\partial \hat{u}}{\partial t} . \tag{4.6.34}$$

Plugging in the derivatives of the time evolution operator from Eq. (157b) and its Hermitian conjugate, and multiplying both sides of the equation by $i \hbar$, we get

$$i \hbar \frac{d}{d t} \hat{A}_{\mathrm{H}}=-\hat{u}^{\dagger} \hat{H} \hat{A}_{\mathrm{S}} \hat{u}+i \hbar \hat{u}^{\dagger} \frac{\partial \hat{A}_{\mathrm{S}}}{\partial t} \hat{u}+\hat{u}^{\dagger} \hat{A}_{\mathrm{S}} \hat{H} \hat{u} \tag{4.6.35}$$

If for the Schrödinger-picture's Hamiltonian the condition similar to Eq. (179) is satisfied, then, according to Eqs. (177) or (182), the Hamiltonian commutes with the time evolution operator and its Hermitian conjugate, and may be swapped with any of them. [40] Hence, we may rewrite Eq. (198a) as

$$i\hbar\frac{d}{dt}\hat{A}_{\mathrm{H}}=-\hat{H}\hat{u}^{\dagger}\hat{A}_{\mathrm{S}}\hat{u}+i\hbar\hat{u}^{\dagger}\frac{\partial\hat{A}_{\mathrm{S}}}{\partial t}\hat{u}+\hat{u}^{\dagger}\hat{A}_{\mathrm{S}}\hat{u}\hat{H}\equiv i\hbar\hat{u}^{\dagger}\frac{\partial\hat{A}_{\mathrm{S}}}{\partial t}\hat{u}+\left[\hat{u}^{\dagger}\hat{A}_{\mathrm{S}}\hat{u},\hat{H}\right]. \tag{4.6.36}$$

Now using the definition (190) again, for both terms on the right-hand side, we may write

$$i\hbar\frac{d}{dt}\hat{A}_{\mathrm{H}}=i\hbar\left(\frac{\partial\hat{A}}{\partial t}\right)_{\mathrm{H}}+\left[\hat{A}_{\mathrm{H}},\hat{H}\right]. \tag{4.6.37}$$

This is the so-called Heisenberg equation of motion.

Let us see how this equation looks for the same problem of the spin- $1/2$ precession in a z-oriented, time-independent magnetic field, described in the z-basis by the Hamiltonian matrix (164), which does not depend on time. In this basis, Eq. (199) for the vector operator of spin reads [41]

$$i\hbar\begin{pmatrix}\dot{\mathbf{S}}_{11} & \dot{\mathbf{S}}_{12}\\ \dot{\mathbf{S}}_{21} & \dot{\mathbf{S}}_{22}\end{pmatrix}=\frac{\hbar\Omega}{2}\left[\begin{pmatrix}\mathbf{S}_{11} & \mathbf{S}_{12}\\ \mathbf{S}_{21} & \mathbf{S}_{22}\end{pmatrix},\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right]=\hbar\Omega\begin{pmatrix}0 & -\mathbf{S}_{12}\\ \mathbf{S}_{21} & 0\end{pmatrix} \tag{4.6.38}$$

Once again, the equations for different matrix elements are decoupled, and their solution is elementary:

$$\begin{array}{ll}\mathbf{S}_{11}(t)=\mathbf{S}_{11}(0)=\text{const}, & \mathbf{S}_{22}(t)=\mathbf{S}_{22}(0)=\text{const},\\ \mathbf{S}_{12}(t)=\mathbf{S}_{12}(0)e^{+i\Omega t}, & \mathbf{S}_{21}(t)=\mathbf{S}_{21}(0)e^{-i\Omega t}.\end{array} \tag{4.6.39}$$

According to Eq. (190), the initial values of the Heisenberg-picture matrix elements are just the Schrödinger-picture ones, so that using Eq. (117) we may rewrite this solution in either of two forms:

$$\begin{aligned}\mathbf{S}(t)&=\frac{\hbar}{2}\left[\mathbf{n}_x\begin{pmatrix}0 & e^{+i\Omega t}\\ e^{-i\Omega t} & 0\end{pmatrix}+\mathbf{n}_y\begin{pmatrix}0 & -ie^{+i\Omega t}\\ ie^{-i\Omega t} & 0\end{pmatrix}+\mathbf{n}_z\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right]\\ &\equiv\frac{\hbar}{2}\begin{pmatrix}\mathbf{n}_z & \mathbf{n}_-e^{+i\Omega t}\\ \mathbf{n}_+e^{-i\Omega t} & -\mathbf{n}_z\end{pmatrix},\quad\text{where }\mathbf{n}_\pm\equiv\mathbf{n}_x\pm i\mathbf{n}_y.\end{aligned}$$

