Chapter 5

Simple Applications of the CCM to the Rabi Hamiltonian

In many cases, the non–perturbative nature of the CCM permits calculations based on very simple model states (typically the noninteracting state) to be performed well beyond the perturbative region without convergence problems. However, this is not always the case, as the calculations presented in this chapter indicate. In fact, for the Rabi system, where the ground state undergoes a major character change, it can be shown that the calculation fails due to an essential incompleteness, to arbitrary finite order, in the CCM ansatz for the ground–state wave function for a particularly simple, yet in principle valid, choice of the CCM model state and correlation operator. For a different but equally simple choice, we also show that the non–Hermiticity of the CCM can lead to the breakdown of the method.

5.1 Earlier CCM analyses of the Rabi Hamiltonian

Of particular relevance for this thesis is the recent application of the CCM to a multimode Rabi Hamiltonian by Wong and Lo [Wo96b]. Although their calculation was done in the context of a quantum system tunneling between two levels in the presence of a phonon bath, their model Hamiltonian represents a simple generalization of the Rabi Hamiltonian to the case of multiple bosonic modes, and the Rabi Hamiltonian may thus be regarded as a special case of the model studied by Wong and Lo. Their results for the ground-state energy of the multimode Rabi system are qualitatively acceptable, and furthermore they find that the CCM results give no indication of the spurious discontinuous localization–delocalization transition of the two–level system observed in earlier variational studies (see [Lo95] and references therein).

Several comments regarding the work of Wong and Lo [Wo96b] are however in order. Firstly, they apply the CCM to a unitary transformed version of the Rabi Hamiltonian (4.1), which leaves the spectrum unaffected. However, their choice of unitary transform destroys the parity symmetry (4.2) associated with the Hamiltonian. As a result, their CCM results for the ground–state energy are, by their own admission, quantitatively inaccurate for intermediate coupling, and it is furthermore not possible in their approach to readily obtain accurate CCM results for the first excited state.

A more minor criticism of the CCM analysis of Wong and Lo relates to their use of the so–called successive coupled cluster approximation (SCCA), a variant of the standard SUB-N CCM approximation. At a particular order of approximation in the SCCA, the similarity transformed Hamiltonian $e^{-S}He^{S}$ is allowed to act on the CCM model state $|\Phi\rangle$, and the CCM coefficients and ground–state energy are determined via term–by–term comparison, with any remaining nonvanishing terms being neglected. At the subsequent level of approximation, terms are added to the cluster correlation operator S in such a manner that their contribution cancels the nonvanishing terms in the previous order of approximation, and the procedure is repeated. The advantage of this approximation scheme is that it naturally tends to select the most important terms which are to be included in the cluster correlation operator, and in some cases (see, *e.g.* [Wo94, Wo96a]), the SCCA leads to rapid, accurate convergence of the CCM. However, not only is the intuitively simple physical meaning of the SUB-N approximation scheme lost, but it is also not clear that the SCCA may be rigorously justified, particularly since there is no gaurantee in the SCCA that the set of configurations $\{C_I^{\dagger}|\Phi\rangle\}$, where the index I runs over all possible configurations generated within the SCCA, satisfies the requirement of completeness.

5.2 Evidence for a spurious symmetry–breaking phase transition

We turn now to our CCM calculations for the Rabi Hamiltonian. For ease of reference, we shall refer to a particular choice of CCM model state and corresponding creation operators as a CCM *scheme*. We have considered a variety of CCM schemes for the Rabi Hamiltonian (see Table D.1 in Appendix D). An obvious choice for the model state $|\Phi\rangle$ is the positive–parity $g = 0$ ground state $|0\rangle|\downarrow\rangle$ of H_{Rabi}, which we shall refer to as the *noninteracting* model state. For our first NCCM calculation of the Rabi ground–state energy, we use the noninteracting model state and the correlation operator [Bi96]

$$\begin{aligned} S &= S_1 + S_2 \\ S_1 &= \sum_{n=1}^{\infty} s_n^{(1)} \left(b^\dagger\right)^n , \qquad S_2 = \sum_{n=1}^{\infty} s_n^{(2)} \left(b^\dagger\right)^{n-1} \sigma^+ , \end{aligned} \tag{5.1}$$

which we shall refer to as Scheme I. For this scheme, the nested commutator expansion (3.8) for the similarity transformed Hamiltonian $e^{-S} H_{\text{Rabi}} e^S$ terminates at third order in S, and it is straightforward to show that the CCM ground–state energy assumes the form

$$E_0^{\text{NCCM,I}} = -\frac{1}{2}\omega_0 + 4g\left\{s_1^{(1)} s_1^{(2)} + s_2^{(2)}\right\} . \tag{5.2}$$

In the SUB-N approximation scheme, both S_1 and S_2 truncate at $n = N$, and the $2N$ coefficients $\left\{s_n^{(1)}, s_n^{(2)}\right\}$, $n = 1, 2, \ldots, N$ are determined via the NCCM equations (3.16). Explicit expressions for the similarity transformed Hamiltonian and NCCM equations for Scheme I are given in Appendix D.

