Fundamentals of Quantum Technology
Week 4: An Atom in a Classical Field

Recommended literature: Gerry, Knight (ch. 4.1, 4.2, 4.4; Appendix A.2)

1 Atom-field Hamiltonian

We consider an electron bound by an atomic potential that interacts with a classical driving field. Following a convenient gauge choice as well as the employment of the dipole approximation $\mathbf{A}(\mathbf{r},t) \approx \mathbf{A}(t)$, the effective Hamiltonian turns out to be

$$H' = H_0 + H_1,$$

where

$$H_0 = \frac{\mathbf{P}^2}{2m} + V(r)$$

is the atomic Hamiltonian, and the interaction Hamiltonian is given by

$$H_1 = e\mathbf{r}\cdot\mathbf{E}(t) \equiv -\mathbf{d}\cdot\mathbf{E}(t).$$

Here $\mathbf{d} = -e\mathbf{r}$ is the **dipole operator**. We focus on the case of a single-mode field, $\mathbf{E}(t) = \mathbf{E}_0\cos(\omega t)$. The effect of H_1 can be treated using perturbation theory, but in class you saw that such a treatment has considerable limitations.

2 The semiclassical Rabi model

The semiclassical Rabi model allows to solve this problem in a *nonperturbative* manner, by discarding all electronic energy levels other than the ground state $|g\rangle$ and a single excited state $|e\rangle$, which is separated from the ground state by an energy gap $E_e - E_g \equiv \hbar\omega_0$ such that $\omega_0 \approx \omega$ (*near resonance*). The restriction to two energy levels allows us to write the Hamiltonian as an operator on a 2D Hilbert space:

$$H = \frac{\hbar\omega_0}{2}\sigma_z + (\mathcal{V}\sigma_+ + \mathcal{V}^*\sigma_-)\cos(\omega t) = \begin{pmatrix} \frac{\hbar\omega_0}{2} & \mathcal{V}\cos(\omega t) \\ \mathcal{V}^*\cos(\omega t) & -\frac{\hbar\omega_0}{2} \end{pmatrix},$$

where $\mathcal{V} = -\langle e|\,\mathbf{d}\cdot\mathbf{E}_0\,|g\rangle$. A useful way to solve the dynamics of $|\psi(t)\rangle$ under such a Hamiltonian – where one part of it is diagonal in a known basis while the rest is not – is by moving to the **interaction picture**. We apply a unitary transformation to $|\psi(t)\rangle$, namely we define

$$|\psi_I(t)\rangle = e^{iH_0 t/\hbar}\,|\psi(t)\rangle,$$

where $H_0 \equiv \frac{\hbar\omega_0}{2}\sigma_z$. The state $|\psi_I\rangle$ evolves according to a Schrödinger equation that includes only $H - H_0$, transformed into the interaction picture,

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi_I(t)\rangle = e^{iH_0 t/\hbar}(H - H_0)\,e^{-iH_0 t/\hbar}\,|\psi_I(t)\rangle \equiv H_I\,|\psi_I(t)\rangle.$$

In a matrix representation,

$$\begin{aligned} H_I &= \begin{pmatrix} e^{i\omega_0 t/2} & 0 \\ 0 & e^{-i\omega_0 t/2} \end{pmatrix} \begin{pmatrix} 0 & \mathcal{V}\cos(\omega t) \\ \mathcal{V}^*\cos(\omega t) & 0 \end{pmatrix} \begin{pmatrix} e^{-i\omega_0 t/2} & 0 \\ 0 & e^{i\omega_0 t/2} \end{pmatrix} \\ &= \begin{pmatrix} 0 & \mathcal{V}\cos(\omega t)\, e^{i\omega_0 t} \\ \mathcal{V}^*\cos(\omega t)\, e^{-i\omega_0 t} & 0 \end{pmatrix} \\ &\approx \frac{1}{2}\begin{pmatrix} 0 & \mathcal{V}e^{i(\omega_0-\omega)t} \\ \mathcal{V}^* e^{-i(\omega_0-\omega)t} & 0 \end{pmatrix}, \end{aligned}$$

where in the last step we employed the **rotating wave approximation** (RWA).

Exercise

Within the interaction picture, write the equation of motion for the density operator of the system.

