Appendix A

Derivation of the General Model Hamiltonian

Here we present a first–principles derivation (in the context of quantum optics) of the general Hamiltonian (2.1).

A.1 The two–level atom

Consider an two–level atom, with the two relevant atomic states labeled $|a\rangle$ and $|b\rangle$, and let $\hbar\omega_0 = E_b - E_a$ denote the energy gap between the states. Choose the origin of the atomic energy scale midway between the levels, so that $E_a = -\frac{1}{2}\hbar\omega_0$, and $E_b = \frac{1}{2}\hbar\omega_0 = E_a + \hbar\omega_0$. The Pauli matrices (supplemented by the 2×2 unit matrix), form a convenient operator basis in the two–dimensional matrix space corresponding to the atom, and we may thus, with a suitable choice of the z–axis, write the Hamiltonian for the atom as

$$H_{\text{atom}} = \frac{1}{2}\hbar\omega_0\sigma^z . \tag{A.1}$$

A.2 Quantization of the electromagnetic field

Consider now the quantization of the free (zero charge and current density) electromagnetic field [Man]. After eliminating from Maxwell's equations (in rationalized Gaussian units) the electric $[\mathbf{E}(\mathbf{r},t)]$ and magnetic $[\mathbf{B}(\mathbf{r},t)]$ fields in favour of the classical scalar $[\Phi(\mathbf{r},t)]$ and vector $[\mathbf{A}(\mathbf{r},t)]$ potentials via

$$\mathbf{B} = \nabla\times\mathbf{A}\ , \qquad \mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{A}}{\partial t} \tag{A.2}$$

and then enforcing the Coulomb or transverse gauge $\nabla\cdot\mathbf{A} = 0$, one finds that $\mathbf{A}$ satisfies the wave equation

$$\frac{1}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2} - \nabla^2\mathbf{A} = 0\ , \tag{A.3}$$

whilst Φ is identically zero. We now treat the field as though it were confined to a cubical box of volume $V = L^3$ and impose periodic boundary conditions. If necessary, one may take the limit $V\to\infty$ at the end of the calculation. We expand the vector potential in a Fourier series

$$\mathbf{A}(\mathbf{r},t) \ = \ -i\sum_{\mathbf{k}}\sum_{s=1}^{2}\sqrt{\frac{\hbar c^2}{2V\omega_k}}\left\{b_{\mathbf{k},s}(t)\, e^{i\mathbf{k}\cdot\mathbf{r}} \ - \ b^*_{\mathbf{k},s}(t)\, e^{-i\mathbf{k}\cdot\mathbf{r}}\right\}\hat{e}_{\mathbf{k},s}\ , \tag{A.4}$$

with $\omega_k = c|\mathbf{k}|$, where the $\mathbf{k}$–sum is over all wave vectors

$$\mathbf{k} = \frac{2\pi}{L}(n_x, n_y, n_z) \qquad (n_x, n_y, n_z = 0, \pm1, \pm2, \ldots) \tag{A.5}$$

satisfying the boundary conditions, and where $\hat{e}_{\mathbf{k},s}, s = 1,2$ represent unit vectors along the two independent directions perpendicular to the wave vector $\mathbf{k}$, thereby also satisfying the requirement of transversality imposed by the Coulomb gauge. Thus (A.4) corresponds to an expansion of the vector potential $\mathbf{A}$ in terms of linearly polarized travelling wave modes. The fact that (A.4) must satisfy the wave equation (A.3) determines the time dependence of the Fourier coefficients as

$$b_{\mathbf{k},s}(t) = b_{\mathbf{k},s} e^{-i\omega_k t} \,, \qquad \text{(A.6)}$$

and the constant in (A.4) has been chosen so that the total energy

$$H_{\text{field}} = \frac{1}{2} \int_V \left(\mathbf{E}^2 + \mathbf{B}^2 \right) \, d^3\mathbf{r} \qquad \text{(A.7)}$$

of the radiation field then assumes the time–independent form

$$H_{\text{field}} = \sum_{\mathbf{k}} \sum_{s=1}^{2} \hbar\omega_k b^*_{\mathbf{k},s} b_{\mathbf{k},s} \,. \qquad \text{(A.8)}$$

By analogy with a system of decoupled harmonic oscillators, this form for the classical field energy suggests that the field may be quantized by promoting the Fourier coefficients $b_{\mathbf{k},s}(t)$ in the expansion (A.4) to operators $b_{\mathbf{k},s}$ satisfying Bose commutation relations. Confining ourselves to two perpendicularly polarized modes, of frequencies ω_1 and ω_2 and which we shall label modes 1 and 2, and neglecting the constant zero point energy of the two modes, we may then write for the field the Hamiltonian

$$H_{\text{field}} = \hbar\omega_1 \, b_1^\dagger b_1 + \hbar\omega_2 \, b_2^\dagger b_2 \qquad \text{(A.9)}$$

where the bosonic operators satisfy the standard commutation relations (2.2). Furthermore, $\mathbf{E}_n$, the electric field corresponding to mode n, now becomes an operator of the form

$$\mathbf{E}_n(\mathbf{r},t) \;=\; -\,\epsilon_n \left\{ b_n\, e^{i\mathbf{k}\cdot\mathbf{r}} \;+\; b_n^\dagger\, e^{-i\mathbf{k}\cdot\mathbf{r}} \right\} \hat{e}_{\mathbf{k},n} \qquad (n=1,2) \qquad \text{(A.10)}$$

where $\epsilon_n = \sqrt{\frac{\hbar\omega_k}{2V}}$ denotes the electric field per quantum (photon) in mode n, $\hat{e}_{\mathbf{k},n} \cdot \hat{e}_{\mathbf{k},m} = \delta_{n,m}$ since the fields are perpendicularly polarized, and with a similar expression for the magnetic field. There are many subtleties in the quantization of the electromagnetic field that have been ignored here (see *e.g.* [Mar], [Coh] or [Hua]).

A.3 The dipole interaction Hamiltonian

In order to determine the interaction Hamiltonian for the coupling of the atom to the field modes, we neglect any interaction with the magnetic field, and make the co–called dipole approximation [Mar, Man]. If we take the origin for $\mathbf{r}$ at the atomic center of mass, and assume that the fields do not vary appreciably over distances of the order of the atomic dimensions so that we may take $\mathbf{k}\cdot\mathbf{r} = 0$, then the dipole interaction between the atom and the two field modes has the form

$$H_{\text{int}} = -\mathbf{p}\cdot(\mathbf{E}_1 + \mathbf{E}_2)\ . \qquad \text{(A.11)}$$

Here the atomic dipole moment operator $\mathbf{p}$ for the N atomic electrons, each of charge e, located at positions $\mathbf{r}_i, i = 1, 2, \ldots, N$ has the form

$$\mathbf{p} \;=\; N\,e \left(\frac{1}{N} \sum_{i=1}^{N} \mathbf{r}_i \right) \;\equiv\; e\mathbf{r}\ , \qquad \text{(A.12)}$$

and

$$\mathbf{E}_n(\mathbf{r},t) \;=\; -\,\epsilon_n \left\{ b_n \;+\; b_n^\dagger \right\} \hat{e}_{\mathbf{k},n} \qquad (n=1,2) \qquad \text{(A.13)}$$

due to the dipole approximation. By the atomic parity selection rule, the diagonal elements of the matrix representing the dipole operator $\mathbf{p}$ in the atomic basis $\{|a\rangle, |b\rangle\}$ are zero, and we only consider atomic levels such that the off–diagonal elements

$$\begin{aligned} \mathbf{p}_{ab} &= \langle a|\mathbf{p}|b\rangle = \langle a|ex|b\rangle\hat{x} + \langle a|ey|b\rangle\hat{y} + \langle a|ez|b\rangle\hat{z} \\ \mathbf{p}_{ba} &= \langle b|\mathbf{p}|a\rangle = \mathbf{p}^*_{ab}\,, \end{aligned} \tag{A.14}$$

with $\hat{z}$ representing the atomic quantization axis, are nonzero. It is then straightforward to show that the interaction Hamiltonian (A.11) assumes the form

$$\begin{aligned} H_{\text{int}} &= \hbar\left(b_1^\dagger + b_1\right)\left(\text{Re}\,[\beta_1]\,\sigma^x - \text{Im}\,[\beta_1]\,\sigma^y\right) \\ &\quad + \hbar\left(b_2^\dagger + b_2\right)\left(\text{Re}\,[\beta_2]\,\sigma^x - \text{Im}\,[\beta_2]\,\sigma^y\right) \end{aligned} \tag{A.15}$$

where

$$\beta_n = \mathcal{P}_n\sqrt{\frac{\omega_n}{2\hbar\mathcal{V}}} \qquad (n = 1, 2) \tag{A.16}$$

and $\mathcal{P}_n$ denotes the component of $\mathbf{p}_{ab}$ along $\hat{e}_n$.

We may now, without loss of generality, take the parameters β_1 and β_2 to be pure real and pure imaginary, respectively, as shown by the following argument: Choose the atomic quantization axis $\hat{z}$ so as to be perpendicular to the plane defined by the orthogonal polarization axes of the two modes. Orient $\hat{x}$ and $\hat{y}$ such that $\hat{e}_n$ makes an angle α_n with $\hat{x}$, with $\alpha_2 = \alpha_1 + \pi/2$, and α_1 as yet arbitrary. By the atomic angular momentum selection rule (or, more formally, via the Wigner-Eckhardt theorem) $\langle a|y|b\rangle = \pm i\langle a|x|b\rangle$. Thus

$$\mathcal{P}_n = \mathbf{p}_{ab}\cdot\hat{e}_n = e\,\langle a|x|b\rangle e^{\pm i\alpha_n}\,. \tag{A.17}$$

We are free to choose α_1 such that $e^{\pm i\alpha_1}$ cancels the phase of $\langle a|x|b\rangle$, so that $\mathcal{P}_1 = e|\langle a|x|b\rangle|$ is pure real, and $\mathcal{P}_2 = \pm e|\langle a|x|b\rangle|i$ is pure imaginary. Thus the interaction Hamiltonian (A.15) may be written in the final form

$$H_{\text{int}} = \hbar\eta_1 \left(b_1^\dagger + b_1\right)\sigma^x - \hbar\eta_2 \left(b_2^\dagger + b_2\right)\sigma^y \tag{A.18}$$

where

$$\eta_n = e|\langle a|x|b\rangle|\sqrt{\frac{\omega_n}{2\hbar\mathcal{V}}} \qquad (n = 1,2) \tag{A.19}$$

denotes the (purely real) dipole coupling constant for mode n. Combining the Hamiltonians (A.1), (A.9) and (A.18), and setting $\hbar = 1$, we obtain the general model Hamiltonian (2.1).

Appendix B

Useful Identities and Commutation Relations

For the model Hamiltonians considered here, the Hausdorff expansion (3.8) often involves commutators either of Pauli matrices or of operators which obey bosonic commutation relations. Here we therefore present several identities for such operators which are useful in the application of the CCM to these models.

B.1 Operators for two–level systems

The Pauli matrices $\sigma^k, k \in \{x, y, z\}$, and the raising and lowering operators σ^+ and σ^- respectively, have the following form in the eigenbasis of σ^z:

$$\sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} , \qquad I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\sigma^x = \frac{1}{2}\left(\sigma^+ + \sigma^-\right) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} , \qquad \sigma^y = \frac{i}{2}\left(\sigma^- - \sigma^+\right) = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\sigma^+ = \sigma^x + i\sigma^y = \begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix} , \qquad \sigma^- = \sigma^x - i\sigma^y = \begin{bmatrix} 0 & 0 \\ 2 & 0 \end{bmatrix} . \tag{B.1}$$

Note that some authors choose to define $\sigma^\pm = \frac{1}{2}\sigma^x \pm i\sigma^y$, resulting in a rescaling of the dipole coupling constant η in our model Hamiltonians.