Since the $g = 0$ ground state has even parity, we expect the ground state to have the same parity for $g > 0$. Thus the NCCM calculation based on Scheme I is restricted to states of positive parity. In this case, terms in the cluster correlation operator S with n odd are zero, there are only N CCM coefficients to solve for in the SUB-N approximation, and the CCM ground–state energy then depends only on the single coefficient $s_2^{(2)}$. Starting from $g = 0$, we solve for increasing values of the coupling by using the solution at the previous coupling as input to the iterative routine for solving the CCM equations. For simplicity, we only quote results for the scaled resonant ($\omega = \omega_0 = 1$) Rabi Hamiltonian.

We find that the even–parity NCCM Scheme I results provide strong evidence for spontaneous breaking of the parity symmetry Π_{Rabi} [Bi96]. For all $N \geq 6$, the positive–parity ground–state solution terminates at a finite value of the coupling which we shall denote by $g_c^{(N)}$. There is a qualitative difference in the nature of the termination depending on whether $N/2$ is even or odd. Here we restrict ourselves to the simpler case where $N/2$ is odd (see [Bi96] for a fuller discussion of the case where $N/2$ is even). The ground–state energy results for $N = 10, 30, 50$ at resonance are shown in Figure 5.1. The termination points $\left\{g_c^{(N)}\right\}$ of the positive–parity NCCM Scheme I results are clearly visible.

The termination in the positive–parity NCCM Scheme I ground–state solution is real rather than numerical. For any N, the NCCM equations (3.16) can in this case be rewritten as a polynomial in $s_2^{(2)}$ (see Appendix D), and the termination in the ground–state solution then corresponds to the vanishing of the relevant real root for $s_2^{(2)}$ at the termination point $g_c^{(N)}$ [Bi97]. Figure 5.2 shows these critical values of the coupling as a function of the cutoff N. An investigation of the behaviour of E_g and its derivatives just below the critical coupling [Bi96] suggests a fit of $g_c^{(N)}$ to the form $a - bN^{\gamma}$, with $\gamma = -2/3$. Using a least–squares fit, we find $a = 0.665$ and $b = 0.722$, and the NCCM based on Scheme I therefore strongly suggests a parity–breaking phase transition at $g_c \equiv \lim_{N\to\infty} g_c^{(N)} = 0.665$.

Figure 5.1: *The ground–state energy E_0 of the scaled resonant ($\omega = \omega_0 = 1$) Rabi Hamiltonian as a function of the coupling g as determined via a SUB-N, N=10,30,50, NCCM analysis based on Scheme I (see Table D.1), compared to results obtained via a CI diagonalization in a basis of 101 even–parity states.*

