Chapter 2

The Model Hamiltonians

In this chapter we introduce the general Hamiltonian which spans the entire class of non–adiabatic systems considered here. We discuss the two special cases of the general model whose analysis forms the remainder of the thesis. The symmetries associated with these systems are of particular interest, and these are discussed in detail.

2.1 The general model Hamiltonian

The most general form for the fully quantized Hamiltonian describing a two–level fermion interacting with two independent bosonic field modes in the dipole approximation is given by

$$\begin{aligned} H &= \frac{1}{2}\omega_0\,\sigma^z + \omega_1\, b_1^\dagger b_1 + \omega_2\, b_2^\dagger b_2 \\ &\quad + \eta_1\,\left(b_1^\dagger + b_1\right)\sigma^x - \eta_2\,\left(b_2^\dagger + b_2\right)\sigma^y\,, \end{aligned} \tag{2.1}$$

where ω_0 is the fermionic level splitting, ω_1 and ω_2 are the frequencies of the two modes and η_1 and η_2 the corresponding dipole coupling constants linking the bosonic modes to the fermion and thus indirectly to each other. The operators b_1, b_2 and $b_1^\dagger, b_2^\dagger$ are boson annihilation and creation operators, respectively, satisfying the standard commutation relations

$$\begin{aligned} \left[b_1, b_1^\dagger\right] &= \left[b_2, b_2^\dagger\right] = 1 \\ [b_1, b_2] &= \left[b_1^\dagger, b_2^\dagger\right] = \left[b_1, b_2^\dagger\right] = \left[b_2, b_1^\dagger\right] = 0\,, \end{aligned} \tag{2.2}$$

and $\sigma^x, \sigma^y, \sigma^z$ are Pauli matrices which form a convenient basis for the two–dimensional fermionic subspace of the full Hilbert space relevant to the Hamiltonian (2.1). The origin of the fermionic energy scale has been chosen such that the lower (upper) fermionic state corresponds to energy $-\frac{1}{2}\omega_0$ ($\frac{1}{2}\omega_0$), and the constant zero point energy $\frac{1}{2}\omega_1 + \frac{1}{2}\omega_2$ of the field modes has been neglected. For convenience, we employ units such that $\hbar = 1$. A derivation of the general model Hamiltonian (2.1) in the context of quantum optics is given in Appendix A.

There is a parity symmetry associated with the Hamiltonian (2.1). We define an operator

$$N \equiv b_1^\dagger b_1 + b_2^\dagger b_2 + \frac{1}{2}\,(\sigma^z + 1) \tag{2.3}$$

which counts the number of bosonic and fermionic quanta (excitations) and

introduce the parity operators (with eigenvalues ± 1)

$$\begin{aligned}
\Pi_1 &\equiv \exp\left\{i\pi\left[b_1^\dagger b_1 + \frac{1}{2}(\sigma_y + 1)\right]\right\} = -\exp\left\{i\pi b_1^\dagger b_1\right\}\sigma_y \\
\Pi_2 &= \exp\left\{i\pi\left[b_2^\dagger b_2 + \frac{1}{2}(\sigma_x + 1)\right]\right\} = -\exp\left\{i\pi b_2^\dagger b_2\right\}\sigma_x \\
\Pi &= -i\Pi_1\Pi_2 \\
&= \exp\left\{i\pi\left[b_1^\dagger b_1 + b_2^\dagger b_2 + \frac{1}{2}(\sigma_z + 1)\right]\right\} \\
&= -\exp\left\{i\pi b_1^\dagger b_1\right\}\exp\left\{i\pi b_2^\dagger b_2\right\}\sigma_z\,. \qquad (2.4)
\end{aligned}$$

Then

$$\begin{aligned}
[H, \Pi_1] &= i\hbar\omega_0 \exp\left\{i\pi b_1^\dagger b_1\right\}\sigma_x \\
[H, \Pi_2] &= -i\hbar\omega_0 \exp\left\{i\pi b_2^\dagger b_2\right\}\sigma_y \\
[H, \Pi] &= 0\,, \qquad (2.5)
\end{aligned}$$

where we have used the relevant identities from Appendix B. The eigenstates of the Hamiltonian (2.1) may thus be chosen to be states of definite Π parity.

