Coupled cluster analysis of model non–adiabatic Hamiltonians

by

David Michael van der Walt

Submitted in partial fulfillment of the requirements for the degree

Philosophiae Doctor (Physics)

in the Faculty of Science

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Abstract

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In this thesis, we undertake a theoretical many–body investigation into the ground and first excited states of a class of model non–adiabatic Hamiltonians describing the interaction of a two–level fermionic system with one or more modes of a quantized bosonic field. These models are of topical interest in quantum optics, solid state physics and quantum chemistry, and we focus here in particular on the Rabi Hamiltonian (or Jaynes–Cummings model without the rotating wave approximation) in quantum optics, and the linear $E \otimes e$ Jahn–Teller and pseudo Jahn–Teller systems in quantum chemistry.

Due to their simplicity, these Hamiltonians exhibit interesting symmetries, allowing them to serve as useful testing grounds for quantum many–

body techniques. Here we analyze these models by means of the the coupled cluster method (CCM). The CCM has an impressive record as a powerful and versatile *ab initio* method, having been successfully applied in nuclear physics, quantum chemistry, lattice gauge and continuum field theories, and spin and electron lattice models. For comparison, we also present results for our model Hamiltonians obtained via a variety of other many–body methods. In particular, we present an excellent variational calculation for the Rabi Hamiltonian in which the importance of the incorporation of the correct symmetry in the variational ansatz is highlighted, as well as an elegant operator method useful in the analysis of the linear $E \otimes e$ Jahn–Teller and pseudo Jahn–Teller models.

The CCM analysis of the class of Hamiltonians considered here displays a critical dependence on the choice of the model state and corresponding creation operators which characterize the method. For certain physically reasonable choices, we present a formal demonstration of an essential incompleteness, to any finite order, in the CCM ansatz for the ground–state wave function of the system. As a result, the CCM results for these systems strongly suggest a phase transition which does not in fact exist. We also show that, for certain other choices of the model state and creation operators, the CCM breaks down as a result of the non–Hermiticity of the method.

This breakdown of the CCM is closely related to the marked change in character of the ground state of the systems considered here. Using a model state which mimics this change in character, excellent CCM results for these systems can be obtained; in particular, we present a simple yet extremely accurate CCM calculation for the linear $E \otimes e$ Jahn–Teller and pseudo Jahn–

Teller models. The dependence of the CCM results for the Hamiltonians considered here on the choice of the model state and creation operators is of considerable importance, given that the CCM formalism does not *a priori* specify this choice beyond the overall symmetry requirements of the Hamiltonian. The results demonstrate that the gross physical properties of the exact solution need to be reproduced by the model state if even qualitatively correct behaviour is to be obtained from a CCM calculation.

Samevatting

Gekoppelde–bondel–analise van model nie–adiabatiese Hamilton operatore

deur

David Michael van der Walt

Voorgelê ter gedeeltelike vervulling van die vereistes vir die graad

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In hierdie tesis word 'n teoretiese veeldeeltjie–ondersoek geloods na die grondtoestand en die laagste opgewekte toestand van 'n bepaalde klas nie–adiabatiese model–Hamilton operatore wat die interaksie beskryf tussen 'n tweevlak fermionsisteem en een of meer modes van 'n gekwantiseerde bosoniese veld. Hierdie modelle is tans van belang in kwantumoptika, vastetoestandfisika en kwantumchemie, en ons fokus hier spesifiek op die Rabi Hamilton operator (of Jaynes–Cummings model sonder die roterende–golf–benadering) in kwantumoptika, en die lineêre $E \otimes e$ Jahn–Teller en kwasi–Jahn–Teller sisteme in kwantumchemie.

As gevolg van hul eenvoud vertoon hierdie Hamilton operatore interes-

sante simmetrieë, wat hul in staat stel om as 'n toetsterrein te dien vir veeldeeltjietegnieke. Ons analiseer hierdie modelle hier deur middel van die gekoppelde–bondel–tegniek (CCM). Die CCM het 'n indrukwekkende rekord, en is al suksesvol aangewend in kernfisika, kwantumchemie, rooster–yk– en kontinuumveldteorië, en spin– en elektron–matriksmodelle. Ter vergelyking wys ons ook resultate vir ons model–Hamilton operatore wat deur middel van 'n verskeidenheid ander metodes verkry is. In die besonder bied ons 'n akkurate variasie berekening vir die Rabi Hamilton operator aan wat die belang van die insluiting van die korrekte simmetrieë in die variasie aanname beklemtoon, asook 'n elegante operatormetode wat in die analise van die lineêre $E \otimes e$ Jahn–Teller en kwasi–Jahn–Teller sisteme benut kan word.

Die CCM analise van die klas Hamilton operatore wat hier beskou word toon 'n kritiese afhanklikheid van die keuse van modeltoestand en ooreenstemmende skeppingsoperatore wat die metode karakteriseer. Vir bepaalde fisies verantwoordbare keuses, toon ons formeel aan dat daar 'n essentiële ontoereikendheid bestaan, tot enige eindige orde, in die CCM–aanname vir die grondtoestand–golffunksie van die sisteem. As gevolg hiervan bied die CCM resultate sterk getuienis vir 'n fase–oorgang wat in werklikheid nie bestaan nie. Ons toon ook aan dat die CCM, vir sekere ander keuses van die modeltoestand en skeppingsoperatore, faal as gevolg van die nie–Hermitiese aard van die metode.

Hierdie mislukkings van die CCM is nou verwant aan die skerp gedragsverandering in die grondtoestand van die sisteme wat ons hier beskou. Mits 'n modeltoestand gebruik word wat hierdie gedragsverandering naboots, kan uitstekende CCM resultate vir hierdie sisteme verkry word; ons vertoon in besonder 'n eenvoudige dog uiters akkurate CCM berekening vir die lineêre $E \otimes e$ Jahn–Teller en kwasi–Jahn–Teller sisteme. Die modeltoestand- en skeppingsoperatorafhanklikheid van die CCM resultate vir die Hamilton operatore wat hier beskou word is van groot belang, gegewe dat die CCM nie *a priori* die keuse van of die modeltoestand of skeppingsoperatore voorskryf buiten die oorkoepelende simmetrieë van die Hamilton operator nie. Die resultate demonstreer dat die uitstaande fisieke eienskappe van die eksakte oplossing in die modeltoestand vervat moet word indien selfs kwalitatief korrekte gedrag deur middel van 'n CCM berekening verlang word.

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