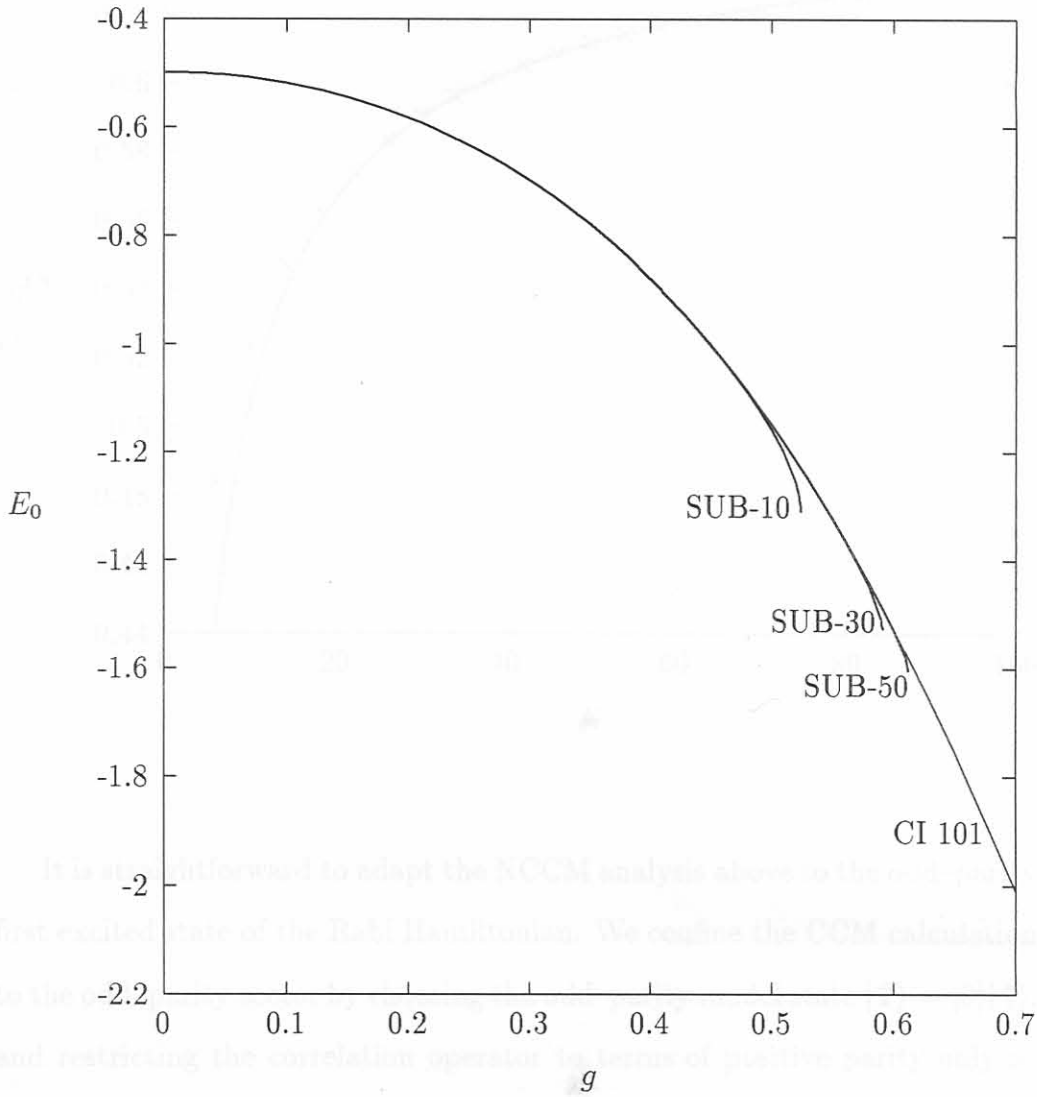
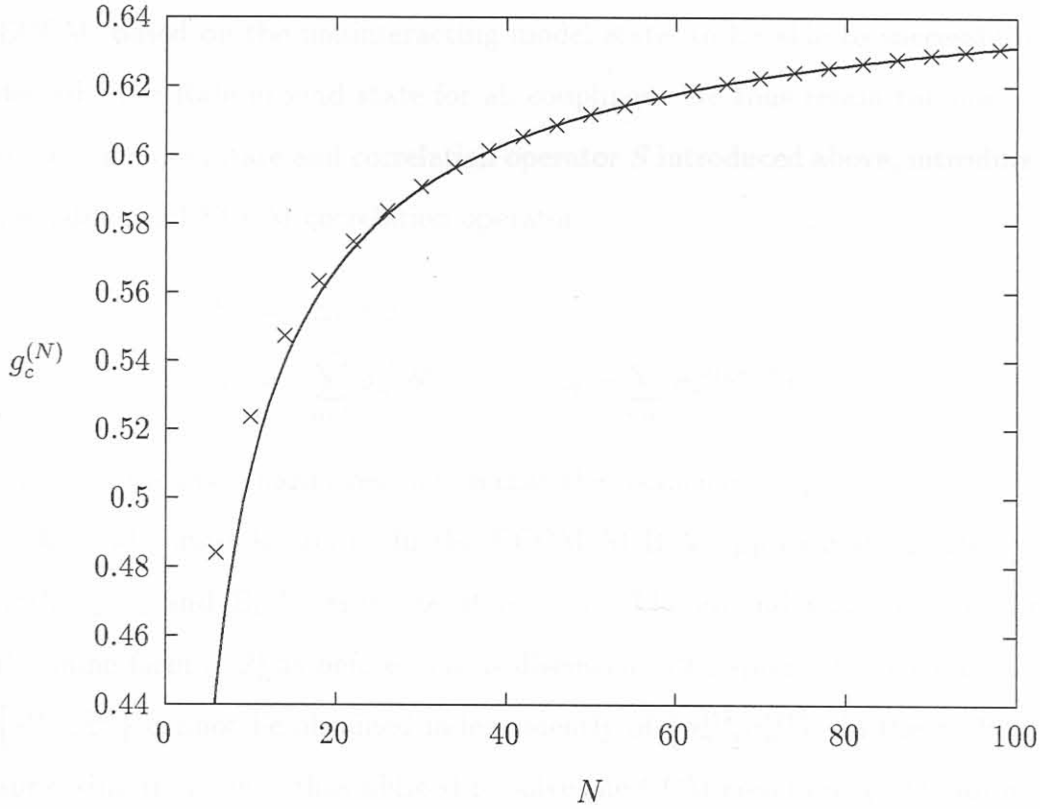


Figure 5.2: *The critical coupling* $g_c^{(N)}$ *as a function of the level of approximation* N *in the NCCM Scheme I analysis of the scaled resonant* ($\omega = \omega_0 = 1$) *Rabi Hamiltonian. The solid line is the function* $0.665 - 0.722N^{-2/3}$ *obtained from a least-squares fit to* $g_c^{(N)}$ *for* $62 \leq N \leq 98$.