In the following identities, $k, l, m \in \{x, y, z\}$, n is an arbitrary integer, and α is an arbitrary real number:

$$\left(\sigma^k\right)^2 = \left(\sigma^k\right)^{2n} = I , \qquad \left(\sigma^k\right)^{2n+1} = \sigma^k$$

$$\exp\left\{i\alpha\pi\left[\tfrac{1}{2}\left(\sigma^k + 1\right)\right]\right\} = \left[\cos\left(\alpha\tfrac{\pi}{2}\right) + i\sin\left(\alpha\tfrac{\pi}{2}\right)\sigma^k\right]\exp\left(i\alpha\tfrac{\pi}{2}\right)$$

$$\exp\left\{i\pi\left[\tfrac{1}{2}\left(\sigma^k + 1\right)\right]\right\} = -\sigma^k \quad (\alpha = 1) . \tag{B.2}$$

The latter identity is particularly useful in verifying the commutation relations between the various parity operators (2.4) and the general model Hamiltonian (2.1) in Chapter 2.

We make frequent use of the following products and commutation relations (here $k, l, m \in \{x, y, z\}$ with $k \neq l$, and ϵ_{klm} is the totally antisymmetric Levi–Civita symbol):

$$\begin{array}{lll}
\sigma^k\sigma^l = i\epsilon_{klm}\sigma_m\ , & \sigma^l\sigma^k = -i\epsilon_{klm}\sigma_m\ , & \left[\sigma^k, \sigma^l\right] = 2i\epsilon_{klm}\sigma_m \\
\sigma^z\sigma^+ = \sigma^+\ , & \sigma^+\sigma^z = -\sigma^+\ , & [\sigma^z, \sigma^+] = 2\sigma^+ \\
\sigma^z\sigma^- = -\sigma^-\ , & \sigma^-\sigma^z = \sigma^-\ , & [\sigma^z, \sigma^-] = -2\sigma^- \\
\sigma^x\sigma^+ = 1 - \sigma^z\ , & \sigma^+\sigma^x = 1 + \sigma^z\ , & [\sigma^x, \sigma^+] = -2\sigma^z \\
\sigma^x\sigma^- = 1 + \sigma^z\ , & \sigma^-\sigma^x = 1 - \sigma^z\ , & [\sigma^x, \sigma^-] = 2\sigma^z \\
\sigma^y\sigma^+ = i\,(1 - \sigma^z)\ , & \sigma^+\sigma^y = i\,(1 + \sigma^z)\ , & [\sigma^y, \sigma^+] = -2i\sigma^z \\
\sigma^y\sigma^- = -i\,(1 + \sigma^z)\ , & \sigma^-\sigma^y = -i\,(1 - \sigma^z)\ , & [\sigma^y, \sigma^-] = -2i\sigma^z \\
\sigma^+\sigma^- = 2\,(1 + \sigma^z)\ , & \sigma^-\sigma^+ = 2\,(1 - \sigma^z)\ , & [\sigma^+, \sigma^-] = 4\sigma^z\ .
\end{array} \tag{B.3}$$

B.2 General commutation relations

Let A, B, C, D denote arbitrary operators. We make frequent use of the following standard identities:

$$\begin{aligned}
[A, BC] &= [A, B]\ C + B\ [A, C] \\
[AB, C] &= A\ [B, C] + [A, C]\ B\ .
\end{aligned} \tag{B.4}$$

If $[A, B] = [A, D] = 0$ and also $[C, B] = [C, D] = 0$, then

$$\begin{aligned}
[AB, CD] &= [A, C]\,B\ D + C\ A\,[B, D] \\
&= [A, C]\,D\ B + A\ C\,[B, D]\ .
\end{aligned} \tag{B.5}$$

B.2.1 The Hausdorff expansion

For arbitrary operators A and B, we define

$$[B,A]_0 \equiv B\ , \qquad [B,A]_{m+1} = [[B,A]_m\,,A] \qquad (m=0,1,2,\ldots)\ . \tag{B.6}$$

Note that $[B,A]_1 = [B,A]$, the usual commutator. Let $C(k,m)$ denote the binomial coefficient $\frac{k!}{m!(k-m)!}$. Then it can readily be shown by induction that, for any $n \in \{0,1,2,\ldots\}$,

$$\begin{aligned} A^n B &= A^{n-k} \sum_{m=0}^{k} (-1)^m\ C(k,m)\ [B,A]_m\ A^{k-m} \qquad \forall\ k \in \{0,1,2,\ldots,n\} \\ &= \sum_{m=0}^{n} (-1)^m\ C(n,m)\ [B,A]_m\ A^{n-m} \qquad (k=n)\ . \end{aligned} \tag{B.7}$$

Assuming that the exponential is well-defined, one may thus write

$$\begin{aligned} e^{-A}Be^{A} &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} A^n B\, e^A \\ &= \sum_{n=0}^{\infty}\sum_{m=0}^{n} \frac{(-1)^{n+m}}{m!(n-m)!} [B,A]_m\ A^{n-m}\ e^A \\ &= \sum_{m=0}^{\infty}\sum_{n=m}^{\infty} \frac{(-1)^{n-m}}{m!(n-m)!} [B,A]_m\ A^{n-m}\ e^A \\ &= \left(\sum_{m=0}^{\infty} \frac{[B,A]_m}{m!}\right)\left(\sum_{k=0}^{\infty} \frac{(-1)^k}{k!} A^k\right) e^A \\ &= \sum_{m=0}^{\infty} \frac{1}{m!} [B,A]_m\ , \end{aligned} \tag{B.8}$$

which is the Hausdorff or nested commutator expansion (3.8) for the similarity transform of B through A (see also [Mer] for an alternative proof). The commutator

$$\begin{aligned} [A^n,B] &= \sum_{m=0}^{n} (-1)^m C(n,m)\,[B,A]_m\, A^{n-m} - BA^n \\ &= \sum_{m=1}^{n} (-1)^m C(n,m)\,[B,A]_m\, A^{n-m} \qquad (n \geq 0) \end{aligned} \tag{B.9}$$

will also be useful in what follows.

B.2.2 Operators for which the commutator is a number

Consider now two otherwise arbitrary operators A and B for which the commutator is a c–number, say $[A, B] = z$. Then, since $[A, B]_m = 0 \;\forall\; m \geq 2$, it is clear from (B.9) above that

$$[A, B^n] = nB^{n-1}z \quad (n \geq 0) \, . \tag{B.10}$$

Let $f(B)$ now be an arbitrary function of B only, subject to the usual restriction that a convergent power series expansion

$$f(B) = \sum_{n=0}^{\infty} a_n B^n \tag{B.11}$$

exists. It is clear from (B.10) that we may formally write

$$[A, f(B)] = \frac{d\, f(B)}{d\, B}\, z \, , \tag{B.12}$$

where, for the purposes of evaluating the derivative, the operator B is treated as a real variable (see, *e.g.* [Mer] or [Hak]). We have also generalized (B.12) to show that, for any integer $n \geq 0$,

$$[A^n, f(B)] = \sum_{m=1}^{n} C(n,m)\, f^{(m)}(B)\, z^m\, A^{n-m}, \tag{B.13}$$

where $f^{(m)}(B)$ is a convenient shorthand for $\frac{d^m\, f(B)}{d\, B^m}$, and we define $f^{(0)}(B) \equiv f(B)$. The relation (B.13) is easily proved by induction. A final identity which we have often used is the Glauber–Weyl formula [Mer]

$$e^A e^B = e^{A+B+z/2} \, . \tag{B.14}$$

B.3 Bosonic commutation relations

For the bosonic annihilation and creation operators, b and $b^\dagger$ respectively, the standard commutation relation reads $\left[b, b^\dagger\right] = 1$, so that the relations (B.12) and (B.13) apply with $A = b$, $B = b^\dagger$ and $z = 1$ or $A = b^\dagger$, $B = b$ and $z = -1$. Thus for f an arbitrary function of the given argument only,

$$\left[b, f(b^\dagger)\right] = \frac{d\, f(b^\dagger)}{d\, b^\dagger} \quad \text{and} \quad \left[b^\dagger, f(b)\right] = -\frac{d\, f(b)}{d\, b} \,. \tag{B.15}$$

In particular, for any integer $n \geq 0$

$$\begin{aligned} \left[b, \left(b^\dagger\right)^n\right] &= n \left(b^\dagger\right)^{n-1} \\ \left[b^\dagger, b^n\right] &= -n b^{n-1} \\ \left[b^\dagger b, \left(b^\dagger\right)^n\right] &= b^\dagger \left[b, \left(b^\dagger\right)^n\right] = n \left(b^\dagger\right)^n \\ \left[b^\dagger b, b^n\right] &= \left[b^\dagger, b^n\right] b = -n b^n \,, \end{aligned} \tag{B.16}$$

and for all $n, k \geq 0$

$$\left[b^n, \left(b^\dagger\right)^k\right] = \sum_{m=1}^{Min(n,k)} \frac{n!k!}{m!(n-m)!(k-m)!} \left(b^\dagger\right)^{k-m} b^{n-m} \,. \tag{B.17}$$

Other useful identities include

$$\begin{aligned} e^b e^{b^\dagger} &= e^{b+b^\dagger+1/2} \\ \left[b, b^\dagger b\right]_m &= b \\ \left[\left(b^\dagger b\right)^n, b\right] &= b\left\{\left(b^\dagger b - 1\right)^n - \left(b^\dagger b\right)^n\right\} \\ \left[\exp\left\{i\alpha\pi\, b^\dagger b\right\}, b\right] &= b\, \exp\left\{i\alpha\pi\, b^\dagger b\right\} \left(e^{-i\alpha\pi} - 1\right) \\ \left[\exp\left\{i\pi\, b^\dagger b\right\}, b\right] &= -2\, b\, \exp\left\{i\pi\, b^\dagger b\right\} \qquad (\alpha = 1) \\ \left[b^\dagger, b^\dagger b\right]_m &= (-1)^m b^\dagger \,. \end{aligned}$$

$$\begin{aligned}
\left[\left(b^\dagger b\right)^n, b^\dagger\right] &= b^\dagger \left\{\left(b^\dagger b + 1\right)^n - \left(b^\dagger b\right)^n\right\} \\
\left[\exp\left\{i\alpha\pi\, b^\dagger b\right\}, b^\dagger\right] &= b^\dagger \exp\left\{i\alpha\pi\, b^\dagger b\right\} \left(e^{i\alpha\pi} - 1\right) \\
\left[\exp\left\{i\pi\, b^\dagger b\right\}, b^\dagger\right] &= -2\, b^\dagger \exp\left\{i\pi\, b^\dagger b\right\} \qquad (\alpha = 1) \\
\left[b^\dagger b, b\right]_0 &= \left[b^\dagger b, b^\dagger\right]_0 = b^\dagger b \\
\left[b^\dagger b, b\right]_1 &= -b \qquad \left[b^\dagger b, b^\dagger\right]_1 = b^\dagger \\
\left[b^\dagger b, b\right]_m &= \left[b^\dagger b, b^\dagger\right]_m = 0 \quad \forall\ m \geq 2\,, \qquad \text{(B.18)}
\end{aligned}$$

where it is important to note that the relations (B.15) are in general only valid in the case where f is strictly a function of the indicated argument only, so that a power series expansion for f of the form (B.11) exists.

