1 Change of variables

Consider the scaled Schrödinger equation

$$\dot{\psi} = -iH(t)\psi, \quad \psi(0) = \psi_0, \quad H(t) = H_s + f(t)a + \bar{f}(t)a^\dagger. \tag{1}$$

Here, $f(t)$ is a scalar complex-valued control function. $H_s = H_s^\dagger$ is the system Hamiltonian matrix, which we assume to be real, Hermitian and independent of time. The lowering and raising matrices are denoted a and $a^\dagger$, respectively. These real matrices satisfy

$$a = \begin{bmatrix} 0 & 1 & & & & \\ & 0 & \sqrt{2} & & & \\ & & 0 & \sqrt{3} & & \\ & & & 0 & \sqrt{4} & \\ & & & & \ddots & \ddots \end{bmatrix}, \quad a^\dagger = \begin{bmatrix} 0 & & & & & \\ 1 & 0 & & & & \\ & \sqrt{2} & 0 & & & \\ & & \sqrt{3} & 0 & & \\ & & & \ddots & \ddots & \end{bmatrix} \tag{2}$$

We can decompose the control function into its real and imaginary parts,

$$f(t) = f_r(t) + i f_i(t),$$

and write the Hamiltonian matrix in (1) as

$$H(t) = H_s + f_r(t)\left(a + a^\dagger\right) + i f_i(t)\left(a - a^\dagger\right) =: H_s + K(t) + iS(t).$$

Here, K and S are real-valued matrices with $K^\dagger = K$ and $S^\dagger = -S$.

1.1 Time-independent change of variables

Because H_s is Hermitian, it has real eigenvalues and can always be diagonalized by a unitary matrix V. By the change of variables, $u(t) = V\psi(t)$, where V is independent of time, Schrödinger's equation (1) becomes

$$\dot{u} = -iVH(t)V^\dagger u, \quad VH(t)V^\dagger = H_0 + f(t)\tilde{a} + \bar{f}(t)\tilde{a}^\dagger,$$

where $\tilde{a} = VaV^\dagger$ and H_0 is a real diagonal matrix.

1.2 Time-dependent unitary transformations

Consider the unitary tranformation

$$\psi(t) = U^\dagger(t)v(t), \quad U^\dagger U = I.$$

We have

$$\begin{aligned} \dot{\psi} &= \dot{U}^\dagger v + U^\dagger \dot{v}, \\ H\psi &= HU^\dagger v \end{aligned}$$

Thus, (1) gives

$$\dot{U}^\dagger v + U^\dagger \dot{v} = -iHU^\dagger v,$$

By using the identity $U\dot{U}^\dagger = -\dot{U}U^\dagger$ and reorganizing the terms,

$$\dot{v} = -iUHU^\dagger v + \dot{U}U^\dagger = -i\left(UHU^\dagger + i\dot{U}U^\dagger\right)v.$$

Thus, the transformed problem becomes

$$\dot{v} = -i\tilde{H}(t)v, \quad \tilde{H} = UHU^\dagger + i\dot{U}U^\dagger. \tag{3}$$

1.3 The interaction picture

We can construct a unitary transformation based on the time-independent system Hamiltonian H_s in (2),

$$U(t) = \exp(iH_s t).$$

We have $\dot{U}(t) = iH_s \exp(iH_s t)$, which gives

$$\dot{U}U^\dagger = iH_s \exp(iH_s t)\exp(-iH_s t) = iH_s.$$

From the definition of the matrix exponential,

$$\exp(iH_s t) = I + itH_s + \frac{1}{2}(it)^2 H_s^2 + \frac{1}{6}(it)^3 H_s^3 + \dots.$$

Thus it is clear that $U = \exp(iH_s t)$ commutes with H_s and $UH_sU^\dagger = H_s$. As a result, the constant (time-independent) part of the transformed Hamiltonian cancels. From (3), the transformed problem becomes

$$\dot{v} = -i\tilde{H}(t)v, \quad \tilde{H}(t) = f(t)UaU^\dagger + \bar{f}(t)Ua^\dagger U^\dagger. \tag{4}$$

This formulation of Schrödinger's equation is known as the interaction picture.