It is straightforward to adapt the NCCM analysis above to the odd-parity first excited state of the Rabi Hamiltonian. We confine the CCM calculation to the odd-parity sector by choosing the odd-parity model state $|\Phi\rangle = |0\rangle|\uparrow\rangle$, and restricting the correlation operator to terms of positive parity only as before. The results are very similar to those obtained for the ground state, with the odd-parity solution terminating at $g_c^{\text{odd}} = 0.601$.

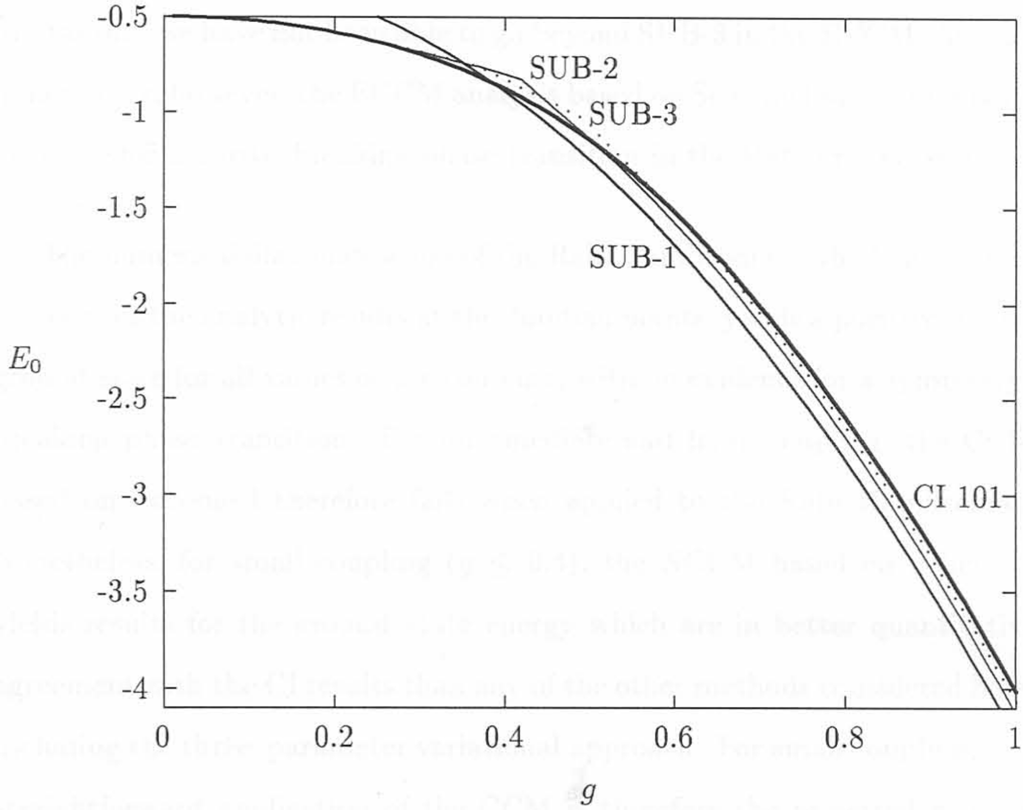
Motivated by the results obtained by Arponen and others for the LMG model (see [Ar82, Ar83a, Ar83b, Ro89] and the discussion in Chapter 3), we also apply the ECCM to the Rabi Hamiltonian [Bi98]. The ECCM, based on a single symmetric model state, is capable of correctly describing a symmetry–breaking phase transition. One might therefore expect the ECCM, based on the noninteracting model state, to be able to successfully describe the Rabi ground state for all couplings. We thus retain the noninteracting model state and correlation operator S introduced above, introduce the additional ECCM correlation operator

$$\begin{aligned} \Sigma &= \Sigma_1 + \Sigma_2 \\ \Sigma_1 &= \sum_{n=1}^{\infty} \sigma_n^{(1)} b^n , \qquad \Sigma_2 = \sum_{n=1}^{\infty} \sigma_n^{(2)} b^{n-1} \sigma^- , \end{aligned} \tag{5.3}$$