The simplicity of the last expression is spectacular. (Remember, it covers any initial conditions and all three spatial components of spin!) On the other hand, for some purposes the previous form may be more convenient; in particular, its Cartesian components give our earlier results (194)-(196). [42]

One of the advantages of the Heisenberg picture is that it provides a more clear link between classical and quantum mechanics, found by P. Dirac. Indeed, analytical classical mechanics may be used to derive the following equation of time evolution of an arbitrary function $A\left(q_j,p_j,t\right)$ of the generalized coordinates q_j and momenta p_j of the system, and time t : [43]

$$\frac{dA}{dt}=\frac{\partial A}{\partial t}-\{A,H\}_{\mathrm{P}}, \tag{4.6.40}$$

where H is the classical Hamiltonian function of the system, and $\{\ldots\ldots\}$ is the so-called Poisson bracket defined, for two arbitrary functions $A\left(q_j,p_j,t\right)$ and $B\left(q_j,p_j,t\right)$, as

$$\{A,B\}_{\mathrm{P}}\equiv\sum_j\left(\frac{\partial A}{\partial p_j}\frac{\partial B}{\partial q_j}-\frac{\partial A}{\partial q_j}\frac{\partial B}{\partial p_j}\right). \tag{4.6.41}$$

Comparing Eq. (203) with Eq. (199), we see that the correspondence between the classical and quantum mechanics (in the Heisenberg picture) is provided by the following symbolic relation

$$\{A,B\}_{\mathrm{P}}\leftrightarrow\frac{i}{\hbar}[\hat{A},\hat{B}]. \tag{4.6.42}$$

This relation may be used, in particular, for finding appropriate operators for the system's observables, if their form is not immediately evident from the correspondence principle.

Finally, let us discuss one more alternative picture of quantum dynamics. It is also attributed to Dirac, and is called either the "Dirac picture", or (more frequently) the interaction picture. The last name stems from the fact that this picture is very useful for the perturbative (approximate) approaches to systems whose Hamiltonians may be partitioned into two parts,

$$\hat{H}=\hat{H}_0+\hat{H}_{\text{int}}\ , \tag{4.6.43}$$

where $\hat{H}_0$ is the sum of relatively simple Hamiltonians of the component subsystems, while the second term in Eq. (206) represents their weak interaction. (Note, however, that all relations in the balance of this section are exact and not directly based on the interaction weakness.) In this case, it is natural to consider, together with the full operator $\hat{u}\left(t, t_0\right)$ of the system's evolution, which obeys Eq. (157b), a similarly defined unitary operator $\hat{u}_0\left(t, t_0\right)$ of evolution of the "unperturbed system" described by the Hamiltonian $\hat{H}_0$ alone:

$$i\hbar\frac{\partial}{\partial t}\hat{u}_0=\hat{H}_0\hat{u}_0, \tag{4.6.44}$$

and also the following interaction evolution operator,

$$\hat{u}_{\text{I}}\equiv\hat{u}_0^{\dagger}\hat{u} \tag{4.6.45}$$

The motivation for these definitions become more clear if we insert the reciprocal relation,

$$\hat{u}\equiv\hat{u}_0\hat{u}_0^{\dagger}\hat{u}=\hat{u}_0\hat{u}_{\text{I}}, \tag{4.6.46}$$

and its Hermitian conjugate,

$$\hat{u}^{\dagger}=\left(\hat{u}_0\hat{u}_{\text{I}}\right)^{\dagger}=\hat{u}_{\text{I}}^{\dagger}\hat{u}_0^{\dagger}, \tag{4.6.47}$$

into the basic Eq. (189):

$$\begin{aligned}\langle\alpha|\hat{A}|\beta\rangle &=\left\langle\alpha\left(t_0\right)\left|\hat{u}^{\dagger}\left(t, t_0\right)\hat{A}_{\text{S}}\hat{u}\left(t, t_0\right)\right|\beta\left(t_0\right)\right\rangle\\ &=\left\langle\alpha\left(t_0\right)\left|\hat{u}_{\text{I}}^{\dagger}\left(t, t_0\right)\hat{u}_0^{\dagger}\left(t, t_0\right)\hat{A}_{\text{s}}\hat{u}_0\left(t, t_0\right)\hat{u}_{\text{I}}\left(t, t_0\right)\right|\beta\left(t_0\right)\right\rangle .\end{aligned}$$