Appendix C

Explicit Forms for Variational Expressions

Here explicit expressions are shown for the expectation values of the Rabi Hamiltonian, the operator σ^z and the boson number operator $b^\dagger b$ in the various variational states considered in Chapter 4. The equations which determine the corresponding variational parameters are also shown. The analytic behaviour of these parameters in the limit of small coupling is discussed in cases where this is useful for numerical purposes.

C.1 The mixed–parity two–parameter ansatz (4.30)

The expectation value of H_{Rabi} in the state (4.30) is given by

$$\begin{aligned}\langle H_{\text{Rabi}}\rangle^{\text{Var}}(x,y) &\equiv \langle \Psi^{\text{Var}}(x,y)|H_{\text{Rabi}}|\Psi^{\text{Var}}(x,y)\rangle \\ &= -\frac{1}{2}\omega_0\left(\frac{1-y^2}{1+y^2}\right)+\omega\, x^2+8g\left(\frac{yx}{1+y^2}\right) . \end{aligned} \tag{C.1}$$

The minimization of (C.1) with respect to the variational parameters x and y yields the following results [Qi98] for the optimal values x_{opt} and y_{opt}, and the variational ground–state energy $E_0^{\text{Var}} = \langle H_{\text{Rabi}}\rangle^{\text{Var}}(x_{\text{opt}}, y_{\text{opt}})$:

$$y_{\text{opt}} = x_{\text{opt}} = 0 \; , \quad E_0^{\text{Var}} = -\frac{1}{2}\omega_0 \tag{C.2}$$

for $g \le \sqrt{\omega\omega_0}/4$, and

$$\begin{aligned} y_{\text{opt}} &= \pm\sqrt{\frac{16g^2-\omega\omega_0}{16g^2+\omega\omega_0}} \\ x_{\text{opt}} &= \mp\frac{1}{8g\omega}\sqrt{256g^4-\omega^2\omega_0^2} \\ E_0^{\text{Var}} &= -\frac{4g^2}{\omega}-\frac{\omega\omega_0^2}{64g^2} \end{aligned} \tag{C.3}$$

for $g > \sqrt{\omega\omega_0}/4$. As a check, note that the correct limiting behaviour

$$y_{\text{opt}} \to \pm 1 \; , \quad x_{\text{opt}} \to \mp\frac{2g}{\omega} \; , \quad E_0^{\text{Var}} \to -\frac{4g^2}{\omega} \tag{C.4}$$

obtains as $g \to \infty$.

The expectation values of σ^z and $b^\dagger b$ are given by

$$\begin{aligned} \langle\sigma^z\rangle^{\text{Var}} &= \left(\frac{y_{\text{opt}}^2-1}{y_{\text{opt}}^2+1}\right) \\ \langle b^\dagger b\rangle^{\text{Var}} &= x_{\text{opt}}^2 \; , \end{aligned} \tag{C.5}$$

with x_{opt} and v_{opt} determined via (C.2) and (C.3).

C.2 The good–parity two–parameter ansatz (4.38)

The expectation value of H_{Rabi} in the state (4.38) is given by

$$\begin{aligned} \langle H_{\text{Rabi}}\rangle_{\pm}^{\text{PBV2}}(x,v) &\equiv \langle\Psi_{\pm}^{\text{PBV2}}(x,v)|H_{\text{Rabi}}|\Psi_{\pm}^{\text{PBV2}}(x,v)\rangle \\ &= -\frac{1}{2}\omega_0\left(\frac{1-v^2}{1+v^2}\right) \\ &\quad +\omega\left(\frac{x^2}{1+v^2}\right)\left(\left[\tanh x^2\right]^{\pm 1}+v^2\left[\coth x^2\right]^{\pm 1}\right) \\ &\quad +8g\left(\frac{xv}{1+v^2}\right)\left(1-e^{-4x^2}\right)^{-1/2} \end{aligned} \tag{C.6}$$

The derivative of $\langle H_{\text{Rabi}}\rangle_{\pm}^{\text{PBV2}}(x,v)$ with respect to v yields the first equation,

$$\begin{aligned} 0 &= \left[4\,g\,x_{\text{opt}}\left(1-\exp\left\{-4x_{\text{opt}}^2\right\}\right)^{-1/2}\right]v_{\text{opt}}^2 \\ &\quad -\left[\omega_0 \mp \omega\, x_{\text{opt}}^2\left(\tanh x_{\text{opt}}^2-\coth x_{\text{opt}}^2\right)\right]v_{\text{opt}} \\ &\quad -\left[4\,g\,x_{\text{opt}}\left(1-\exp\left\{-4x_{\text{opt}}^2\right\}\right)^{-1/2}\right], \end{aligned} \tag{C.7}$$

to be satisfied by the optimal values x_{opt} and v_{opt}. For the case of positive parity (*i.e.* for the ground state), the derivative of $\langle H_{\text{Rabi}}\rangle_{+}^{\text{PBV2}}(x,v)$ with respect to x yields the second variational equation

$$\begin{aligned} 0 &= \omega\, x_{\text{opt}}\left(\tanh x_{\text{opt}}^2+v_{\text{opt}}^2\coth x_{\text{opt}}^2\right) \\ &\quad +\omega\, x_{\text{opt}}^3\left(\left[\operatorname{sech} x_{\text{opt}}^2\right]^2-v_{\text{opt}}^2\left[\operatorname{csch} x_{\text{opt}}^2\right]^2\right) \\ &\quad +4\,g\,v_{\text{opt}}\left(1-\exp\left\{-4x_{\text{opt}}^2\right\}\right)^{-1/2}\times \\ &\quad \left(1-\frac{4x_{\text{opt}}^2\exp\left\{-4x_{\text{opt}}^2\right\}}{1-\exp\left\{-4x_{\text{opt}}^2\right\}}\right). \end{aligned} \tag{C.8}$$

The corresponding expression for the negative–parity (first excited) state is obtained by making the substitutions

$$\begin{aligned} \tanh x_{\text{opt}}^2 &\longleftrightarrow \coth x_{\text{opt}}^2 \\ \left[\operatorname{sech} x_{\text{opt}}^2\right]^2 &\longleftrightarrow -\left[\operatorname{csch} x_{\text{opt}}^2\right]^2. \end{aligned} \tag{C.9}$$

Note that (C.7), being quadratic in $v_{\rm opt}$, is easily solved to yield an analytic expression for the parameter $v_{\rm opt}$ in terms of $x_{\rm opt}$, so that the variational (PBV) approach based on the two–parameter state (4.38) thus only requires the numerical solution of one non–linear equation (C.8) in the single unknown $x_{\rm opt}$.

The expectation values of σ^z and the photon number operator $b^\dagger b$ in the state (4.38) are given by

$$\begin{aligned}
\langle\sigma^z\rangle^{\rm PBV2} &= \left(\frac{v_{\rm opt}^2-1}{v_{\rm opt}^2+1}\right) \\
\langle b^\dagger b\rangle^{\rm PBV2} &= \frac{x_{\rm opt}^2}{v_{\rm opt}^2+1}\left(\tanh x_{\rm opt}^2 + v_{\rm opt}^2\coth x_{\rm opt}^2\right) , \qquad \text{(C.10)}
\end{aligned}$$

with $x_{\rm opt}$ and $v_{\rm opt}$ determined via the variational equations (C.7) and (C.8).

C.3 The good–parity three–parameter ansatz (4.41)

In the state (4.41), $H_{\rm Rabi}$ has the expectation value

$$\begin{aligned}
\langle H_{\rm Rabi}\rangle_\pm^{\rm PBV3}(x_1,x_2,v) &\equiv \langle\Psi_\pm^{\rm PBV3}(x_1,x_2,v)|H_{\rm Rabi}|\Psi_\pm^{\rm PBV3}(x_1,x_2,v)\rangle \\
&= A_v^2\left[\frac{1}{2}\omega_0(v^2-1)\right. \\
&+ \omega\left(x_1^2\left[\tanh x_1^2\right]^{\pm1} + v^2x_2^2\left[\coth x_2^2\right]^{\pm1}\right) \\
&+ \left. 8gvB_\pm(x_1,x_2)\right] \qquad \text{(C.11)}
\end{aligned}$$

with

$$B_\pm(x_1,x_2) = A_{1,\pm}A_{2,\mp}\left\{(x_2+x_1)e^{-(x_1-x_2)^2/2} \pm (x_2-x_1)e^{-(x_1+x_2)^2/2}\right\} . \qquad \text{(C.12)}$$

The minimization of $\langle H_{\mathrm{Rabi}}\rangle_{\pm}^{\mathrm{PBV3}}(x_1, x_2, v)$ with respect to v yields a quadratic equation for v_{opt} in terms of $x_{1,\mathrm{opt}}$ and $x_{2,\mathrm{opt}}$. The solution with the lowest energy is always given by

$$v_{\mathrm{opt}} = \frac{\omega_0 + \omega C_{\pm}(x_{1,\mathrm{opt}}, x_{2,\mathrm{opt}})}{8gB_{\pm}(x_{1,\mathrm{opt}}, x_{2,\mathrm{opt}})} - \sqrt{1 + \left(\frac{\omega_0 + \omega C_{\pm}(x_{1,\mathrm{opt}}, x_{2,\mathrm{opt}})}{8gB_{\pm}(x_{1,\mathrm{opt}}, x_{2,\mathrm{opt}})}\right)^2}, \quad \text{(C.13)}$$

where

$$C_{\pm}(x_1, x_2) = -x_1^2\left[\tanh x_1^2\right]^{\pm 1} + x_2^2\left[\coth x_2^2\right]^{\pm 1}.$$