and drop the even–parity restriction that the coefficients $\left\{s_n^{(1)}, s_n^{(2)}, \sigma_n^{(1)}, \sigma_n^{(2)}\right\}$ with n odd must be zero. In the ECCM SUB-N approximation scheme, both S_1, S_2 and Σ_1, Σ_2 truncate at $n = N$. The ground–state energy has the same form (5.2) as before, but as discussed in Chapter 3 the coefficients $\left\{s_n^{(1)}, s_n^{(2)}\right\}$ cannot be obtained independently of $\left\{\sigma_n^{(1)}, \sigma_n^{(2)}\right\}$. In the SUB-$N$ approximation one is thus obliged to solve the CCM equations (3.14) for all $4N$ unknowns. The ECCM functional $\overline{H}_{\mathrm{Rabi}} = \langle\Phi|e^{\Sigma}e^{-S}H_{\mathrm{Rabi}}e^{S}|\Phi\rangle$, which is required in order to set up these equations, is shown in Appendix D.

In the SUB-1 approximation, the ECCM Scheme I equations can be solved analytically (see Appendix D). At resonance ($\omega = \omega_0 = 1$), one finds, for $g \leq 1/4$, only the trivial solution where all four SUB-1 ECCM coefficients are identically zero. In this coupling regime the ECCM approximation to the exact ground state is thus simply the evĕn–parity noninteracting model state $|0\rangle|\downarrow\rangle$, with corresponding energy $E_0 = -1/2$. For $g > 1/4$, the SUB-1 ECCM equations also allow for a mixed–parity solution corresponding to the lower energy $E_0 = -4g^2 - 1/4$. Thus the SUB-1 ECCM ground–state energy is continuous but not differentiable at the crossover point $g = 1/4$ where the symmetry of the ground state is broken. This result in plotted in Figure 5.3,

Figure 5.3: *The ground–state energy E_0 of the scaled resonant ($\omega = \omega_0 = 1$) Rabi Hamiltonian as a function of the coupling g as determined via a SUB-1 (solid line), SUB-2 (thin solid line) and SUB-3 (dotted line) ECCM analysis based on Scheme I (see Table D.1), compared to results obtained via a CI diagonalization in a basis of 101 even–parity states (thick solid line).*



where we also present the results of a numerical SUB-N, $N = 2, 3$, ECCM calculation of the Rabi ground–state energy as a function of the coupling g. Here similar behaviour occurs to that observed in the SUB-1 case. Although the ground–state energy approximates the CI result quite closely for all g, it is evident from the graph there is a narrow coupling region around $g \sim 0.4$ where smooth SUB-2 and SUB-3 ECCM solutions cannot be found. In Table 5.1, we tabulate some of the SUB-3 ECCM coefficients, and it is clear from the behaviour of the coefficients with odd index n that the symmetry of the ECCM ground state is in fact broken at $g \approx 0.37$. This in good agreement with the NCCM SUB-2 result based on the same scheme, for which the even–parity ground–state solution terminates at $g = 0.397$. Due to numerical limitations, we have not been able to go beyond SUB-3 in the ECCM. At least in low order, however, the ECCM analysis based on Scheme I provides further evidence for a parity–breaking phase transition in the Rabi ground state.

The numerical diagonalization of the Rabi Hamiltonian, which accurately reproduces the analytic results at the Juddian points, yields a positive–parity ground state for all values of the coupling, with no evidence for a symmetry–breaking phase transition. For intermediate and large coupling, the CCM based on Scheme I therefore fails when applied to the Rabi Hamiltonian. Nonetheless, for small coupling ($g \leq 0.4$), the NCCM based on Scheme I yields results for the ground–state energy which are in better quantitative agreement with the CI results than any of the other methods considered here, including the three–parameter variational approach. For small coupling, this straightforward application of the CCM is therefore the preferred *a priori* method for determining the Rabi ground–state energy accurately and quickly.

Table 5.1: *The behaviour of the SUB-3 ECCM Scheme I coefficients as a function of the coupling g for the ground state of the scaled resonant ($\omega = \omega_0 = 1$) Rabi Hamiltonian. Coefficients of both even and odd order n are nonzero for $g \geq 0.38$, indicating that the ECCM ground state is of mixed parity in this coupling regime. The odd order coefficients vanish abruptly between $g = 0.38$ and $g = 0.37$, and are effectively zero for $g \leq 0.37$, where the ground state is therefore of positive parity.*