This relation shows that any long bracket (187), i.e. any experimentally verifiable result of quantum mechanics, may be expressed as

$$\langle\alpha|\hat{A}|\beta\rangle=\left\langle\alpha_{\text{I}}(t)\left|\hat{A}_{\text{I}}(t)\right|\beta_{\text{I}}(t)\right\rangle, \tag{4.6.48}$$

if we assume that both the state vectors and the operators depend on time, with the vectors evolving only due to the interaction operator $\hat{u}_{\text{I}}$,

$$\left\langle\alpha_1(t)\right|\equiv\left\langle\alpha\left(t_0\right)\right|\hat{u}_1^{\dagger}\left(t, t_0\right), \quad\left|\beta_1(t)\right\rangle\equiv\hat{u}_1\left(t, t_0\right)\left|\beta\left(t_0\right)\right\rangle, \tag{4.6.49}$$

while the operators' evolution being governed by the unperturbed operator $\hat{u}_0$:

$$\hat{A}_{\text{I}}(t)\equiv\hat{u}_0^{\dagger}\left(t, t_0\right)\hat{A}_{\text{S}}\hat{u}_0\left(t, t_0\right). \tag{4.6.50}$$

These relations describe the interaction picture of quantum dynamics. Let me defer an example of its use until the perturbative analysis of open quantum systems in Sec. 7.6, and end this section with a proof that the interaction evolution operator (208) satisfies the following natural equation,

$$i\hbar\frac{\partial}{\partial t}\hat{u}_1=\hat{H}_1\hat{u}_1, \tag{4.6.51}$$

where $\hat{H}_{\text{I}}$ is the interaction Hamiltonian formed from $\hat{H}_{\text{int}}$ in accordance with the same rule (214):

$$\hat{H}_{\text{I}}(t)\equiv\hat{u}_0^{\dagger}\left(t, t_0\right)\hat{H}_{\text{int}}\hat{u}_0\left(t, t_0\right) \tag{4.6.52}$$

The proof is very straightforward: first using the definition (208), and then Eqs. (157b) and the Hermitian conjugate of Eq. (207), we may write

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\hat{u}_1 &\equiv i\hbar\frac{\partial}{\partial t}\left(\hat{u}_0^\dagger\hat{u}\right) \equiv i\hbar\frac{\partial\hat{u}_0^\dagger}{\partial t}\hat{u}+\hat{u}_0^\dagger i\hbar\frac{\partial\hat{u}}{\partial t} = -\hat{H}_0\hat{u}_0^\dagger\hat{u}+\hat{u}_0^\dagger\hat{H}\hat{u} = -\hat{H}_0\hat{u}_0^\dagger\hat{u}+\hat{u}_0^\dagger\left(\hat{H}_0+\hat{H}_{\text{int}}\right)\hat{u} \\
&\equiv -\hat{H}_0\hat{u}_0^\dagger\hat{u}+\hat{u}_0^\dagger\hat{H}_0\hat{u}+\hat{u}_0^\dagger\hat{H}_{\text{int}}\,\hat{u} \equiv \left(-\hat{H}_0\hat{u}_0^\dagger+\hat{u}_0^\dagger\hat{H}_0\right)\hat{u}+\hat{u}_0^\dagger\hat{H}_{\text{int}}\,\hat{u}.
\end{aligned}
$$

Since $\hat{u}_0^\dagger$ may be represented as an integral of an exponent of $\hat{H}_0$ over time (similar to Eq. (181) relating $\hat{u}$ and $\hat{H}$), these operators commute, so that the parentheses in the last form of Eq. (217) vanish. Now plugging $\hat{u}$ from the last form of Eq. (209), we get the equation,

$$
i\hbar\frac{\partial}{\partial t}\hat{u}_{\text{I}} = \hat{u}_0^\dagger\hat{H}_{\text{int}}\hat{u}_0 u_{\text{I}} \equiv \left(\hat{u}_0^\dagger\hat{H}_{\text{int}}\hat{u}_0\right)\hat{u}_{\text{I}}, \tag{4.6.53}
$$

which is clearly equivalent to the combination of Eqs. (215) and (216).