For the ground state, we are then left with the two coupled non-linear equations to be solved numerically for $x_{1,\mathrm{opt}}$ and $x_{2,\mathrm{opt}}$, namely

$$\begin{aligned}
0 &= \omega\, x_{1,\mathrm{opt}}\left(\tanh x_{\mathrm{opt}}^2 + x_{1,\mathrm{opt}}^2\left[\mathrm{sech}\, x_{\mathrm{opt}}^2\right]^2\right) \\
&+ 4\, g\, v_{\mathrm{opt}} x_{1,\mathrm{opt}}\left(1 + \exp\left\{-2x_{1,\mathrm{opt}}^2\right\}\right)^{-3/2}\left(1 - \exp\left\{-2x_{2,\mathrm{opt}}^2\right\}\right)^{-1/2} \times \\
&\quad \exp\left\{-2x_{1,\mathrm{opt}}^2\right\} \times \left(\left[x_{2,\mathrm{opt}} + x_{1,\mathrm{opt}}\right]\exp\left\{-\frac{1}{2}\left[x_{1,\mathrm{opt}} - x_{2,\mathrm{opt}}\right]^2\right\}\right. \\
&\quad \left. + \left[x_{2,\mathrm{opt}} - x_{1,\mathrm{opt}}\right]\exp\left\{-\frac{1}{2}\left[x_{1,\mathrm{opt}} + x_{2,\mathrm{opt}}\right]^2\right\}\right) \\
&+ 2\, g\, v_{\mathrm{opt}}\left(1 + \exp\left\{-2x_{1,\mathrm{opt}}^2\right\}\right)^{-1/2}\left(1 - \exp\left\{-2x_{2,\mathrm{opt}}^2\right\}\right)^{-1/2} \times \\
&\quad \left[x_{2,\mathrm{opt}}^2 - x_{1,\mathrm{opt}}^2 + 1\right] \times \\
&\quad \left(\exp\left\{-\frac{1}{2}\left[x_{1,\mathrm{opt}} - x_{2,\mathrm{opt}}\right]^2\right\} - \exp\left\{-\frac{1}{2}\left[x_{1,\mathrm{opt}} + x_{2,\mathrm{opt}}\right]^2\right\}\right) \qquad \text{(C.14)}
\end{aligned}$$

and

$$\begin{aligned}
0 &= \omega v_{\mathrm{opt}}^2\, x_{2,\mathrm{opt}}\left(\coth x_{\mathrm{opt}}^2 - x_{2,\mathrm{opt}}^2\left[\mathrm{csch}\, x_{\mathrm{opt}}^2\right]^2\right) \\
&- 4\, g\, v_{\mathrm{opt}} x_{2,\mathrm{opt}}\left(1 + \exp\left\{-2x_{1,\mathrm{opt}}^2\right\}\right)^{-1/2}\left(1 - \exp\left\{-2x_{2,\mathrm{opt}}^2\right\}\right)^{-3/2} \times \\
&\quad \exp\left\{-2x_{2,\mathrm{opt}}^2\right\} \times \left(\left[x_{2,\mathrm{opt}} + x_{1,\mathrm{opt}}\right]\exp\left\{-\frac{1}{2}\left[x_{1,\mathrm{opt}} - x_{2,\mathrm{opt}}\right]^2\right\}\right. \\
&\quad \left. + \left[x_{2,\mathrm{opt}} - x_{1,\mathrm{opt}}\right]\exp\left\{-\frac{1}{2}\left[x_{1,\mathrm{opt}} + x_{2,\mathrm{opt}}\right]^2\right\}\right) \\
&+ 2\, g\, v_{\mathrm{opt}}\left(1 + \exp\left\{-2x_{1,\mathrm{opt}}^2\right\}\right)^{-1/2}\left(1 - \exp\left\{-2x_{2,\mathrm{opt}}^2\right\}\right)^{-1/2} \times
\end{aligned}$$

$$\left[x_{1,\text{opt}}^2 - x_{2,\text{opt}}^2 + 1\right] \times$$
$$\left(\exp\left\{-\frac{1}{2}\left[x_{1,\text{opt}} - x_{2,\text{opt}}\right]^2\right\} + \exp\left\{-\frac{1}{2}\left[x_{1,\text{opt}} + x_{2,\text{opt}}\right]^2\right\}\right) . \quad \text{(C.15)}$$

The corresponding expressions for the first excited state are obtained by making the substitutions

$$\begin{aligned}
\exp\left\{-2x_{i,\text{opt}}^2\right\} &\longleftrightarrow -\exp\left\{-2x_{i,\text{opt}}^2\right\} \qquad (i = 1, 2) \\
\exp\left\{-\frac{1}{2}\left[x_{1,\text{opt}} + x_{2,\text{opt}}\right]^2\right\} &\longleftrightarrow -\exp\left\{-\frac{1}{2}\left[x_{1,\text{opt}} + x_{2,\text{opt}}\right]^2\right\} \\
\tanh x_{\text{opt}}^2 &\longleftrightarrow \coth x_{\text{opt}}^2 \\
\left[\text{sech } x_{\text{opt}}^2\right]^2 &\longleftrightarrow -\left[\text{csch } x_{\text{opt}}^2\right]^2 . \qquad \text{(C.16)}
\end{aligned}$$

We note that there are classes of solutions with $x_{1,\text{opt}} = 0$ (ground state) and $x_{2,\text{opt}} = 0$ (excited state), but these do not minimize the energies, and so are not considered.

In the limit of very small couplings, it is possible to obtain asymptotic expressions for the parameters v_{opt}, $x_{1,\text{opt}}$ and $x_{2,\text{opt}}$, for the ground state,

$$\begin{aligned}
v_{\text{opt}} &\rightarrow \frac{-2g}{\omega + \omega_0}, \\
x_{1,\text{opt}} &\rightarrow \frac{2g}{\omega}\left\{1 + \frac{\omega_0}{\omega}\right\}^{-1/2}, \qquad \text{(C.17)} \\
x_{2,\text{opt}} &\rightarrow \frac{2g}{\omega}\left\{1 + \frac{\omega_0}{3\omega}\right\}^{-1/2},
\end{aligned}$$

which yield good starting values for the numerical solution routines.

The situation for the first excited state is more complex, and depends explicitly on whether the system is sub- or supra-resonant. In fact, for the sub-resonant case ($\omega < \omega_0$), the asymptotic forms are the solutions of transcendental equations; however, one can show that in the limit of zero coupling, $x_{1,\text{opt}}$ and v_{opt} are zero, but $x_{2,\text{opt}}$ is a non-zero constant dependent on the frequencies. For the other two cases, the asymptotic expression are

$$\begin{aligned} v_{\text{opt}} &\rightarrow -1 \\ x_{1,\text{opt}} &\rightarrow \frac{\sqrt{6}g}{\omega} \\ x_{2,\text{opt}} &\rightarrow \sqrt{\frac{2g}{\omega}} \end{aligned} \tag{C.18}$$

for the case $\omega_0 = \omega$, and

$$\begin{aligned} v_{\text{opt}} &\rightarrow \frac{\omega_0 - \omega}{2g} \\ x_{1,\text{opt}} &\rightarrow \frac{2g}{\omega}\left\{1 - \frac{\omega_0}{3\omega}\right\}^{-1/2}, \\ x_{2,\text{opt}} &\rightarrow \frac{2g}{\omega}\left\{1 - \frac{\omega_0}{\omega}\right\}^{-1/2}, \end{aligned} \tag{C.19}$$

for the case $\omega_0 < \omega$.

The expectation values of σ^z and the photon number operator $b^\dagger b$ in the three–parameter variational state (4.41) are given by

$$\begin{aligned} \langle \sigma^z \rangle^{\text{PBV3}} &= \left(\frac{v_{\text{opt}}^2 - 1}{v_{\text{opt}}^2 + 1} \right) \\ \left\langle b^\dagger b \right\rangle^{\text{PBV3}} &= \frac{1}{v_{\text{opt}}^2 + 1} \left(x_{1,\text{opt}}^2 \tanh x_{1,\text{opt}}^2 + v_{\text{opt}}^2 x_{2,\text{opt}}^2 \coth x_{2,\text{opt}}^2 \right). \end{aligned} \tag{C.20}$$

It is often useful to express the wavefunctions for Hamiltonians such as the Rabi Hamiltonian in terms of their expansion in a basis of products of oscillator and two-level states, as these are often the form in which initial conditions are formulated. We present here the expansions for the three-parameter ansätze for the ground and first excited states:

$$
\begin{aligned}
|\Psi_+^{\mathrm{PBV3}}(x_1,x_2,v)\rangle &= A_v\left[A_{1,+}\,e^{-x_1^2/2}\sum_{n=0}^{\infty}\frac{x_1^{2n}}{\sqrt{(2n)!}}|2n\rangle|\downarrow\rangle\right.\\
&\quad\left.+\ vA_{2,-}\,e^{-x_2^2/2}\sum_{n=0}^{\infty}\frac{x_2^{2n+1}}{\sqrt{(2n+1)!}}|2n+1\rangle|\uparrow\rangle\right]\\
|\Psi_-^{\mathrm{PBV3}}(x_1,x_2,v)\rangle &= A_v\left[A_{1,-}\,e^{-x_1^2/2}\sum_{n=0}^{\infty}\frac{x_1^{2n+1}}{\sqrt{(2n+1)!}}|2n+1\rangle|\downarrow\rangle\right.\\
&\quad\left.+\ vA_{2,+}\,e^{-x_2^2/2}\sum_{n=0}^{\infty}\frac{x_2^{2n}}{\sqrt{(2n)!}}|2n\rangle|\uparrow\rangle\right]. \qquad \text{(C.21)}
\end{aligned}
$$

The expansions for the two-parameter states can be found by setting $x_1 = x_2 = x$ in these equations.

Appendix D

Explicit Forms for CCM Expressions

We present here explicit expressions for the similarity transformed Hamiltonian (3.5) and the CCM equations (3.14) for the various CCM schemes employed in the ground–state analysis of the Rabi Hamiltonian (see Table D.1). Where quantities other than the ground–state energy are required, we also give expressions for the energy functional $\overline{H}_{\text{Rabi}}$ and the expectation value of these quantities in the CCM.

In Table D.2, we also show how the four ground–state CCM schemes may be modified to deal with the odd–parity first excited state of the Rabi Hamiltonian. It is intuitively clear, however, that the first excited state results may be obtained from the ground–state formalism by making the replacement $\omega_0 \rightarrow -\omega_0$, and in practice we have taken this simpler route to generate, in addition to the ground–state results, first excited state results for the each of the CCM schemes considered here.

Table D.1: *The four schemes, labelled I—IV, employed in the ground–state CCM analysis of the (unrotated) Rabi Hamiltonian, showing the choice of model state* $|\Phi\rangle$ *and cluster correlation operators for each scheme. For all schemes, the cluster correlation operator* S*, which is required for the calculation of the NCCM ground–state energy, is shown. For Schemes I and III, the operator* $\tilde{S}$*, which is required for the calculation of other ground–state properties of the system in the NCCM, is shown, and for Scheme I, the operator* Σ *required for an ECCM ground–state energy calculation is also shown.*

Scheme	Model state $\|\Phi\rangle$	Cluster correlation operators S, $\tilde{S}$, Σ
I	$\|0\rangle\|\downarrow\rangle$	$S = S_1 + S_2$ $S_1 = \sum_{n=1}^{\infty} s_n^{(1)} (b^\dagger)^n$ $S_2 = \sum_{n=1}^{\infty} s_n^{(2)} (b^\dagger)^{n-1} \sigma^+$ $\tilde{S} = 1 + \tilde{S}_1 + \tilde{S}_2$ $\tilde{S}_1 = \sum_{n=1}^{\infty} \tilde{s}_n^{(1)} b^n$ $\tilde{S}_2 = \sum_{n=1}^{\infty} \tilde{s}_n^{(2)} b^{n-1} \sigma^-$ $\Sigma = \Sigma_1 + \Sigma_2$ $\Sigma_1 = \sum_{n=1}^{\infty} \sigma_n^{(1)} b^n$ $\Sigma_2 = \sum_{n=1}^{\infty} \sigma_n^{(2)} b^{n-1} \sigma^-$
II	$\|0\rangle\|\downarrow\rangle$	$S = \sum_{n=1}^{\infty} s_n \left(c^\dagger\right)^n, \quad c^\dagger = b^\dagger \sigma^x$
III	$\|\Psi_+\rangle$ [see (4.16)]	$S = \sum_{n=1}^{\infty} s_n \left(c^\dagger\right)^n, \quad c^\dagger = b^\dagger \sigma^x + 2g/\omega$ $\tilde{S} = 1 + \sum_{n=1}^{\infty} \tilde{s}_n c^n, \quad c = b \sigma^x + 2g/\omega$
IV	$\|\Psi_+^{\mathrm{PBV2}}(x_{\mathrm{opt}}, v_{\mathrm{opt}})\rangle$ [see (4.38)]	$S = \sum_{n=1}^{\infty} s_n \left(c^\dagger\right)^n, \quad c^\dagger = b^\dagger \sigma^x$