Solution

We define $\rho_I = |\psi_I\rangle\langle\psi_I|$, and write

$$\rho_I = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} = \begin{pmatrix} \rho_{11} & \rho_{21}^* \\ \rho_{21} & 1-\rho_{11} \end{pmatrix}.$$

For convenience, let us denote $\mathcal{D}(t) = \mathcal{V}e^{i(\omega_0-\omega)t}$. This density operator evolves in time according to

$$\begin{aligned} \dot{\rho}_I &= \frac{i}{\hbar}[\rho_I, H_I] = \frac{i}{2\hbar}\left[\begin{pmatrix} \mathcal{D}^*\rho_{12} & \mathcal{D}\rho_{11} \\ \mathcal{D}^*\rho_{22} & \mathcal{D}\rho_{21} \end{pmatrix} - \begin{pmatrix} \mathcal{D}\rho_{21} & \mathcal{D}\rho_{22} \\ \mathcal{D}^*\rho_{11} & \mathcal{D}^*\rho_{12} \end{pmatrix}\right] \\ &= \frac{1}{\hbar}\begin{pmatrix} \mathrm{Im}[\mathcal{D}\rho_{21}] & i\mathcal{D}\left(\rho_{11}-\frac{1}{2}\right) \\ -i\mathcal{D}^*\left(\rho_{11}-\frac{1}{2}\right) & -\mathrm{Im}[\mathcal{D}\rho_{21}] \end{pmatrix}, \end{aligned}$$

yielding a set of two coupled equations

$$\begin{aligned} \dot{\rho}_{11} &= \frac{1}{\hbar}\mathrm{Im}[\mathcal{D}\rho_{21}], \\ \dot{\rho}_{21} &= -\frac{i}{\hbar}\mathcal{D}^*\left(\rho_{11}-\frac{1}{2}\right). \end{aligned}$$

These equations may be solved by plugging one equation into the other, but a more transparent form of them arises once we adopt a special representation of the density operator.

3 The Bloch vector representation

A density matrix of a two-level system can always be written in the following way:

$$\rho = \frac{1}{2}\left(\mathbb{I} + s_1\sigma_x + s_2\sigma_y + s_3\sigma_z\right) = \frac{1}{2}\left(\mathbb{I} + \mathbf{s}\cdot\vec{\sigma}\right) = \frac{1}{2}\begin{pmatrix} 1+s_3 & s_1 - is_2 \\ s_1 + is_2 & 1-s_3 \end{pmatrix},$$

where the s_i are real numbers and $|\mathbf{s}| = \sqrt{s_1^2+s_2^2+s_3^2} \leq 1$. Indeed, the Pauli matrices together with $\mathbb{I}$ constitute a basis for the space of 2×2 matrices, and it is straightforward to check that a matrix of the above form is Hermitian and obeys $\mathrm{Tr}\rho = 1$. As you will show at home, for a pure state we necessarily have that $|\mathbf{s}| = 1$, so that a pure state can be simply represented by a unit vector $\mathbf{s}$ living on the unit sphere in 3D.

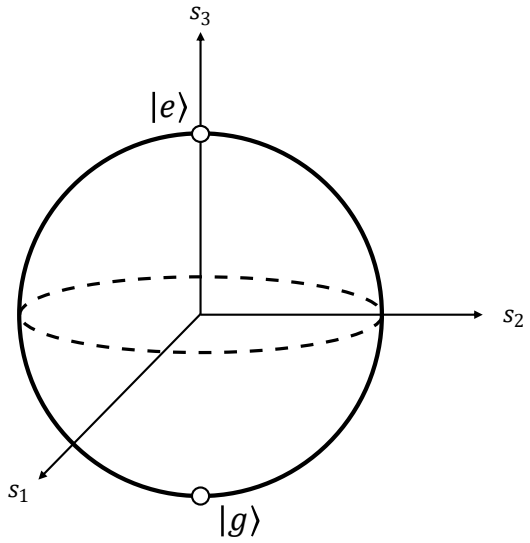

Figure 1: The pure states of a two-level system, represented as points on the Bloch sphere. The north pole ($s_3 = 1$) represents the excited state, and the south pole ($s_3 = -1$) represents the ground state.

For a pure state, we can specify $\mathbf{s}$ by the two angles $0 \leq \phi < 2\pi$ and $0 \leq \theta \leq \pi$ which are used in polar coordinates,

$$\mathbf{s} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)\,.$$

At home you will show that the correspondence between this Bloch vector representation and the state vector representation is given by

$$|\psi\rangle = e^{i\varphi}\left[\cos\left(\frac{\theta}{2}\right)|e\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|g\rangle\right].$$

Note that the overall phase factor $e^{i\varphi}$ *cannot* be determined by $\mathbf{s}$ (but is generally unimportant).

