Quantum optics meets quantum many-body theory

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QUANTUM OPTICS MEETS QUANTUM MANY–BODY THEORY: COUPLED CLUSTER STUDIES OF THE RABI HAMILTONIAN

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The Rabi Hamiltonian, which describes the interaction of a single mode of electromagnetic radiation with a two–level system, is one of the fundamental models of quantum optics. It is also of wider interest as it provides a generic model for the interaction of bosons and fermions. To allow for a systematic analysis of the strong–coupling behaviour, we have applied the coupled cluster method (CCM) to the Rabi Hamiltonian to calculate its spectrum. We find strong evidence for the existence of a somewhat subtle quantum phase transition.

1 Introduction

The prototypical model for the interaction of a single mode of a quantised electromagnetic field with a two-level system, popular in quantum optics [1,2] and more recently in studies of quantum chaos [3] is the Rabi Hamiltonian, given by

$$H = \frac{1}{2}\omega_0\sigma^z + \omega b^\dagger b + g(\sigma^+ + \sigma^-)(b^\dagger + b), \qquad (1)$$

where σ^z, σ^+ and σ^- are Pauli matrices, and b and $b^\dagger$ are bosonic annihilation and creation operators respectively, obeying the commutation relation $[b, b^\dagger] = 1$. There is a conserved parity Π associated with the Hamiltonian (1),

$$Pi = \exp[i\pi N], \quad N \equiv b^\dagger b + \frac{1}{2}(\sigma^z + 1). \qquad (2)$$

Although the Rabi Hamiltonian (1) does not appear to be integrable, (and see, however, Ref. 4), it clearly becomes so if the rotating wave approximation (RWA) is made, leading to the Jaynes-Cummings model.[1] In the RWA the terms $g(b^\dagger\sigma^+ + b\sigma^-)$ are neglected, so that $[H_{\text{RWA}}, N] = 0$ and the model is exactly soluble by a series of 2×2 diagonalisations.

Historically, most calculations based on (1) have made use of the RWA for applications where $g/\omega << 1$, and of diagonalisation in large but finite vector spaces for $g/\omega \sim 1$. In the present work, we report on the results obtained from the application of the coupled cluster method (CCM) to the Hamiltonian of Eq. (1). The CCM is well known in the quantum many–body theory community, and the reader is referred to the literature (see, e.g., Ref. 5) for a detailed discussion of the

CCM. For the formalism for the application of the CCM to the Rabi Hamiltonian, the reader is referred to previous work.[6]

2 Ground State Results: Normal Coupled Cluster Method (NCCM)

We turn now to our results for the ground–state energy for the Hamiltonian (1) with $\omega_0 > 0$. For simplicity, we will only quote results for the case of a scaled Hamiltonian at resonance ($\omega = \omega_0 = 1$). Since the Rabi Hamiltonian is not integrable, some approximation has to be made. The simplest is the SUB–N approximation, in which the CCM correlation operator is truncated so as include at most N–body excitations relative to the chosen model state.[5]

We find that the ground–state energy shows evidence for spontaneous breaking of the parity symmetry. For each N, the solution with positive parity terminates at a finite value of g which we indicate by $g_c^{(N)}$. It is possible to find solutions above this coupling with mixed symmetry; these solutions reproduce the expected large–g behaviour, but appear to be rather unreliable for $g < 2$.

In Figure 1 we show the ground–state energy E_g as a function of the coupling g for several SUB-N approximations, together with configuration–interaction (CI) method results from a diagonalisation of (1) in a basis of 100 positive parity states. For $g < g_c^{(N)}$, the agreement between the results of the CCM and CI calculations is very good. The termination points of the CCM solutions with positive parity are clearly visible. Note that there is a difference in the nature of the termination of the positive parity solutions depending on whether $\frac{N}{2}$ is odd or even.[6] In the same reference, an attempt is made to determine critical indices for a possible parity–breaking transition using the coherent anomaly method (CAM) of Suzuki.[7] The results of this analysis suggest that there may be an essential singularity in the ground state energy at $g \approx 0.665$.

Similar behaviour is certainly known to exist in some comparable exactly integrable models, for example at the isotropic Heisenberg point for a 1D chain of spin–1/2 atoms interacting via the XXZ Hamiltonian. The CCM has been applied to this model in both 1D and 2D, and equally strong evidence for similar critical behaviour has been observed in various truncation schemes.[8]

The CI and CCM results appear to be contradictory, in that the CI calculations give no indication of a possible phase transition and always yield a positive–parity ground state. However, the application of a unitary transformation to the Hamiltonian yields states which always have mixed parity, so it is by no means clear that the CI results are reliable in the prediction of a possible phase transition. More detailed investigations of the CI results are in progress.