Table D.2: *The four schemes, labelled I'—IV', employed in the CCM analysis of the first excited state of the Rabi Hamiltonian, showing the choice of model state $|\Phi\rangle$ and cluster correlation operators for each scheme. For all primed schemes, the cluster correlation operator S is identical to that used for the corresponding unprimed (ground-state) scheme, and the model state is chosen so as to incorporate the odd-parity symmetry of the first excited state.*

Scheme	Model state $\|\Phi\rangle$	Cluster correlation operators S, $\tilde{S}$, Σ
I'	$\|0\rangle\|\uparrow\rangle$	$S = S_1 + S_2$ $S_1 = \sum_{n=1}^{\infty} s_n^{(1)} (b^\dagger)^n$ $S_2 = \sum_{n=1}^{\infty} s_n^{(2)} (b^\dagger)^{n-1}\sigma^+$ $\tilde{S} = 1 + \tilde{S}_1 + \tilde{S}_2$ $\tilde{S}_1 = \sum_{n=1}^{\infty} \tilde{s}_n^{(1)} b^n$ $\tilde{S}_2 = \sum_{n=1}^{\infty} \tilde{s}_n^{(2)} b^{n-1}\sigma^-$ $\Sigma = \Sigma_1 + \Sigma_2$ $\Sigma_1 = \sum_{n=1}^{\infty} \sigma_n^{(1)} b^n$ $\Sigma_2 = \sum_{n=1}^{\infty} \sigma_n^{(2)} b^{n-1}\sigma^-$
II'	$\|0\rangle\|\uparrow\rangle$	$S = \sum_{n=1}^{\infty} s_n \left(c^\dagger\right)^n$, $\quad c^\dagger = b^\dagger\sigma^x$
III'	$\|\Psi_-\rangle$ [see (4.16)]	$S = \sum_{n=1}^{\infty} s_n \left(c^\dagger\right)^n$, $\quad c^\dagger = b^\dagger\sigma^x + 2g/\omega$ $\tilde{S} = 1 + \sum_{n=1}^{\infty} \tilde{s}_n c^n$, $\quad c = b\sigma^x + 2g/\omega$
IV'	$\|\Psi_-^{\mathrm{PBV2}}(x_{\mathrm{opt}}, v_{\mathrm{opt}})\rangle$ [see (4.38)]	$S = \sum_{n=1}^{\infty} s_n \left(c^\dagger\right)^n$, $\quad c^\dagger = b^\dagger\sigma^x$

D.1 NCCM Scheme I

For Scheme I, we obtain the following form for the similarity transformed Hamiltonian:

$$
\begin{aligned}
e^{-S}H_{\text{Rabi}}e^{S} &= \frac{1}{2}\omega_0\sigma^z + \omega b^\dagger b + g\left(b^\dagger + b\right)\left(\sigma^+ + \sigma^-\right) \\
&+ \sum_{n=1}^{\infty} s_n^{(1)}\left\{n\omega\left(b^\dagger\right)^n + ng\left(b^\dagger\right)^{n-1}\left(\sigma^+ + \sigma^-\right)\right\} \\
&+ \sum_{n=1}^{\infty} s_n^{(2)}\left\{[(n-1)\omega + \omega_0]\left(b^\dagger\right)^{n-1}\sigma^+ \right. \\
&\qquad \left. + g(n-1)\left(b^\dagger\right)^{n-2}\sigma^-\sigma^+ - 4g\left(b^\dagger\right)^{n-1}\left(b^\dagger + b\right)\sigma^z\right\} \\
&-4g\sum_{n=1}^{\infty}\sum_{n'=1}^{\infty} s_n^{(1)}s_{n'}^{(2)}\left\{n\left(b^\dagger\right)^{n+n'-2}\sigma^z\right\} \\
&-4g\sum_{n=1}^{\infty}\sum_{n'=1}^{\infty} s_n^{(2)}s_{n'}^{(2)}\left\{(n-1)\left(b^\dagger\right)^{n+n'-3}\sigma^z\sigma^+ \right. \\
&\qquad \left. + \left(b^\dagger\right)^{n+n'-2}\left(b^\dagger + b\right)\sigma^+\right\} \\
&-4g\sum_{n=1}^{\infty}\sum_{n'=1}^{\infty}\sum_{n''=1}^{\infty} s_n^{(1)}s_{n'}^{(2)}s_{n''}^{(2)}\left\{n\left(b^\dagger\right)^{n+n'+n''-3}\sigma^+\right\} . \qquad \text{(D.1)}
\end{aligned}
$$

The energy functional

$$
\begin{aligned}
\overline{H} &= \langle\Phi|\tilde{S}e^{-S}H_{\text{Rabi}}e^{S}|\Phi\rangle \\
&= -\frac{1}{2}\omega_0 + 4g\ s_2^{(2)} + 4g\ s_1^{(1)}s_1^{(2)} \\
&+ \sum_{k=1}^{\infty} k!\ \tilde{s}_k^{(1)}\left\{\omega k\ s_k^{(1)} + 4g\ s_k^{(2)} + 4g(k+1)\ s_{k+2}^{(2)} + 4g\sum_{n=1}^{k+1} n\ s_n^{(1)}s_{k+2-n}^{(2)}\right\} \\
&+4\sum_{k=1}^{\infty}(k-1)!\ \tilde{s}_k^{(2)}\left\{g\delta_{k,2} + gk\ s_k^{(1)} + [\omega(k-1) + \omega_0]\ s_k^{(2)} \right. \\
&\qquad -4g\sum_{n=1}^{k+1}(n-1)\ s_n^{(2)}s_{k+2-n}^{(2)} - 4g\sum_{n=1}^{k-1} s_n^{(2)}s_{k-n}^{(2)} \\
&\qquad \left. -4g\sum_{n=1}^{k}\sum_{n'=1}^{k+1-n} n\ s_n^{(1)}s_{n'}^{(2)}s_{k+2-n-n'}^{(2)}\right\} . \qquad \text{(D.2)}
\end{aligned}
$$

may now be used to set up the CCM equations (3.14) for $\left\{s_k^{(1)}, s_k^{(2)};\ k=1,2,3,\ldots\right\}$,

$$\begin{aligned}
0 &= \omega k\ s_k^{(1)} + 4g\ s_k^{(2)} + 4g(k+1)\ s_{k+2}^{(2)} + 4g\sum_{n=1}^{k+1} n\ s_n^{(1)} s_{k+2-n}^{(2)} \\
0 &= g\delta_{k,2} + gk\ s_k^{(1)} + \left[\omega(k-1)+\omega_0\right]\ s_k^{(2)} - 4g\sum_{n=1}^{k+1}(n-1)\ s_n^{(2)} s_{k+2-n}^{(2)} \\
&\quad -4g\sum_{n=1}^{k-1} s_n^{(2)} s_{k-n}^{(2)} - 4g\sum_{n=1}^{k}\sum_{n'=1}^{k+1-n} n\ s_n^{(1)} s_{n'}^{(2)} s_{k+2-n-n'}^{(2)}\ ,
\end{aligned} \tag{D.3}$$

and for $\left\{\tilde{s}_k^{(1)}, \tilde{s}_k^{(2)};\ k=1,2,3,\ldots\right\}$:

$$\begin{aligned}
0 &= 4g\delta_{k,1}\ s_1^{(2)} + \omega k!\ \tilde{s}_k^{(1)} + 4g(k-1)!\ \tilde{s}_k^{(2)} + 4g\sum_{n=Max[k-1,1]}^{\infty} n!\ \tilde{s}_n^{(1)} s_{n+2-k}^{(2)} \\
&\quad -16g\sum_{n=k}^{\infty}\sum_{n'=1}^{n+1-k}(n-1)!\ \tilde{s}_n^{(2)} s_{n'}^{(2)} s_{n+2-k-n'}^{(2)} \\
0 &= g\ \delta_{k,2} + g\delta_{k,1}\ s_1^{(1)} + gk!\ \tilde{s}_k^{(1)} + g(k-1)!(1-\delta_{k,1})(1-\delta_{k,2})\ \tilde{s}_{k-2}^{(1)} \\
&\quad +(k-1)!\left[\omega(k-1)+\omega_0\right]\ \tilde{s}_k^{(2)} + g\sum_{n=Max[k-1,1]}^{\infty} n!(n+2-k)\ \tilde{s}_n^{(1)} s_{n+2-k}^{(1)} \\
&\quad -4g\sum_{n=Max[k-1,1]}^{\infty} n!\ \tilde{s}_n^{(2)} s_{n+2-k}^{(2)} - 8g\sum_{n=k+1}^{\infty}(n-1)!\ \tilde{s}_n^{(2)} s_{n-k}^{(2)} \\
&\quad -8g\sum_{n=k}^{\infty}\sum_{n'=1}^{n+1-k}(n-1)!n'\ \tilde{s}_n^{(2)} s_{n'}^{(1)} s_{n+2-k-n'}^{(2)}\ .
\end{aligned} \tag{D.4}$$

Note that equations (D.3) may be solved for $\left\{s_k^{(1)}, s_k^{(2)}\right\}$, so that these coefficients are known quantities when solving (D.4). The expectation value of σ^z assumes the form

$$\langle\sigma^z\rangle^{\mathrm{NCCM,I}} = -1 + 8\sum_{k=1}^{\infty}(k-1)!\ \tilde{s}_k^{(2)} s_k^{(2)}\ . \tag{D.5}$$

D.1.1 Termination of the even–parity NCCM Scheme I calculation

If the CCM calculation is restricted to the even–parity sector, then

$$s_n^{(1)} = s_n^{(2)} = 0 \tag{D.6}$$

for all odd n, and the only coefficient required in order to determine the CCM ground–state energy is $z \equiv s_2^{(2)}$. In the SUB-2 approximation, the equations (D.3) then reduce to

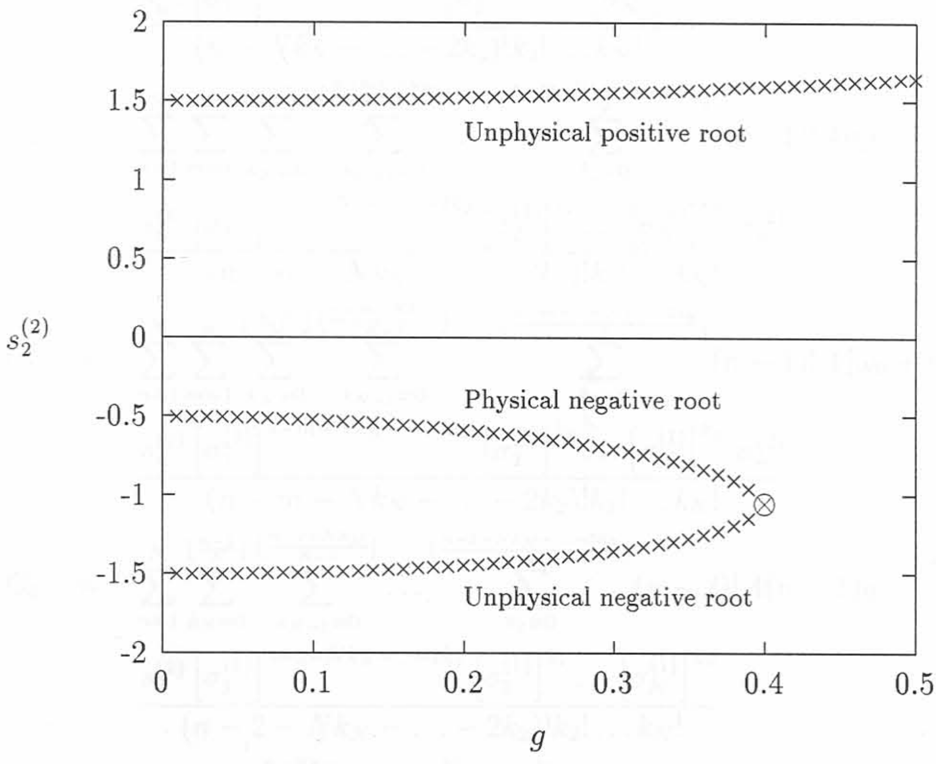
$$z^3 - \frac{\omega_0}{4g} z^2 - \frac{\omega(\omega+\omega_0)}{16g^2} z - \frac{\omega}{16g} = 0 \, . \tag{D.7}$$