When $H_s = H_0$ is real and diagonal,

$$H_0 = \begin{bmatrix} \omega_1 & & & \\ & \omega_2 & & \\ & & \omega_3 & \\ & & & \ddots \end{bmatrix}, \quad U(t) = \exp(iH_0 t) = \begin{bmatrix} e^{i\omega_1 t} & & & \\ & e^{i\omega_2 t} & & \\ & & e^{i\omega_3 t} & \\ & & & \ddots \end{bmatrix}$$

The lowering operator transforms according to

$$UaU^\dagger = \begin{bmatrix} e^{i\omega_1 t} & & & \\ & e^{i\omega_2 t} & & \\ & & e^{i\omega_3 t} & \\ & & & \ddots \end{bmatrix} \begin{bmatrix} 0 & 1 & & \\ & 0 & \sqrt{2} & \\ & & 0 & \sqrt{3} \\ & & & \ddots & \ddots \end{bmatrix} \begin{bmatrix} e^{-i\omega_1 t} & & & \\ & e^{-i\omega_2 t} & & \\ & & e^{-i\omega_3 t} & \\ & & & \ddots \end{bmatrix} =$$

$$\begin{bmatrix} 0 & e^{-i\Delta\omega_1 t} & & & \\ & 0 & \sqrt{2}e^{-i\Delta\omega_2 t} & & \\ & & 0 & \sqrt{3}e^{-i\Delta\omega_3 t} & \\ & & & \ddots & \ddots \end{bmatrix} =: D(t)a,$$

where $\Delta\omega_k = \omega_{k+1} - \omega_k$ and $D(t)$ is the diagonal matrix

$$D(t) = \begin{bmatrix} e^{-i\Delta\omega_1 t} & & & \\ & \sqrt{2}e^{-i\Delta\omega_2 t} & & \\ & & \sqrt{3}e^{-i\Delta\omega_3 t} & \\ & & & \ddots \end{bmatrix}, \quad \Delta\omega_N = 0.$$

Then,

$$UaU^\dagger = Da, \quad Ua^\dagger U^\dagger = a^\dagger D^\dagger.$$

Note that the value of $\Delta\omega_N$ is arbitrary because it is not needed to evaluate Da. Thus, when the system Hamiltonian is diagonal, the transformed problem corresponding to (4) becomes

$$\dot{v} = -i\widetilde{H}(t)v, \quad \widetilde{H}(t) = f(t)D(t)a + \bar{f}(t)a^\dagger D^\dagger(t). \tag{5}$$

The structure of the transformed Hamiltonian indicates how resonance can be induced in the system. For example, by taking $f(t) = \Omega e^{i\Delta\omega_1 t}$, the Hamiltonian matrix becomes

$$\tilde{H}(t) = \begin{bmatrix} 0 & \Omega & & & \\ \bar{\Omega} & 0 & f(t)\sqrt{2}e^{-i\Delta\omega_2 t} & & \\ & \bar{f}(t)\sqrt{2}e^{i\Delta\omega_2 t} & 0 & f(t)\sqrt{3}e^{-i\Delta\omega_3 t} & \\ & & & & \\ & & \ddots & \ddots & \ddots \end{bmatrix}.$$

In this case, the dynamics of the system will be dominated by an oscillation between the ground state and the first excited state, with frequency Ω. One shortcoming this approach is that the function $f(t) = \Omega e^{i\Delta\omega_1 t}$ is complex-valued. To be realized in the laboratory it must however be real-valued. We can instead use the ansatz

$$
\begin{aligned}
f(t) &= \alpha \cos(\Delta\omega_1 t) + \beta \sin(\Delta\omega_1 t) \\
&= \frac{\alpha}{2}\left(\exp(i\omega_1 t) + \exp(-i\omega_1 t)\right) - \frac{\beta i}{2}\left(\exp(i\omega_1 t) - \exp(-i\omega_1 t)\right) \\
&= \exp(i\omega_1 t)\left(\frac{\alpha}{2} - \frac{\beta i}{2}\right) + \exp(-i\omega_1 t)\left(\frac{\alpha}{2} + \frac{\beta i}{2}\right)
\end{aligned}
$$

We may write the matrix $D(t)$ as

$$
D(t) = \exp(-i\Delta\omega_1 t)\widetilde{D}(t), \quad \widetilde{D}(t) = \begin{bmatrix} 1 & & & \\ & \sqrt{2}e^{i(\Delta\omega_1 - \Delta\omega_2)t} & & \\ & & \sqrt{3}e^{i(\Delta\omega_1 - \Delta\omega_3)t} & \\ & & & \ddots \end{bmatrix}.
$$

Thus,

$$
f(t)D(t) = \left(\frac{\alpha}{2} - \frac{\beta i}{2}\right)\widetilde{D}(t) + \exp(-2i\omega_1 t)\left(\frac{\alpha}{2} + \frac{\beta i}{2}\right).
$$