As Eq. (215) shows, if the energy scale of the interaction H_{int} is much smaller than that of the background Hamiltonian H_0, the interaction evolution operators $\hat{u}_1$ and $\hat{u}_1^\dagger$, and hence the state vectors (213) evolve relatively slowly, without fast background oscillations. This is very convenient for the perturbative approaches to complex interacting systems, in particular to the "open" quantum systems that weakly interact with their environment $-$ see Sec. 7.6.

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[30] Moreover, we will be able to derive Eq. (1.25) from Eq. (158) - see below.

[31] I have switched the state index notation from j to n, which was used for numbering stationary states in Chapter 1 , to emphasize the special role played by the stationary states a_n in quantum dynamics.

[32] See, e.g., EM Eq. (5.100). As a reminder, we have already used this expression for the derivation of Eq. (3).

[33] See, e.g., CM Sec. 4.5, in particular Eq. (4.72), and EM Sec. 5.5, in particular Eq. (5.114) and its discussion.

[34] This is one more (hopefully, redundant :-) illustration of the difference between the averaging over the statistical ensemble and that over time: in Eqs. (170), (173)-(174), and also in quite a few relations below, only the former averaging has been performed, so the results are still functions of time.

[35] Note that according to this relation, the gyromagnetic ratio γ may be interpreted just as the angular frequency of the spin precession per unit magnetic field - hence the name. In particular, for electrons, $|\gamma_{\text{e}}| \approx 1.761\times10^{11}\ \text{s}^{-1}\ \text{T}^{-\ 1}$; for protons, the ratio is much smaller, $\gamma_{\text{p}} \equiv g_{\text{p}}e/2m_{\text{p}} \approx 2.675\times10^{8}\ \text{s}^{-1}\ \text{T}^{-1}$, mostly because of their larger mass m_{p}, at a g-factor of the same order as for the electron: $g_{\text{p}} \approx 5.586$. For heavier spin-1/2 particles, e.g., atomic nuclei with such spin, the values of γ are correspondingly smaller - e.g., $\gamma \approx 8.681\times10^{6}\ \text{s}^{-1}\ \text{T}^{-1}$ for the ^{57}Fe nucleus.

[36] We will run into such situations in Chapter 7 , but will not need to apply Eq. (186) there.

[37] It may be found, for example, in Chapter 5 of J. Sakurai's textbook - see References.

[38] Note that this strict relation is similar in structure to the first of the symbolic Eqs. (94), with the state bases $\{v\}$ and $\{u\}$ loosely associated with the time moments, respectively, t and t_0.

[39] We could of course use this solution, together with Eq. (157), to obtain all the above results for this system within the Schrödinger picture. In our simple case, the use of Eqs. (161) for this purpose was more straightforward, but in some cases, e.g., for some time-dependent Hamiltonians, an explicit calculation of the time-evolution matrix may be the best (or even only practicable) way to proceed.

[40] Due to the same reason, $\hat{H}_{\text{H}} \equiv \hat{u}^\dagger\hat{H}_{\text{s}}\hat{u} = \hat{u}^\dagger\hat{u}\hat{H}_{\text{S}} = \hat{H}_{\text{s}};$ this is why the Hamiltonian operator's index may be dropped in Eqs. (198)-(199).

[41] Using the commutation relations (155), this equation may be readily generalized to the case of an arbitrary magnetic field $\mathscr{B}(t)$ and an arbitrary state basis - the exercise highly recommended to the reader.

[42] Note that the "values" of the same Heisenberg operator at different moments of time may or may not commute. For example, consider a free 1D particle, with the time-independent Hamiltonian $\hat{H} = \hat{p}^2/2m$. In this case, Eq. (199) yields the following equations: $i\hbar\dot{\hat{x}} = [\hat{x},\hat{H}] = i\hbar\hat{p}/m$ and $i\hbar\dot{\hat{p}} = [\hat{p},\hat{H}] = 0$, with simple solutions (similar to those for the classical motion): $\hat{p}(t) = \text{const} = \hat{p}(0)$ and $\hat{x}(t) = \hat{x}(0)+\hat{p}(0)t/m$, so that $[\hat{x}(0),\hat{x}(t)] = [\hat{x}(0),\hat{p}(0)]t/m \equiv [\hat{x}_{\text{s}},\hat{p}_{\text{s}}]\,t/m = i\hbar t/m \neq 0$, for $t \neq 0$.

[43] See, e.g., CM Eq. (10.17). The notation there does not use the subscript "P" that is employed in Eqs. (203)(205) to distinguish the classical Poisson bracket (204) from the quantum anticommutator (34).