g	n	$s_n^{(1)}$	$s_n^{(2)}$	$\sigma_n^{(1)}$	$\sigma_n^{(2)}$
0.50	1	-5.126×10^{-1}	1.717×10^{-1}	-7.549×10^{-1}	1.843×10^{-1}
	2	1.348×10^{-1}	-1.902×10^{-1}	1.020×10^{-1}	-9.711×10^{-2}
	3	1.164×10^{-2}	-3.941×10^{-2}	2.366×10^{-2}	-3.648×10^{-2}
0.45	1	-3.508×10^{-1}	1.217×10^{-1}	-5.315×10^{-1}	1.457×10^{-1}
	2	1.359×10^{-1}	-1.992×10^{-1}	1.391×10^{-1}	-1.312×10^{-1}
	3	1.157×10^{-2}	-3.620×10^{-2}	2.727×10^{-2}	-3.927×10^{-2}
0.40	1	-2.095×10^{-1}	7.465×10^{-2}	-3.123×10^{-1}	9.821×10^{-2}
	2	1.184×10^{-1}	-1.876×10^{-1}	1.456×10^{-1}	-1.508×10^{-1}
	3	9.046×10^{-3}	-2.363×10^{-2}	1.884×10^{-2}	-2.850×10^{-2}
0.39	1	-1.706×10^{-1}	6.100×10^{-2}	-2.529×10^{-1}	8.194×10^{-2}
	2	1.137×10^{-1}	-1.841×10^{-1}	1.458×10^{-1}	-1.547×10^{-1}
	3	7.747×10^{-3}	-1.939×10^{-2}	1.568×10^{-2}	-2.402×10^{-2}
0.38	1	-1.195×10^{-1}	4.287×10^{-2}	-1.762×10^{-1}	5.885×10^{-2}
	2	1.086×10^{-1}	-1.802×10^{-1}	1.458×10^{-1}	-1.588×10^{-1}
	3	5.701×10^{-3}	-1.366×10^{-2}	1.121×10^{-2}	-1.742×10^{-2}
0.37	1	3.356×10^{-17}	-1.206×10^{-17}	4.888×10^{-17}	-1.683×10^{-17}
	2	1.031×10^{-1}	-1.761×10^{-1}	1.453×10^{-1}	-1.628×10^{-1}
	3	-1.649×10^{-18}	3.807×10^{-18}	-3.222×10^{-18}	5.063×10^{-18}
0.36	1	2.350×10^{-21}	-8.791×10^{-22}	3.414×10^{-21}	-1.207×10^{-21}
	2	9.971×10^{-2}	-1.729×10^{-1}	1.383×10^{-1}	-1.601×10^{-1}
	3	-1.208×10^{-22}	2.550×10^{-22}	-1.423×10^{-22}	2.939×10^{-22}
0.35	1	9.415×10^{-27}	-3.648×10^{-27}	1.344×10^{-26}	-4.852×10^{-27}
	2	9.624×10^{-2}	-1.696×10^{-1}	1.313×10^{-1}	-1.573×10^{-1}
	3	-4.714×10^{-28}	9.446×10^{-28}	-2.732×10^{-28}	9.122×10^{-28}
0.30	1	6.794×10^{-60}	-2.858×10^{-60}	8.247×10^{-60}	-3.350×10^{-60}
	2	7.775×10^{-2}	-1.505×10^{-1}	9.785×10^{-2}	-1.411×10^{-1}
	3	-1.556×10^{-61}	3.143×10^{-61}	4.082×10^{-61}	-1.579×10^{-61}

5.3 Incompleteness of the CCM ground–state ansatz

It is possible to illustrate numerically that the breakdown of the method is formally due to the incompleteness, to any finite order, of the exponential CCM ansatz (3.3) for the ground–state wave function for the model state and creation operators of Scheme I. We investigate whether it is possible, to good approximation for all values of the coupling g, to write

$$|\Psi_{CI}\rangle(g) = e^S|\Phi\rangle \ . \qquad (5.4)$$

Here $|\Psi_{CI}\rangle(g)$ represents the (essentially exact) positive–parity ground–state ket determined as a function of g via the CI diagonalization, $|\Phi\rangle = |0\rangle|\downarrow\rangle$ is the noninteracting model state, and S is the cluster correlation operator (5.1) of Scheme I in the SUB-N approximation, restricted to terms of even parity as before. We expand both sides of (5.4) in a basis consisting of bosonic oscillator states multiplied by eigenfunctions of σ^z, and determine the coefficients $\left\{s_n^{(1)}(g), s_n^{(2)}(g)\right\}$, $n = 2, 4, 6, \ldots, N$, via term–by–term comparison. Due to the intermediate normalization condition (3.4) imposed by the CCM, the state $|\Psi_{CI}\rangle(g)$ must be scaled so that the coefficient of $|0\rangle|\downarrow\rangle$ is unity. For the sequence $s_2^{(i)}(g), s_4^{(i)}(g), \ldots, s_n^{(i)}(g), \ldots; i = 1, 2$, we numerically determine the ratio

$$R^{(i)}(g) \equiv \lim_{n\to\infty} \left| \frac{s_{n+2}^{(i)}(g)}{s_n^{(i)}(g)} \right| , \qquad i = 1, 2 \ . \qquad (5.5)$$

