Chapter 1

Introduction

Non–adiabatic models of a two–level fermionic system interacting with either one or two independent modes of a quantized bosonic field are of topical interest for several reasons. Firstly, these models serve as generic prototypes for a wide variety of physical systems. In quantum optics, models of this form are employed to describe the resonant or near–resonant interaction of a two–level atom with either a single or two perpendicularly polarized modes of a quantized electromagnetic field [Sh93, Mi91]. In the case of a single electromagnetic mode, the model is known as the Rabi Hamiltonian, or equivalently as the Jaynes–Cummings model without the rotating wave approximation (RWA). In quantum chemistry, models of this form describe the vibronic coupling between two electronic levels and two degenerate nuclear vibrational modes in a molecule or crystal. This is known as the linear $E \otimes e$ Jahn–Teller model in the case where the electronic levels are degenerate, and as the linear $E \otimes e$ pseudo Jahn–Teller model in the case where the electronic

levels are non–degenerate [Berb]. The term *non–adiabatic* arises in the context of quantum chemistry, and refers to the intimate coupling between the electronic and nuclear motions which occurs when it is no longer possible for the electrons to adiabatically follow the generally slower displacements of the more massive nuclei. Yet another realization of these models is provided by the two–site polaron in solid state physics, describing the interaction of an electron confined to two sites in a crystal lattice with the quantized phononic field of the lattice [Mah, Hak].

Judd [Ju77, Ju79] and subsequently Reik [Re87], guided by the results of early numerical diagonalizations [Lo58, Th68], proved the existence of analytic solutions for the linear $E \otimes e$ Jahn–Teller and Rabi Hamiltonians at isolated values of the coupling. Complete analytic solutions, valid for all couplings, are however only known for a few special cases of the class of non–adiabatic Hamiltonians considered here. Given their physical relevance, these models have therefore been the subject of much theoretical investigation. Recent many–body analyses of the Rabi Hamiltonian include the use of time–independent perturbation theory (TIPT) [Gr84b, Ph89, Qi98], a variational approach [Qi98], and several methods aimed at finding numerically exact results for the Rabi spectrum [Lo96, Fe96, Qi98]. Several variational calculations have also recently been performed for the linear $E \otimes e$ Jahn–Teller system [Lo91, Hu98].

The theoretical models considered here always represent, to a greater or lesser degree, an idealized simplification of the real physical system under consideration. It is in the very simplicity of these models, however, that

their further utility lies. Besides the isolated analytic solutions, quasi–exact numerical results for these models are also available, or relatively easy to obtain. Furthermore, simple Hamiltonians such as these often contain interesting symmetries, and as such are ideal testing grounds for approximate many–body methods.

Finally, apart from their practical value, these models represent some of the simplest non–trivial examples of quantum many–body physics. The straightforward appearance of these models hides a wealth of interesting quantum behaviour, which is readily contrasted with that of their classical or semi–classical counterparts [Bl96]. It is instructive to note that, despite intensive investigation, a complete analytic description of even the ground state of the Rabi Hamiltonian has not yet been found.

In this thesis, we therefore analyze several of these Hamiltonians from the perspective of quantum many–body theory. As a starting point, it is worth summarizing the characteristics which a good many–body method should embody:

1. It should be a microscopic or *ab initio* method, *i.e.* it should be a first–principles approach which readily reveals the physical significance of both its approximation scheme and its results. This requirement is generally not met by, *e.g.*, a large scale numerical diagonalization, or a quantum Monte Carlo calculation.
2. A related but different requirement is that the method should always be exact in principle, *i.e.*, it should reproduce the exact result in the limit

where the method is applied to infinite order, or equivalently, is applied without any form of approximation. This excludes perturbation theory, which fails in this respect when applied to non–perturbative systems.

3. It should be universal, *i.e.* the method should be applicable, with very little or ideally no modification of its standard form, to any given many–body system. This requirement excludes, *e.g.*, the method of canonical transformation, which generally requires either a lucky guess, a trial–and–error approach, or an inordinate amount of physical insight.

4. The method should be capable of systematic improvement, and should yield results that converge uniformly as the order to which the method is applied is increased. In general, this excludes the variational method.

5. Finally, the application of the method should be computationally simple or, at the very least, tractable.

The coupled cluster method (CCM) is one of the few quantum many–body techniques which can lay claim to satisfying almost all the criteria listed above. This non–perturbative method, originally developed in nuclear physics by Coester and Kümmel [Co58, Co60], has since been successfully applied in the analysis of the many–body ground–state in quantum chemistry [Ci66, Bar78, Pu82, Mo87, No87, No88, Bar89, Wo94, Wo96a], the electron gas [Bi78, Em84], quantum tunneling in the presence of a phonon bath [Wo96b], lattice gauge [Bi93, Le93, Ba96, Le98] and continuum field [Fu87, Ar90] theories, and spin and electron lattice models [Ro90, Bi91b]. An alternative formulation of the CCM, the so–called extended coupled cluster method (ECCM) introduced by Arponen [Ar83a], has also been successfully

applied [Ar83a, Ar83b, Ro89] to the Lipkin–Meshkov–Glick (LMG) model [Li65] in nuclear physics. This is a particularly important application of the method, given that the nucleus in the LMG model is known to exhibit a phase transition from a spherically symmetric to a deformed shape. Both the normal and extended CCM have also been reformulated in order to study excited states [Em81, Ar83a, Ar87].