For $g \to 0$ at scaled resonance ($\omega = \omega_0 = 1$), equation (D.7) has one real root corresponding to a positive, and two real roots corresponding to a negative ground–state energy. One of the latter roots describes the exact ground state at $g = 0$, and the other gives a spurious solution with lower energy. As the coupling g is increased, these two roots meet and form a complex conjugate pair at

$$g_c^{(2)} = 3\left(20 + 14\sqrt{7}\right)^{-1/2} = 0.3972 \, . \tag{D.8}$$

Thus the physical even–parity SUB-2 solution terminates at this point, above which there exist only a single real root corresponding to an unphysical positive ground–state energy, and a pair of complex conjugate roots corresponding to a complex ground–state energy. This behaviour is illustrated in Figure D.1. In the even–parity SUB-N approximation, it may be shown using *Mathematica* [Mat] that the CCM equations (D.3) may always be reduced to a polynomial of order $N + 1$ in z, and for all $N/2$ odd behaviour similar to that in the SUB-2 case is observed. In the case $N/2$ even, there is no unphysical negative root for $s_2^{(2)}$ which, together with the physical root, can form a complex pair at finite coupling, and the physical solution therefore does not terminate. In this case, however, the CCM ground–state energy corresponding to the physical root peels off the exact ground–state energy in the same coupling region where the $N/2$ odd solution terminates.

Figure D.1: *The behaviour of the three roots for the single CCM coefficient* $s_2^{(2)}$ *in the even–parity SUB-2 NCCM Scheme I analysis of the scaled resonant* $(\omega = \omega_0 = 1)$ *Rabi Hamiltonian. The termination point at* $g = g_c^{(2)} = 0.3972$, *where the physical and unphysical negative roots meet to form a complex conjugate pair, is indicated by the symbol* $\otimes$.



D.2 ECCM Scheme I

The similarity transform $e^{-S}H_{\text{Rabi}}e^{S}$ has the same form as for the NCCM, but the functional $\overline{H}$ in the ECCM SUB-N approximation is now given by

$$\overline{H} = \langle\Phi|e^{\Sigma}e^{-S}H_{\text{Rabi}}e^{S}|\Phi\rangle = \sum_{i=1}^{11} C_i \tag{D.9}$$

with

$$C_1 = -\frac{1}{2}\omega_0$$

$$C_2 = 4g\,\sigma_1^{(2)}$$

$$C_3 = \sum_{n=1}^{N}\sum_{k_N=0}^{\lfloor\frac{n}{N}\rfloor}\sum_{k_{N-1}=0}^{\lfloor\frac{n-Nk_N}{N-1}\rfloor}\cdots\sum_{k_2=0}^{\lfloor\frac{n-Nk_N-\ldots-3k_3}{2}\rfloor} n!\,n\omega \frac{s_n^{(1)}\left[\sigma_1^{(1)}\right]^{n-Nk_N-\ldots-2k_2}\left[\sigma_2^{(1)}\right]^{k_2}\cdots\left[\sigma_N^{(1)}\right]^{k_N}}{(n-Nk_N-\ldots-2k_2)!k_2!\ldots k_N!}$$

$$C_4 = \sum_{n=1}^{N}\sum_{m=1}^{n}\sum_{k_N=0}^{\lfloor\frac{n-m}{N}\rfloor}\sum_{k_{N-1}=0}^{\lfloor\frac{n-m-Nk_N}{N-1}\rfloor}\cdots\sum_{k_2=0}^{\lfloor\frac{n-m-Nk_N-\ldots-3k_3}{2}\rfloor}(n-1)!\,4ng \frac{s_n^{(1)}\left[\sigma_1^{(1)}\right]^{n-m-Nk_N-\ldots-2k_2}\left[\sigma_2^{(1)}\right]^{k_2}\cdots\left[\sigma_N^{(1)}\right]^{k_N}\sigma_m^{(2)}}{(n-m-Nk_N-\ldots-2k_2)!k_2!\ldots k_N!}$$

$$C_5 = \sum_{n=1}^{N}\sum_{m=1}^{n}\sum_{k_N=0}^{\lfloor\frac{n-m}{N}\rfloor}\sum_{k_{N-1}=0}^{\lfloor\frac{n-m-Nk_N}{N-1}\rfloor}\cdots\sum_{k_2=0}^{\lfloor\frac{n-m-Nk_N-\ldots-3k_3}{2}\rfloor}(n-1)!\,4\left[\omega_0+(n-1)\omega\right] \frac{s_n^{(2)}\left[\sigma_1^{(1)}\right]^{n-m-Nk_N-\ldots-2k_2}\left[\sigma_2^{(1)}\right]^{k_2}\cdots\left[\sigma_N^{(1)}\right]^{k_N}\sigma_m^{(2)}}{(n-m-Nk_N-\ldots-2k_2)!k_2!\ldots k_N!}$$

$$C_6 = \sum_{n=1}^{N}\sum_{k_N=0}^{\lfloor\frac{n-2}{N}\rfloor}\sum_{k_{N-1}=0}^{\lfloor\frac{n-2-Nk_N}{N-1}\rfloor}\cdots\sum_{k_2=0}^{\lfloor\frac{n-2-Nk_N-\ldots-3k_3}{2}\rfloor}(n-2)!\,4(n-1)g \frac{s_n^{(2)}\left[\sigma_1^{(1)}\right]^{n-2-Nk_N-\ldots-2k_2}\left[\sigma_2^{(1)}\right]^{k_2}\cdots\left[\sigma_N^{(1)}\right]^{k_N}}{(n-2-Nk_N-\ldots-2k_2)!k_2!\ldots k_N!}$$

$$C_7 = \sum_{n=1}^{N}\sum_{k_N=0}^{\lfloor\frac{n}{N}\rfloor}\sum_{k_{N-1}=0}^{\lfloor\frac{n-Nk_N}{N-1}\rfloor}\cdots\sum_{k_2=0}^{\lfloor\frac{n-Nk_N-\ldots-3k_3}{2}\rfloor} n!\,4g$$

$$\frac{s_n^{(2)}\left[\sigma_1^{(1)}\right]^{n-Nk_N-\ldots-2k_2}\left[\sigma_2^{(1)}\right]^{k_2}\ldots\left[\sigma_N^{(1)}\right]^{k_N}}{(n-Nk_N-\ldots-2k_2)!k_2!\ldots k_N!}$$

$$C_8 = \sum_{n,n'=1}^{N}\sum_{k_N=0}^{\lfloor\frac{n+n'-2}{N}\rfloor}\sum_{k_{N-1}=0}^{\lfloor\frac{n+n'-2-Nk_N}{N-1}\rfloor}\cdots\sum_{k_2=0}^{\lfloor\frac{n+n'-2-Nk_N-\ldots-3k_3}{2}\rfloor}(n+n'-2)!\,4ng$$

$$\frac{s_n^{(1)}s_{n'}^{(2)}\left[\sigma_1^{(1)}\right]^{n+n'-2-Nk_N-\ldots-2k_2}\left[\sigma_2^{(1)}\right]^{k_2}\ldots\left[\sigma_N^{(1)}\right]^{k_N}}{(n+n'-2-Nk_N-\ldots-2k_2)!k_2!\ldots k_N!}$$

$$C_9 = -\sum_{n,n'=1}^{N}\sum_{m=1}^{Min[n+n'-2,N]}\sum_{k_N=0}^{\lfloor\frac{n+n'-m-2}{N}\rfloor}\sum_{k_{N-1}=0}^{\lfloor\frac{n+n'-m-2-Nk_N}{N-1}\rfloor}\cdots$$

$$\cdots\sum_{k_2=0}^{\lfloor\frac{n+n'-m-2-Nk_N-\ldots-3k_3}{2}\rfloor}(n+n'-3)!\,16(n-1)g$$

$$\frac{s_n^{(2)}s_{n'}^{(2)}\left[\sigma_1^{(1)}\right]^{n+n'-m-2-Nk_N-\ldots-2k_2}\left[\sigma_2^{(1)}\right]^{k_2}\ldots\left[\sigma_N^{(1)}\right]^{k_N}\sigma_m^{(2)}}{(n+n'-m-2-Nk_N-\ldots-2k_2)!k_2!\ldots k_N!}$$

$$C_{10} = -\sum_{n,n'=1}^{N}\sum_{m=1}^{Min[n+n',N]}\sum_{k_N=0}^{\lfloor\frac{n+n'-m}{N}\rfloor}\sum_{k_{N-1}=0}^{\lfloor\frac{n+n'-m-Nk_N}{N-1}\rfloor}\cdots$$

$$\cdots\sum_{k_2=0}^{\lfloor\frac{n+n'-m-Nk_N-\ldots-3k_3}{2}\rfloor}(n+n'-1)!\,16g$$

$$\frac{s_n^{(2)}s_{n'}^{(2)}\left[\sigma_1^{(1)}\right]^{n+n'-m-Nk_N-\ldots-2k_2}\left[\sigma_2^{(1)}\right]^{k_2}\ldots\left[\sigma_N^{(1)}\right]^{k_N}\sigma_m^{(2)}}{(n+n'-m-Nk_N-\ldots-2k_2)!k_2!\ldots k_N!}$$

$$C_{11} = -\sum_{n,n',n''=1}^{N}\sum_{m=1}^{Min[n+n'+n''-2,N]}\sum_{k_N=0}^{\lfloor\frac{n+n'+n''-2-m}{N}\rfloor}\sum_{k_{N-1}=0}^{\lfloor\frac{n+n'+n''-2-m-Nk_N}{N-1}\rfloor}\cdots$$

$$\cdots\sum_{k_2=0}^{\lfloor\frac{n+n'+n''-2-m-Nk_N-\ldots-3k_3}{2}\rfloor}(n+n'+n''-3)!\,16ng\;s_n^{(1)}s_{n'}^{(2)}s_{n''}^{(2)}$$

$$\frac{\left[\sigma_1^{(1)}\right]^{n+n'+n''-m-2-Nk_N-\ldots-2k_2}\left[\sigma_2^{(1)}\right]^{k_2}\ldots\left[\sigma_N^{(1)}\right]^{k_N}\sigma_m^{(2)}}{(n+n'+n''-2-m-Nk_N-\ldots-2k_2)!k_2!\ldots k_N!}\,. \tag{D.10}$$

The $4N$ ECCM Scheme I equations are

$$\frac{\partial\overline{H}}{\partial s_k^{(1)}} = 0 = \frac{\partial\overline{H}}{\partial s_k^{(2)}}\,, \quad \frac{\partial\overline{H}}{\partial\sigma_k^{(1)}} = 0 = \frac{\partial\overline{H}}{\partial\sigma_k^{(2)}} \qquad k=1,2,\ldots,N\,. \tag{D.11}$$

D.2.1 The SUB-1 case

Here the ECCM equations above are analytically soluble, and yield the trivial (even–parity) solution

$$\begin{aligned} s_1^{(1)} &= s_1^{(2)} = \sigma_1^{(1)} = \sigma_1^{(2)} = 0 \\ E_0 &= -\frac{1}{2}\omega_0 \end{aligned} \tag{D.12}$$

for $g \le \sqrt{\omega\omega_0}/4$, and the doubly-degenerate (odd–parity) solution

$$\begin{aligned} s_1^{(1)} &= \sigma_1^{(1)} = \pm\frac{\sqrt{256g^2 - \omega^2\omega_0^2}}{8g\omega} \\ s_1^{(2)} &= \mp\frac{1}{2}\sqrt{\frac{16g^2 - \omega\omega_0}{16g^2 + \omega\omega_0}} \\ \sigma_1^{(2)} &= \mp\frac{\sqrt{256g^2 - \omega^2\omega_0^2}}{64g^2} \\ E_0 &= -\frac{4g^2}{\omega} - \frac{1}{4}\omega_0 \end{aligned} \tag{D.13}$$

for $g > \sqrt{\omega\omega_0}/4$.