3 Excited States (NCCM)

The CCM formalism also permits the calculation of the spectrum of a given Hamiltonian. The standard approach is that of Emrich,[9] in which the excited–state ket is parameterised by means of an excitation operator acting on the CCM ground–state ket. A problem with this approach is that another approximation, namely in the excitation operator, is necessary to enable calculations to be performed.

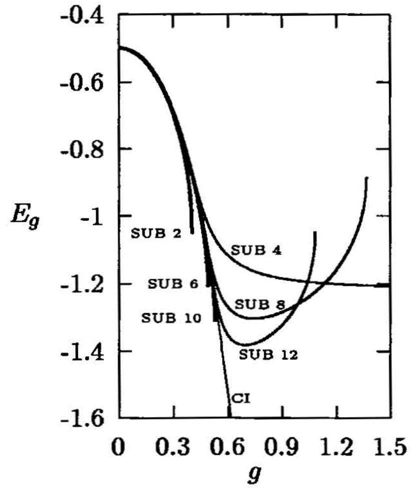

Figure 1: The ground–state energy E_g as a function of the coupling g for the indicated CCM SUB-N approximations for the case $\omega = \omega_0 = 1$. Also shown are the results of a CI calculation in a basis of 100 positive–parity states.

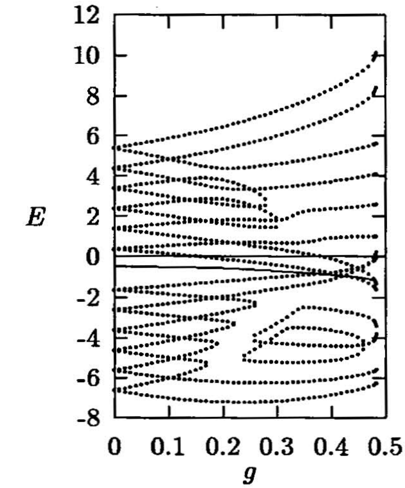

Figure 2: The spectrum of the Rabi Hamiltonian, as determined from linear repsonse theory, for the CCM SUB–6 approximation ($\omega = \omega_0 = 1$). The ground–state energy is shown as the solid line, with the excited states shown as dots. Missing regions in the excited states indicates complex energies. Note the presence of the spurious (negative–energy) excitations.

An alternative method which avoids the need to introduce another truncation is to use the theory of linear response.[10] Here a dynamical matrix is determined, the eigenvalues of which are the excitation energies. At the SUB–N level of approximation, the matrix is of dimension $4N$; however, half of the eigenvalues are spurious due to symmetries in the matrix.

Figure 2 shows the full spectrum (spurious states included) for the SUB–6 approximation for the Rabi Hamiltonian at resonance. The bunching of the states near $g_c^{(6)}$ is noteworthy, and may provide additional support for the possibility of a parity–breaking phase transition in this system.

4 Ground State Results: Extended Coupled Cluster Method (ECCM)

Although the NCCM has been very successfully applied to a wide variety of physical systems, its one major failing is its apparent inability to traverse regions of parameter space near phase transitions. However, a modified version of the CCM ansatz, which makes use of a double similarity transform of the Hamiltonian rather than the single such transform of the NCCM, has been very successful in correcting this shortcoming. This approach is called the extended coupled cluster method.[11]

We have applied the ECCM to the Rabi Hamiltonian to calculate the ground–state energy. Apart from some difficulty in the close proximity of the NCCM critical point, our initial ECCM results are very close to those of the CI. However, the eigenket below the transition region can easily be shown to be of positive parity, while that above the transition is definitely of mixed parity. This result is very different to the conclusions which would be drawn from the CI calculation.

5 Conclusions and Future Work

In contrast to the perturbative or semiclassical treatments of previous work on the Rabi Hamiltonian, we have applied the CCM to the calculation of its spectrum. For the weak–coupling range of parameters typical of optical applications to date the method converges extremely rapidly to yield very accurate results. However, since quantum optics experiments are nowadays being performed with ever–increasing atom–field couplings, it is of considerable interest to explore the full Rabi Hamiltonian with a non–perturbative approach such as the CCM. One outcome has been that for stronger couplings than have hitherto been explored experimentally, our results provide strong evidence for a subtle quantum phase transition. Future work includes higher–order ECCM calculations, and the determination of a suitable order parameter for the transition. In the longer term, the application of the CCM to other Hamiltonians of relevance in quantum optics, such as multi–level systems, is envisaged.

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