Chapter 9

Conclusions

The Rabi and linear $E \otimes e$ Jahn–Teller and pseudo Jahn–Teller Hamiltonians exhibit much interesting physical behaviour, and are relevant in many fields in physics. These non–adiabatic models capture and, by virtue of their simplicity, highlight some of the essential aspects of the interacting many–body problem. Thus the application of the coupled cluster method, with its highly impressive history as a powerful and versatile *ab initio* many–body technique, to such apparently straightforward models is of interest. Indeed, in this thesis, we have found that a CCM analysis of the Rabi and linear $E \otimes e$ JT and PJT Hamiltonians is anything but trivial, and that a thorough investigation of these models is required in order to apply the method successfully.

Analytic solutions for the spectra of the Rabi and linear $E \otimes e$ JT and PJT Hamiltonians are available only at the isolated Juddian values of the parameters which occur in these Hamiltonians. In this thesis, we have presented an elegant operator–based method which simplifies the analysis of the Juddian solutions for the linear $E \otimes e$ JT and PJT models [Bi99b]. For all the Hamiltonians considered here, we have used the isolated analytic solutions as a benchmark for the ground and first excited state results obtained via the configuration–interaction method. We conclude that the numerical diagonalization of these models yields results which are effectively exact, provided that the set of configurations included in the CI method is sufficiently large.

In the analysis of a given many–body Hamiltonian, it is important that the symmetries of the Hamiltonian be taken into account. In general, this not only simplifies the analysis, but also leads to more accurate results. A parity symmetry is associated with each of the Hamiltonians considered here. In the case where the two levels of the fermionic subsystem are degenerate, the eigenstates of the Hamiltonian are doubly degenerate for all values of the coupling strength of the interaction between the fermionic and bosonic degrees of freedom. For finite fermionic level splitting ω_0, however, the parity symmetry lifts this degeneracy; in particular, the ground (first excited) state is then a unique even–parity (odd–parity) state for all values of the coupling.

For the Rabi Hamiltonian with $\omega_0 > 0$, we have presented a simple three–parameter variational calculation which, due to the incorporation of the correct parity symmetry, yields excellent results for both the ground and first excited states of the system; in the physically interesting case of atom–field resonance, the maximal percentage error in the ground–state energy, over the full coupling spectrum, is 0.1 % [Bi99a]. For the linear $E \otimes e$ JT and PJT Hamiltonians, there is, in addition to the parity, also a conserved angular momentum component J. Due to the neglect of the J symmetry, the variational approach employed for the Rabi Hamiltonian does not readily generalize to the linear $E \otimes e$ JT and PJT case of two bosonic modes.

Using the CI results, the physical nature of the ground state of the Rabi and linear $E \otimes e$ JT and PJT Hamiltonians has been thoroughly examined. Although a phase transition does not occur, we have found that the ground state undergoes a change in character in a fairly well-defined transitional region of intermediate coupling. We have shown that this character change, which is closely analogous to the well-known crossover behaviour in the polaron problem, manifests itself in the occupation probabilities for the two levels of the fermionic system. Furthermore, we have found that this change in character also occurs in the even-parity ground-state in the case $\omega_0 = 0$, where the ground state is in fact doubly degenerate. It follows that the character change in the case $\omega_0 > 0$ is therefore not related to the onset of near-degeneracy in the transitional coupling region.

In previous applications of the CCM to both a multimode Rabi Hamiltonian and the linear $E \otimes e$ JT Hamiltonian, the symmetries of these Hamiltonians have been neglected. Our initial attempts at applying the CCM to the ground and first excited states of the Rabi Hamiltonian, with proper consideration of the parity symmetry, were based on the noninteracting model state of Schemes I and II (see Tables D.1). These calculations yielded very accurate results in the weak-coupling regime. However, the results also provided strong evidence for a spurious parity–breaking phase transition in the transitional coupling region [Bi96], even in the case $\omega_0 = 0$. Physically, the breakdown of the method in this regime is a result of the marked character change in the exact ground state, which is not in any way reflected in the noninteracting model state. We have formally demonstrated that the method fails as a direct result of the exponential form of the CCM ansatz for the ground–state wave function, which is incomplete, to any finite order, for the model state $|\Phi\rangle$ and cluster operator S of Scheme I. This is despite the fact that $|\Phi\rangle$ and $S = \sum_i s_i C_i^\dagger$ satisfy the requirement, dictated by the CCM formalism (see Chapter 3), that the set of states $\left\{C_i^\dagger|\Phi\rangle\right\}$ should span the many–body Hilbert space. This incompleteness is a serious defect not only of the CCM, but also of any method which relies on an $\exp S|\Phi\rangle$ parameterization of the ground state.

Subsequently, we showed that accurate CCM results for the ground and first excited state energies of the Rabi Hamiltonian can be obtained, provided that a coupling–dependent model state is chosen which mimics the change in character in the Rabi ground state; a common characteristic of such states is that they are exact in both the limits of zero and infinite coupling. In particular, a CCM calculation based on a model state of the two–parameter variational form (see Scheme IV in Table D.1) yields quantitatively accurate results which, for all couplings, compare favourably with results obtained via the benchmark three–parameter variational calculation. This CCM calculation is however not entirely satisfactory, since it involves considerably more computational effort than the variational analysis, and requires the use of a model state which of itself yields the overwhelming contribution to the exact ground and first excited state energies.

None of the schemes employed in the CCM analysis of the Rabi Hamiltonian effectively generalize to the linear $E \otimes e$ JT and PJT Hamiltonians, since these schemes do not incorporate the J symmetry of the linear $E \otimes e$ models. For these Hamiltonians, however, we have obtained excellent first–order CCM results for the ground and first excited state energies, using as model states the analytic ground state of the linear $E \otimes e$ RPJT Hamiltonian, and the corresponding spin–flipped state, respectively [Bi99b]. These results, which require the solution of only a single transcendental equation, are far superior to those obtained via earlier CCM analyses and other many–body methods, and are quantitatively accurate over the full coupling spectrum for a range of values for the parameter ω_0. Also, in contrast to the Scheme IV calculation for the Rabi Hamiltonian, the CCM energy here dramatically improves on the model–state energy. This is especially true for the (pure) linear $E \otimes e$ JT model in the physically interesting region of intermediate coupling, where the exact energy differs substantially from the model–state energy.

The analyses and results presented in this thesis suggest several avenues for further exploration. It would be of interest to apply the CCM to the polaron problem. This would determine whether the incompleteness of the exponential ansatz for the ground–state wave function is also a feature of other systems which undergo a drastic ground–state character change without a true phase transition. Given the quality of the good–parity variational results for the Rabi Hamiltonian, it would also be interesting to investigate the possibility of constructing a variational ansatz for the linear $E \otimes e$ JT and PJT Hamiltonians which incorporates all the symmetries of these models. Furthermore, the extension of our variational results for the Rabi Hamiltonian, and of our CCM results for the linear $E \otimes e$ JT and PJT Hamiltonians, to higher–lying states would allow for the consideration of both the time– and temperature–dependence of these models. This would permit comparison with experimental results.