D.3 NCCM Scheme II

The similarity transformed Hamiltonian is given by

$$\begin{aligned} e^{-S}H_{\text{Rabi}}e^{S} &= \frac{1}{2}\omega_0 F\left(c^\dagger\right)\sigma^z + \omega c^\dagger c + 2g\left(c^\dagger + c\right) \\ &\quad + \omega\sum_{n=1}^{\infty} n\, s_n \left(c^\dagger\right)^n + 2g\sum_{n=1}^{\infty} n\, s_n \left(c^\dagger\right)^{n-1} \end{aligned} \tag{D.14}$$

with $c^\dagger = b^\dagger\sigma^x$, $\left[c, c^\dagger\right] = \left[b, b^\dagger\right] = 1$ and

$$F\left(c^\dagger\right) \equiv \exp\left[G\left(c^\dagger\right)\right], \quad G\left(c^\dagger\right) \equiv -2\sum_{n=1}^{\infty} s_{2n-1}\left(c^\dagger\right)^{2n-1}. \tag{D.15}$$

Using the overlap form (3.7) of the CCM equations, we obtain the following set of simultaneous equations for $\{s_k;\ k = 1, 2, 3, \ldots\}$ (see also Appendix B):

$$0 \; = \; 2g\delta_{k,1} + \omega k k!\; s_k + 2g(k+1)k!\; s_{k+1} - \frac{1}{2}\omega_0 \langle \Phi | F^{(k)}\left(c^\dagger\right) | \Phi \rangle \,. \quad \text{(D.16)}$$

We have used *Mathematica* [Mat] to evaluate the functional derivative

$$F^{(k)}\left(c^\dagger\right) \equiv \frac{\partial^k F\left(c^\dagger\right)}{\partial\left(c^\dagger\right)^k} = \frac{\partial^k}{\partial\left(c^\dagger\right)^k}\left\{e^{G\left(c^\dagger\right)}\right\} \quad \text{(D.17)}$$

and the form of the equations is greatly simplified by the fact that $\langle \Phi | c^\dagger = 0$.

D.3.1 Analytics for the SUB-1 and SUB-2 cases

In the SUB-1 approximation, one obtains the solution $s_1 = -2g/(\omega + \omega_0)$, valid for all coupling, with corresponding ground–state energy

$$E_0 = -\frac{1}{2}\omega_0 - \frac{4g^2}{\omega + \omega_0}\,. \quad \text{(D.18)}$$

In the SUB-2 case, one finds the analytic solution

$$\begin{aligned} s_1 &= \frac{-\omega\left(\omega + \omega_0\right) + \sqrt{\omega^2\left(\omega+\omega_0\right)^2 - 16g^2\omega\omega_0}}{4g\omega_0} \\ s_2 &= \frac{\omega_0}{2\omega} s_1^2 \end{aligned} \quad \text{(D.19)}$$

with corresponding ground–state energy

$$E_0 = -\frac{1}{2}\omega_0 - \frac{\omega\left(\omega+\omega_0\right)}{2\omega_0} + \frac{\sqrt{\omega^2\left(\omega+\omega_0\right)^2 - 16g^2\omega\omega_0}}{2\omega_0} \quad \text{(D.20)}$$

below $g_c^{(2)} = \frac{1}{4}\sqrt{\frac{\omega}{\omega_0}}\left(\omega + \omega_0\right)$. Above this value of the coupling, there are no physical solutions to the SUB-2 NCCM Scheme II equations. At resonance ($\omega = \omega_0 = 1$), the SUB-2 NCCM Scheme II solution (which is always of even–parity) thus terminates at $g_c^{(2)} = 0.5$.

D.4 NCCM Scheme III

For Scheme III, the similarity transformed Hamiltonian $e^{-S}H_{\text{Rabi}}e^{S}$ assumes the form

$$e^{-S}H_{\text{Rabi}}e^{S} = \frac{1}{2}\omega_0 F\left(c^\dagger\right)\sigma^z + \omega c^\dagger c - \frac{4g^2}{\omega} + \omega\sum_{n=1}^{\infty} n\, s_n \left(c^\dagger\right)^n \tag{D.21}$$

with $c^\dagger = b^\dagger\sigma^x + 2g/\omega$, $\left[c, c^\dagger\right] = \left[b, b^\dagger\right] = 1$ and

$$F\left(c^\dagger\right) \equiv \exp\left[G\left(c^\dagger\right)\right], \quad G\left(c^\dagger\right) \equiv \sum_{n=1}^{\infty} s_n\left\{\left(\frac{4g}{\omega} - c^\dagger\right)^n - \left(c^\dagger\right)^n\right\}. \tag{D.22}$$

The energy functional $\overline{H}$ is given by

$$\begin{aligned}\overline{H} &= \langle\Phi|\tilde{S}e^{-S}H_{\text{Rabi}}e^{S}|\Phi\rangle \\ &= -\frac{1}{2}\omega_0 e^{-8g^2/\omega^2}\sum_{n=1}^{\infty}\tilde{s}_n\left\{\sum_{k=0}^{n} C(n,k)\left(\frac{4g}{\omega}\right)^{n-k}\langle\Phi|F^{(k)}\left(c^\dagger\right)|\Phi\rangle\right\} \\ &\quad -\frac{1}{2}\omega_0 e^{-8g^2/\omega^2}\exp\left\{\sum_{n=1}^{\infty}\left(\frac{4g}{\omega}\right)^n s_n\right\} - \frac{4g^2}{\omega} + \omega\sum_{n=1}^{\infty} n n!\, s_n\tilde{s}_n\end{aligned} \tag{D.23}$$

where $C(n,k)$ denotes the binomial coefficient $\frac{n!}{k!(n-k)!}$ and

$$F^{(k)}\left(c^\dagger\right) \equiv \frac{\partial^k F\left(c^\dagger\right)}{\partial\left(c^\dagger\right)^k}. \tag{D.24}$$

The CCM equations (3.14) for $\{s_k;\ k = 1,2,3,\ldots\}$ (see also Appendix B) are given by

$$\begin{aligned}0 &= -\frac{1}{2}\omega_0 e^{-8g^2/\omega^2}\sum_{n=0}^{k} C(k,n)\left(\frac{4g}{\omega}\right)^{k-n}\langle\Phi|F^{(n)}\left(c^\dagger\right)|\Phi\rangle \\ &\quad + \omega k k!\, s_k,\end{aligned} \tag{D.25}$$

and those for $\{\tilde{s}_k;\ k = 1,2,3,\ldots\}$ by

$$\begin{aligned}0 &= -\frac{1}{2}\omega_0 e^{-8g^2/\omega^2}\sum_{n=1}^{\infty}\tilde{s}_n\left\{\sum_{m=0}^{n} C(n,m)\left(\frac{4g}{\omega}\right)^{n-m}\frac{\partial}{\partial s_k}\left[\langle\Phi|F^{(n)}\left(c^\dagger\right)|\Phi\rangle\right]\right\} \\ &\quad -\frac{1}{2}\omega_0 e^{-8g^2/\omega^2}\exp\left\{\sum_{n=1}^{\infty}\left(\frac{4g}{\omega}\right)^n s_n\right\}\left(\frac{4g}{\omega}\right)^k + \omega k k!\, \tilde{s}_k,\end{aligned} \tag{D.26}$$

so that the expectation value of σ^z assumes the form

$$
\begin{aligned}
\langle\sigma^z\rangle^{\text{NCCM,III}} &= -e^{-8g^2/\omega^2}\sum_{n=1}^{\infty}\tilde{s}_n\left\{\sum_{k=0}^{n}C(n,k)\left(\frac{4g}{\omega}\right)^{n-k}\langle\Phi|F^{(k)}\left(c^\dagger\right)|\Phi\rangle\right\} \\
&\quad -e^{-8g^2/\omega^2}\exp\left\{\sum_{n=1}^{\infty}\left(\frac{4g}{\omega}\right)^n s_n\right\}. \qquad \text{(D.27)}
\end{aligned}
$$

In (D.25), (D.26) and (D.27) we have again used *Mathematica* [Mat] to evaluate the derivatives explicitly, and as before $\langle\Phi|c^\dagger = 0$. For Scheme III, it is not possible to solve even the SUB-1 CCM equations analytically.

D.5 NCCM Scheme IV

Here the similarity transformed Hamiltonian

$$
\begin{aligned}
H_{\text{sim}} &\equiv e^{-S}H_{\text{Rabi}}e^{S} \\
&= \frac{1}{2}\omega_0 F\left(b^\dagger\right)\sigma^z + \omega b^\dagger b + 2g\left(b^\dagger + b\right)\sigma^x \\
&\quad + \omega\sum_{n=1}^{\infty} n\; s_n\left(b^\dagger\sigma^x\right)^n + 2g\sum_{n=1}^{\infty} n\; s_n\left(b^\dagger\sigma^x\right)^{n-1} \qquad \text{(D.28)}
\end{aligned}
$$

with

$$
F\left(b^\dagger\right) \equiv \exp\left[G\left(b^\dagger\right)\right], \qquad G\left(b^\dagger\right) \equiv -2\sum_{n=1}^{\infty} s_{2n-1}\left(b^\dagger\right)^{2n-1}\sigma^x \qquad \text{(D.29)}
$$

obviously has the same form as for Scheme II.

In this section, all expectation values refer to the model state

$$
|\Phi\rangle = |\Psi_+^{\text{PBV2}}(x_{\text{opt}}, v_{\text{opt}})\rangle \qquad \text{(D.30)}
$$

(see (4.38)) of Scheme IV, *i.e.* $\langle A\rangle = \langle\Phi|A|\Phi\rangle$ for arbitrary A. Note also that the optimal values x_{opt} and v_{opt} of the variational parameters are predetermined via (C.7) and (C.8) at each value of the coupling g.