2.2 Special cases of the general Hamiltonian

2.2.1 The Rabi Hamiltonian

The dipole interaction between a two–level atom with level–splitting ω_0 and a single electromagnetic field mode of frequency ω may be modelled by the Rabi Hamiltonian

$$\begin{aligned}
H_{\text{Rabi}} &= \frac{1}{2}\omega_0\,\sigma^z + \omega\, b^\dagger b + \eta\,\left(b^\dagger + b\right)\sigma^x \\
&= \frac{1}{2}\omega_0\,\sigma^z + \omega\, b^\dagger b + 2\,g\,\left(b^\dagger + b\right)\sigma^x\,, \qquad (2.6)
\end{aligned}$$

which is the simplest non–trivial realization of the general model Hamiltonian (2.1), obtained by setting $\omega_1 = \omega, \omega_2 = 0$, and with the coupling conventionally relabelled via $\eta_1 = \eta = 2g, \eta_2 = 0$. This model was originally employed in the context of nuclear magnetic resonance [Ra37, Ra54], and is of topical interest in quantum optics [Sh93, Mi91]. The Hamiltonian (2.6) conserves the parity

$$\Pi_{\text{Rabi}} = \exp\left\{i\pi\left[b^\dagger b + \frac{1}{2}(\sigma_z + 1)\right]\right\}. \tag{2.7}$$

It is important to note that the Rabi Hamiltonian is not a continuous limit of the general model Hamiltonian (2.1), since it operates in a fundamentally different Hilbert space where the additional degrees of freedom corresponding to the second bosonic mode are absent.

2.2.2 The linear $E \otimes e$ Jahn–Teller and pseudo Jahn–Teller Hamiltonians

In the case of degenerate bosonic modes ($\omega_1 = \omega_2 = \omega$) equally coupled ($\eta_1 = \eta_2 = \eta$) to a fermionic system, the general Hamiltonian (2.1) reduces to the linear $E \otimes e$ pseudo Jahn–Teller (PJT) model

$$\begin{aligned} H_{\text{PJT}} &= \frac{1}{2}\omega_0\,\sigma^z + \omega\, b_1^\dagger b_1 + \omega\, b_2^\dagger b_2 \\ &\quad + \eta\,\left(b_1^\dagger + b_1\right)\sigma^x - \eta\,\left(b_2^\dagger + b_2\right)\sigma^y . \end{aligned} \tag{2.8}$$

If, in addition, the fermionic levels are degenerate ($\omega_0 = 0$), then we obtain the (pure) linear $E \otimes e$ Jahn–Teller (JT) Hamiltonian H_{JT}. These models are of relevance not only in quantum optics, but also in quantum chemistry [Berb], where they describe the non–adiabatic vibronic interaction between a

two–fold degenerate or quasi–degenerate electronic level (E) and a doubly–degenerate nuclear vibrational mode (e). The designation "linear" indicates that the vibronic interaction terms, expanded in powers of the nuclear configurational coordinates, have been truncated at first order.

There is another symmetry, besides the parity symmetry (2.4), associated with the PJT Hamiltonian (and therefore also with the JT Hamiltonian) which is not obvious from the form (2.8). If we perform the canonical transformation

$$\begin{aligned} a_1 &\equiv \frac{1}{\sqrt{2}}(b_1 + ib_2) \qquad & a_1^\dagger &\equiv \frac{1}{\sqrt{2}}\left(b_1^\dagger - ib_2^\dagger\right) \\ a_2 &\equiv \frac{1}{\sqrt{2}}(b_1 - ib_2) \qquad & a_2^\dagger &\equiv \frac{1}{\sqrt{2}}\left(b_1^\dagger + ib_2^\dagger\right) , \end{aligned} \tag{2.9}$$

which preserves the commutation relations (2.2), then the Hamiltonian (2.8) and parity operator (2.4) become

$$\begin{aligned} H_{\mathrm{PJT}} &= \frac{1}{2}\omega_0\,\sigma^z \;+\; \omega\, a_1^\dagger a_1 \;+\; \omega\, a_2^\dagger a_2 \\ &\quad + \gamma\,\left(a_1 + a_2^\dagger\right)\sigma^+ \;+\; \gamma\,\left(a_1^\dagger + a_2\right)\sigma^- \qquad (2.10) \\ \Pi_{\mathrm{PJT}} &= \exp\left\{i\pi\left[a_1^\dagger a_1 + a_2^\dagger a_2 + \frac{1}{2}(\sigma_z + 1)\right]\right\} . \qquad (2.11) \end{aligned}$$

where $\gamma \equiv \eta/\sqrt{2}$. In the form (2.10), it is readily seen that, for arbitrary ω_0, H_{PJT} commutes with the operator

$$J \;=\; a_1^\dagger a_1 - a_2^\dagger a_2 + \frac{1}{2}\sigma^z \; . \tag{2.12}$$

The transformation (2.9) and the symmetry $[H_{\mathrm{PJT}}, J] = 0$ have a simple physical meaning. In the quantum optics context, Equations (2.9) correspond to a transformation to field modes of circular rather than linear polarization, with $a_1^\dagger$ ($a_2^\dagger$) denoting an operator which creates a photon of positive

(negative) helicity. The operator J then represents a conserved angular momentum component. Since J also commutes with the parity operator (2.11), the eigenstates of H_{PJT} (and H_{JT}) need thus only be sought amongst those states with definite Π_{PJT} and J.