In addition to its power and scope, the CCM also yields size–extensive results for all ground–state observables, including the ground–state energy, at every level of approximation (the cluster property). This is due to the CCM prescription for calculating the expectation value of an arbitrary ground–state observable, which implies that such expectation values are calculated as a sum over linked diagrams only.

No many–body method is perfect, and the CCM does display some less desirable features. There is no guarantee of uniform convergence in the CCM, although this is often the case in practice. Also, the method can sometimes be computationally expensive, although this is often the result of an injudicious choice for the model state and cluster correlation operator which characterize the CCM.

Perhaps the most serious known criticism of the method is that the CCM, to any finite order, is manifestly non–Hermitian, relying on an independent parameterization of the ground–state bra and ket. Although the CCM is a genuine variational method, this non–Hermiticity implies that an approximate CCM result for the ground–state energy no longer provides an upper

bound to the true ground–state energy [1]. This loss of the upper–bound property is offset by the following factors: firstly, the similarity transformed Hamiltonian which occurs in the CCM formalism is amenable to the Hausdorff expansion, which in most cases either terminates naturally or is resummable to closed form without approximation; secondly, at every level of approximation, the CCM in its purest form is compatible with the Hellman–Feynman theorem.

The primary aim of this thesis is to investigate the applicability of the CCM to the class of non–adiabatic Hamiltonians introduced above. In particular, we apply the CCM to the ground and first excited states of the Rabi Hamiltonian and the linear $E \otimes e$ Jahn–Teller and pseudo Jahn–Teller systems.

For comparison, we also consider the application of other many–body techniques to the Rabi and linear $E \otimes e$ Jahn–Teller systems. We present an operator–based method which simplifies the analysis of the isolated analytic (Juddian) solutions for the linear $E \otimes e$ Jahn–Teller models, and yields explicit closed–form expressions for the wave functions at the Juddian points. We also perform a weak–coupling TIPT calculation, analytic to any finite order, for the Rabi Hamiltonian, as well as a simple variational calculation which yields results, for both the ground and first excited states of the Rabi Hamiltonian, far superior to those obtained by previous methods.

The CCM has previously been applied to the Rabi and linear $E \otimes e$ Jahn–

[1] See also [Sc92] for a discussion of the implementation of a variational principle in certain non–Hermitian systems.

Teller systems. Wong and Lo have used the CCM to calculate the ground–state energy of both the multimode Rabi [Wo96b] and the linear $E \otimes e$ pure (as opposed to pseudo) Jahn–Teller Hamiltonians [Wo94, Wo96a]. In both cases, these authors perform a unitary transformation which destroys at least two of the symmetries of the Hamiltonian, and then apply the CCM to the transformed Hamiltonian. For the linear $E \otimes e$ Jahn–Teller system, where the fermionic levels are degenerate, they obtain very accurate results over the full coupling spectrum. For the Rabi and pseudo Jahn–Teller Hamiltonians, however, the fermionic level splitting is nonzero, and as a result the eigenstates of these systems are of definite symmetry. Thus the approach of Wong and Lo yields quantitatively inaccurate CCM results for the Rabi Hamiltonian in the intermediate coupling regime, does not readily generalize to the pseudo Jahn–Teller system, and also does not allow for a CCM calculation of the first excited state energy.

Our main purpose is to show that it is possible to obtain quantitatively accurate results for the ground and first excited state energies of the Rabi, linear $E \otimes e$ Jahn–Teller, and linear $E \otimes e$ pseudo Jahn–Teller systems within the CCM by maintaining the correct symmetries throughout the analysis. We show that this is in fact possible, provided that a CCM model state is chosen which is also capable of following the change in character which occurs in the ground state of these systems.

We also demonstrate that, for a naive choice of model state and correlation operator, the CCM fails when applied to the Rabi and linear $E \otimes e$ Jahn–Teller Hamiltonians. We show not only that the non–Hermiticity of the

CCM can lead to a breakdown in the method, but also that the method may fail as a result of an essential incompleteness due to the exponential form of the CCM ansatz for the ground–state wave function. Given the broad freedom of choice for the model state and correlation operator implicit in the method, these defects have severe implications not only for the CCM, but also for other methods which employ the exponential form.

To conclude this introduction, we present here an outline of the remainder of this thesis. In Chapter 2 we introduce the general class of model Hamiltonians under consideration. Chapter 3 gives an overview of the coupled cluster method. Chapters 4-6 are devoted to the Rabi Hamiltonian, and Chapters 7-8 to the Jahn–Teller systems. In Chapter 9 we summarize the main results of the thesis, and present conclusions.