At resonance ($\omega = \omega_0 = 1$), we find

$$\begin{aligned} &R^{(1)} < 1,\ R^{(2)} < 1 \qquad &&\text{at} \quad g = 0.665 \\ &R^{(1)} \approx 1,\ R^{(2)} \approx 1 \qquad &&\text{at} \quad g \approx 0.8 \\ &R^{(1)} > 1,\ R^{(2)} > 1 \qquad &&\text{at} \quad g = 1.0\ . \end{aligned} \tag{5.6}$$

In order for a SUB-N CCM calculation to yield an acceptable approximation to the exact ground state, it is essential that one should safely be able to neglect coefficients in S of order $n > N$. Our results for the ratio R indicate that, for the model state and cluster operator of Scheme I, this is not always possible. For $g \gtrsim 0.8$, the exact resonant Rabi ground state cannot be adequately approximated by the exponential form (5.4) *for any finite value of* N, and it is in this sense that the exponential ground–state ansatz renders the CCM incomplete [1]. Note that the CCM breaks down at a value of the coupling below the critical value determined above. This incompleteness is a serious defect not only of the CCM, but also of other methods reliant on the $\exp S$ form, and is compounded by the fact that the model state and creation operators of Scheme I represent perhaps the most obvious choice for a CCM analysis of the Rabi system.

There is some overlap between the breakdown of the CCM observed here and that reported by Arponen [Ar82] who, based on a SUB-2 NCCM analysis of the LMG model, conjectured without proof that a SUB-N NCCM

[1] Note that the incompleteness, to arbitrary finite order, of the CCM based on scheme I does not contradict the fact that the CCM formalism is in principle exact — an expansion of the form (5.4) does exist for arbitrary coupling g, provided that the cluster operator S is not truncated at all. Of course, this is of no practical significance in the application of the method, where a truncation at finite order is unavoidable.

analysis of the LMG ground state based on a spherically symmetric model state would fail for any value of N. In the LMG model, however, a true phase transition occurs in the thermodynamic limit, and the breakdown of the NCCM correctly signals the onset of symmetry–breaking. Also, unlike the situation for the LMG model with a finite number of nucleons, the failure of the CCM for the Rabi Hamiltonian cannot simply be ascribed to the onset of near–degeneracy in the ground state for intermediate coupling. To show this, we have repeated the even–parity NCCM Scheme I calculation for the case of degenerate atomic levels ($\omega_0 = 0$), where the analytic positive– and negative–parity ground states (4.16) are degenerate for all couplings.

For $\omega_0 = 0$, we find that the even–parity NCCM Scheme I ground–state solution again terminates at intermediate coupling. As before, we test the CCM ansatz (3.3) for completeness by writing

$$\begin{aligned} |\Psi_+\rangle &= \sum_{n=0}^{\infty} \frac{x^{2n}}{\sqrt{(2n)!}}|2n\rangle|\downarrow\rangle - \sum_{n=0}^{\infty} \frac{x^{2n+1}}{\sqrt{(2n+1)!}}|2n+1\rangle|\uparrow\rangle \\ &= e^S|\Phi\rangle \,, \end{aligned} \tag{5.7}$$

where $|\Psi_+\rangle$ is the positive–parity ground state (4.16) with $x = 2g/\omega$ (scaled so as to meet the normalization condition (3.4)), and $|\Phi\rangle$ (S) represents the model state (even–parity cluster correlation operator) of Scheme I. Given the explicit expansion (5.7) for the exact ground state $|\Psi_+\rangle$, it can be shown analytically that

$$R_n^{(i)}(g) \equiv \frac{s_{n+2}^{(i)}(g)}{s_n^{(i)}(g)} = \frac{a_{n+1}^{(i)}}{a_n^{(i)}}x^2 = \frac{a_{n+1}^{(i)}}{a_n^{(i)}}\left(\frac{4g^2}{\omega}\right) , \qquad i = 1, 2 \,, \tag{5.8}$$

where the parameters $\{a_n^{(i)}\}; i = 1, 2$ are independent of the coupling g. These parameters obey a set of algebraic recurrence relations which we have not been able to solve in closed form. We therefore scale out the ω–dependence by setting $\omega = 1$, and numerically investigate the ratios