Exercise

Derive the equation of motion for $\mathbf{s}$ in the case of the Rabi model (within the interaction picture).

Solution

We write

$$\rho_I = \frac{1}{2}\begin{pmatrix} 1+s_3 & s_1 - is_2 \\ s_1 + is_2 & 1-s_3 \end{pmatrix}.$$

Substituting this into the equations of motion we got for ρ_{11} and ρ_{21}, we obtain the **optical Bloch equations**,

$$\begin{aligned}
\dot{s}_1 &= \frac{1}{\hbar}\mathrm{Im}\left[\mathcal{D}^*\right]s_3, \\
\dot{s}_2 &= -\frac{1}{\hbar}\mathrm{Re}\left[\mathcal{D}^*\right]s_3, \\
\dot{s}_3 &= \frac{1}{\hbar}\left(\mathrm{Re}\left[\mathcal{D}^*\right]s_2 - \mathrm{Im}\left[\mathcal{D}^*\right]s_1\right).
\end{aligned}$$

These equations assume a compact form if we define a "magnetic field" $\mathbf{\Omega} \equiv \frac{1}{\hbar}\left(\mathrm{Re}\left[\mathcal{D}^*\right], \mathrm{Im}\left[\mathcal{D}^*\right], 0\right)$, yielding the following equation of motion for the pseudo-spin $\mathbf{s}$:

$$\boxed{\dot{\mathbf{s}} = \mathbf{\Omega} \times \mathbf{s}.}$$

This is equivalent to the classical equation of motion for a spin in a magnetic field. On resonance ($\omega = \omega_0$), $\mathbf{\Omega}$ is time-independent ($\mathcal{D} = \mathcal{V}$) and so $\mathbf{s}$ simply performs a precession about the axis of $\mathbf{\Omega}$ at the frequency $|\mathbf{\Omega}| = |\mathcal{V}|/\hbar$ (for instance, if $\mathcal{V}$ is imaginary, then $\hat{s}_2$ is the rotation axis). This gives us a simple description of the dynamics of the two-level system starting from *any* initial state.

Moreover, if we view the two-level system as a qubit – identifying $|0\rangle \equiv |e\rangle$ and $|1\rangle \equiv |g\rangle$ – we may observe how the driving field allows us to **control** the state of the qubit. The driving field rotates $\mathbf{s}$, with $\mathbf{\Omega}$ determining both the rotation axis and the rotation frequency; the duration of the pulse determines the final state of the qubit following the rotation. But to have full control of the qubit, we need an additional axis of rotation.

Suppose that we can control the energy-splitting between $|e\rangle$ and $|g\rangle$, such that the Hamlitonian can be written as

$$H = \frac{\hbar\omega_0}{2}\sigma_z + \left(\mathcal{V}\sigma_+ + \mathcal{V}^*\sigma_-\right)\cos\left(\omega t\right) + \frac{B}{2}\sigma_z,$$

with $\mathcal{V}, \omega, B$ being parameters under our control. If we move to the interaction picture as before (and apply the RWA), we will have additional terms on the diagonal,

$$H_I \approx \frac{1}{2}\begin{pmatrix} B & \mathcal{V}e^{i(\omega_0-\omega)t} \\ \mathcal{V}^*e^{-i(\omega_0-\omega)t} & -B \end{pmatrix}.$$

Exercise

Show that the phase gate can be implemented by applying the field B for a specific duration of time.

Solution

If we do not turn on the Rabi field ($\mathcal{V} = 0$) and let the state evolve according to H_I, then

$$|\psi_I\left(t\right)\rangle = e^{-iH_It/\hbar}\left|\psi_I\left(0\right)\right\rangle,$$

with

$$e^{-iH_It/\hbar} = e^{-iBt/2\hbar}\begin{pmatrix} 1 & 0 \\ 0 & e^{iBt/\hbar} \end{pmatrix}.$$

Recall that the phase gate is given by

$$U_\varphi = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\varphi} \end{pmatrix},$$

and so these operations are identical (up to an unimportant overall phase) if we apply the field B for $t = \hbar\varphi/B$. Note that in the Bloch vector representation, U_φ is equivalent to a rotation about the $\hat{s}_3$ axis by an angle φ.

In general, if we can rotate the Bloch sphere about two non-parallel rotation axes, any rotation of the Bloch sphere can be expressed as a product of such rotations. Since rotations of the sphere are equivalent to the possible unitary operations that can be applied to a qubit, this means that **any single-qubit gate can be constructed from a sequence of such rotations**.