The Hermitian conjugate $c = b\sigma^x$ of $c^\dagger = b^\dagger\sigma^x$ does not annihilate the model state $|\Phi\rangle$. However, since

$$c^2|\Phi\rangle = b^2|\Phi\rangle = x_{\rm opt}^2|\Phi\rangle \ , \tag{D.31}$$

it follows that

$$\begin{aligned} c^m|\Phi\rangle &= x_{\rm opt}^m|\Phi\rangle \ , && m = 2,4,6,\ldots \\ c^m|\Phi\rangle &= x_{\rm opt}^{m-1}c|\Phi\rangle = x_{\rm opt}^{m-1}b\sigma^x|\Phi\rangle && m = 1,3,5,\ldots \ . \end{aligned} \tag{D.32}$$

This, together with the fact that $\left[c, c^\dagger\right] = \left[b, b^\dagger\right] = 1$, allows us to set up the equations for $\{s_k;\ k = 1,2,3,\ldots\}$ by constructing, for $m = 2,4,6,\ldots$, the overlaps

$$\begin{aligned} \langle c^m H_{\rm sim}\rangle &= \left\langle b^m E_0^{\rm NCCM,IV}\right\rangle = x_{opt}^m E_0^{\rm NCCM,IV} \\ &= \langle H_{\rm sim}b^m\rangle + \sum_{r=1}^{m} C(m,r)\left\langle H_{\rm sim}^{(r)}b^{m-r}\right\rangle \\ &= x_{opt}^m E_0^{\rm NCCM,IV} + \sum_{\substack{r=2 \\ r\ \rm even}}^{m} C(m,r)x_{\rm opt}^{m-r}\left\langle H_{\rm sim}^{(r)}\right\rangle \\ &\qquad + \sum_{\substack{r=1 \\ r\ \rm odd}}^{m-1} C(m,r)x_{\rm opt}^{m-r-1}\left\langle H_{\rm sim}^{(r)}b\right\rangle \ , \end{aligned} \tag{D.33}$$

and, for $m = 1,3,5,\ldots$, the overlaps

$$\begin{aligned} \langle c^m H_{\rm sim}\rangle &= \left\langle b^{m-1}b\sigma^x E_0^{\rm NCCM,IV}\right\rangle = x_{opt}^{m-1}E_0^{\rm NCCM,IV}\langle b\sigma^x\rangle \\ &= \sum_{r=0}^{m} C(m,r)\left\langle \sigma^x H_{\rm sim}^{(r)}b^{m-r}\right\rangle \\ &= x_{\rm opt}^{m-1}\langle\sigma^x H_{\rm sim}b\rangle + \sum_{\substack{r=2 \\ r\ \rm even}}^{m-1} C(m,r)x_{\rm opt}^{m-r-1}\left\langle\sigma^x H_{\rm sim}^{(r)}b\right\rangle \\ &\qquad + \sum_{\substack{r=1 \\ r\ \rm odd}}^{m} C(m,r)x_{\rm opt}^{m-r}\left\langle\sigma^x H_{\rm sim}^{(r)}\right\rangle \ . \end{aligned} \tag{D.34}$$

Here $E_0^{\mathrm{NCCM,IV}}$ is the NCCM Scheme IV ground–state energy (6.3), and

$$
\begin{aligned}
H_{\mathrm{sim}}^{(r)} &\equiv \frac{\partial^r H_{\mathrm{sim}}}{\partial\left(b^{\dagger}\right)^r} \\
F^{(r)} &\equiv \frac{\partial^r F\left(b^{\dagger}\right)}{\partial\left(b^{\dagger}\right)^r} \\
\left\langle H_{\mathrm{sim}}^{(r)}\right\rangle &= \frac{1}{2}\omega_0\left\langle F^{(r)}\sigma^z\right\rangle \\
&+\omega\sum_{\substack{n=r+1\\ n\ \mathrm{odd}}}^{\infty}\frac{nn!}{(n-r)!}x_{\mathrm{opt}}^{n-r-1}\left\langle b\sigma^x\right\rangle\ s_n \\
&+\omega\sum_{\substack{n=r\\ n\ \mathrm{even}}}^{\infty}\frac{nn!}{(n-r)!}x_{\mathrm{opt}}^{n-r}\ s_n \\
&+2g\sum_{\substack{n=r+1\\ n\ \mathrm{odd}}}^{\infty}\frac{n!}{(n-r-1)!}x_{\mathrm{opt}}^{n-r-1}\ s_n \\
&+2g\sum_{\substack{n=r+2\\ n\ \mathrm{even}}}^{\infty}\frac{n!}{(n-r-1)!}x_{\mathrm{opt}}^{n-r-2}\left\langle b\sigma^x\right\rangle\ s_n\ , \qquad r\in\{2,4,6,\ldots\} \\
\left\langle H_{\mathrm{sim}}^{(r)}b\right\rangle &= \frac{1}{2}\omega_0\left\langle F^{(r)}b\sigma^z\right\rangle+\left\{\omega x_{\mathrm{opt}}^2+2g\left\langle b\sigma^x\right\rangle\right\}\delta_{r,1} \\
&+\omega\sum_{\substack{n=r\\ n\ \mathrm{odd}}}^{\infty}\frac{nn!}{(n-r)!}x_{\mathrm{opt}}^{n-r}\left\langle b\sigma^x\right\rangle\ s_n \\
&+\omega\sum_{\substack{n=r+1\\ n\ \mathrm{even}}}^{\infty}\frac{nn!}{(n-r)!}x_{\mathrm{opt}}^{n-r-1}\left\langle b^{\dagger}b\right\rangle\ s_n \\
&+2g\sum_{\substack{n=r+2\\ n\ \mathrm{odd}}}^{\infty}\frac{n!}{(n-r-1)!}x_{\mathrm{opt}}^{n-r-2}\left\langle b^{\dagger}b\right\rangle\ s_n \\
&+2g\sum_{\substack{n=r+1\\ n\ \mathrm{even}}}^{\infty}\frac{n!}{(n-r-1)!}x_{\mathrm{opt}}^{n-r-1}\left\langle b\sigma^x\right\rangle\ s_n\ , \qquad r\in\{1,3,5,\ldots\} \\
\left\langle\sigma^x H_{\mathrm{sim}}^{(r)}b\right\rangle &= \frac{1}{2}\omega_0\left\langle F^{(r)}b\sigma^x\sigma^z\right\rangle \\
&+\omega\sum_{\substack{n=r+1\\ n\ \mathrm{odd}}}^{\infty}\frac{nn!}{(n-r)!}x_{\mathrm{opt}}^{n-r-1}\left\langle b^{\dagger}b\right\rangle\ s_n \\
&+\omega\sum_{\substack{n=r\\ n\ \mathrm{even}}}^{\infty}\frac{nn!}{(n-r)!}x_{\mathrm{opt}}^{n-r}\left\langle b\sigma^x\right\rangle\ s_n
\end{aligned}
$$

$$
\begin{aligned}
& + 2g \sum_{\substack{n=r+1 \\ n \text{ odd}}}^{\infty} \frac{n!}{(n-r-1)!} x_{\text{opt}}^{n-r-1} \langle b\sigma^x \rangle \; s_n \\
& + 2g \sum_{\substack{n=r+2 \\ n \text{ even}}}^{\infty} \frac{n!}{(n-r-1)!} x_{\text{opt}}^{n-r-2} \left\langle b^\dagger b \right\rangle \; s_n \,, \qquad r \in \{2,4,6,\ldots\} \\
\left\langle \sigma^x H_{\text{sim}}^{(r)} \right\rangle &= \frac{1}{2}\omega_0 \left\langle F^{(r)} \sigma^x \sigma^z \right\rangle + \{\omega \langle b\sigma^x \rangle + 2g\} \delta_{r,1} \\
& + \omega \sum_{\substack{n=r \\ n \text{ odd}}}^{\infty} \frac{nn!}{(n-r)!} x_{\text{opt}}^{n-r} \; s_n \\
& + \omega \sum_{\substack{n=r+1 \\ n \text{ even}}}^{\infty} \frac{nn!}{(n-r)!} x_{\text{opt}}^{n-r-1} \langle b\sigma^x \rangle \; s_n \\
& + 2g \sum_{\substack{n=r+2 \\ n \text{ odd}}}^{\infty} \frac{n!}{(n-r-1)!} x_{\text{opt}}^{n-r-2} \langle b\sigma^x \rangle \; s_n \\
& + 2g \sum_{\substack{n=r+1 \\ n \text{ even}}}^{\infty} \frac{n!}{(n-r-1)!} x_{\text{opt}}^{n-r-1} \; s_n \,, \qquad r \in \{1,3,5,\ldots\} \\
\langle \sigma^z \rangle &= \frac{v_{\text{opt}}^2 - 1}{v_{\text{opt}}^2 + 1} \\
\left\langle b^\dagger b \right\rangle &= \frac{x_{\text{opt}}^2}{1 + v_{\text{opt}}^2} \left(\tanh x_{\text{opt}}^2 + v_{\text{opt}}^2 \coth x_{\text{opt}}^2 \right) \\
\langle b\sigma^x \rangle &= \frac{2x_{\text{opt}} v_{\text{opt}}}{1 + v_{\text{opt}}^2} \left(1 - \exp\left[-4x_{\text{opt}}^2\right] \right)^{-1/2} \\
\langle b\sigma^x \sigma^z \rangle &= \frac{2x_{\text{opt}} v_{\text{opt}} \exp\left[-2x_{\text{opt}}^2\right]}{1 + v_{\text{opt}}^2} \left(1 - \exp\left[-4x_{\text{opt}}^2\right] \right)^{-1/2} . \qquad \text{(D.35)}
\end{aligned}
$$

We have again used *Mathematica* [Mat] to set up the derivatives $F^{(r)}$ as a function of the set $\left\{G^{(k)}; k = 0,1,2,\ldots\right\}$ with

$$
G^{(k)} \equiv \frac{\partial^k G\left(b^\dagger\right)}{\partial \left(b^\dagger\right)^k} = \begin{cases} -2\sum_{\substack{n=k+1 \\ n \text{ odd}}}^{\infty} \frac{n!}{(n-k)!} \left(b^\dagger\right)^{n-k-1} b^\dagger \sigma^x \; s_n & k \in \{0,2,4,\ldots\} \\ -2\sum_{\substack{n=k \\ n \text{ odd}}}^{\infty} \frac{n!}{(n-k)!} \left(b^\dagger\right)^{n-k} \sigma^x \; s_n & k \in \{1,3,5,\ldots\} \end{cases} \qquad \text{(D.36)}
$$

One may readily prove the identity

$$
\langle \Phi | \exp\left[G\left(b^\dagger\right)\right] = \langle \Phi | \cosh\alpha - \langle \Phi | \left(\frac{\sinh\alpha}{x_{\text{opt}}}\right) b^\dagger \sigma^x \qquad \text{(D.37)}
$$

with

$$\alpha \equiv \sum_{n=0}^{\infty} 2\, s_{2n+1}\, x_{\text{opt}}^{2n+1}\ , \tag{D.38}$$

which is the final element required in order to set up the CCM equations (D.33) and (D.34).

Appendix E

Acronyms and Abbreviations

Acronym/abbrevation	Explanation	Relevant chapters
CCM	Coupled cluster method	1,3,5,6,8
CI	Configuration–interaction	1,4,7
ECCM	Extended coupled cluster method	1,3,5
JT	Jahn–Teller	1,2,7,8
PJT	Pseudo Jahn–Teller	1,2,7,8
LMG	Lipkin–Meshkov–Glick	1,5
NCCM	Normal coupled cluster method	1,3,5,6,8
PAV	Projection after variation	4
PBV	Projection before variation	4
RPJT	Resonant pseudo Jahn–Teller	1,2,7,8
RWA	Rotating–wave approximation	1, 4
TIPT	Time–independent perturbation theory	1,4