$$\begin{aligned} A_n^{(1)} &\equiv \frac{a_{n+1}^{(1)}}{a_n^{(1)}} \\ A_n^{(2)} &\equiv \frac{a_{n+1}^{(2)}}{a_n^{(2)}} \end{aligned} \tag{5.9}$$

as a function of n. We find that both quantities increase uniformly with increasing n. At $n = 51$, the ratio $A_n^{(2)}$ has converged to the value 0.406, and $A_n^{(1)}$ attains the value 0.396. Although the convergence of $A_n^{(1)}$ with increasing n is not rapid enough to state the true limiting value with certainty, the important conclusion is that

$$\begin{aligned} A^{(1)} &\equiv \lim_{n\to\infty} A_n^{(1)} \geq 0.396 \\ A^{(2)} &\equiv \lim_{n\to\infty} A_n^{(2)} = 0.406 \; . \end{aligned} \tag{5.10}$$

Therefore

$$\begin{aligned} R^{(1)}(g) &\equiv \lim_{n\to\infty} R_n^{(1)}(g) = 4A^{(1)}g^2 \geq 1.584g^2 \\ R^{(2)}(g) &\equiv \lim_{n\to\infty} R_n^{(2)}(g) = 4A^{(2)}g^2 = 1.624g^2 \; , \end{aligned} \tag{5.11}$$

and it is clear that

$$\begin{aligned} R^{(1)}(g) &\geq 1 \text{ for } g \geq \frac{1}{\sqrt{1.584}} = 0.795 \\ R^{(2)}(g) &\geq 1 \text{ for } g \geq \frac{1}{\sqrt{1.624}} = 0.785 \; . \end{aligned} \tag{5.12}$$

Thus for $g \geq 0.785$ (and, depending on the true limiting value $A^{(1)}$, possibly even below $g = 0.785$), the exact positive–parity ground state $|\Psi_+\rangle$ cannot, to any finite order, be adequately approximated by the $\exp S$ form required by the CCM. This proof of incompleteness for the case $\omega_0 = 0$ is strengthened by the fact that, unlike the $\omega_0 \neq 0$ case where the exact ground state had to be determined numerically, the state $|\Psi_+\rangle$ is here known analytically.

5.4 An alternative CCM calculation based on the noninteracting model state

Given the above incompleteness for scheme I, we are therefore led to consider alternative CCM schemes for the Rabi Hamiltonian. Using (4.11) and (4.37), it is easily shown that the positive–parity $g \to \infty$ ground state (4.16) may be written in the form

$$|\Psi_+\rangle = e^{-2g^2/\omega^2} \exp\left\{\left(-\frac{2g}{\omega}\right) b^\dagger \sigma^x\right\} |0\rangle|\downarrow\rangle \,. \tag{5.13}$$

Thus for Scheme II (see Table D.1), we retain the noninteracting model state $|\Phi\rangle = |0\rangle|\downarrow\rangle$ of Scheme I, but introduce a new correlation operator

$$S = \sum_{n=1}^{\infty} s_n \left(c^\dagger\right)^n \,, \qquad c^\dagger \equiv b^\dagger \sigma^x \,. \tag{5.14}$$

The nested commutator expansion (3.8), although non–terminating, now assumes a closed (exponential) form, and the CCM ground–state energy is given by

$$E_0^{\mathrm{NCCM,II}} = -\frac{1}{2}\omega_0 + 2g s_1 \,. \tag{5.15}$$

This calculation is also restricted to the positive–parity sector, as is obvious from the form of both the model state and the CCM creation operators. Explicit expressions for the similarity transformed Hamiltonian and NCCM equations for Scheme II are given in Appendix D.

We find that the CCM yields results (not shown here) for the ground–state energy which again fail, in a manner very similar to that observed for Scheme I, at intermediate and large coupling. Although we have not proved this, the breakdown of the NCCM based on Scheme II for intermediate coupling is almost certainly due to an incompleteness similar to that shown for Scheme I. Furthermore, the failure of this approach at large coupling is particularly significant, since it is obvious from (5.13) that the $g \to \infty$ ground state $|\Psi_+\rangle$ is of SUB-1 form with $s_1 = -2g/\omega$. The two–parameter variational calculation presented in Chapter 4, which was based on a trial state of SUB-1 Scheme II form, correctly determines the limiting behaviour of s_1 as $g \to \infty$. For the CCM, which is based on a similarity rather than a unitary transform (see the discussion in Chapter 3), it can however be shown analytically (see Appendix D) that $s_1 = -2g/(\omega + \omega_0)$ in the SUB-1 approximation, and at resonance the SUB-1 result is thus not even correct to leading order. Thus, for Scheme II, the CCM also fails as a result of the non–Hermiticity of the method.