Annals of Physics 378 (2017) 280–302

Contents lists available at ScienceDirect

Annals of Physics

journal homepage: www.elsevier.com/locate/aop

Electronic correlations in the Hubbard model on a bi-partite lattice

Wissam A. Ameen [a,b], Niels R. Walet [a,*], Yang Xian [a]

[a] *Theoretical Physics Division, School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, United Kingdom*

[b] *Physics Department, College of Science, University of Anbar, Anbar, Iraq*

ARTICLE INFO

Article history:
Received 26 April 2016
Accepted 20 January 2017
Available online 23 January 2017

Keywords:
Hubbard model
Spin excitations
Coupled-cluster method

ABSTRACT

In this work we study the Hubbard model on a bi-partite lattice using the coupled-cluster method (CCM). We first investigate how to implement this approach in order to reproduce the lack of magnetic order in the 1D model, as predicted by the exact Bethe-Ansatz solution. This result can only be reproduced if we include an algebraic correlation in some of the coupled-cluster model coefficients. Using the correspondence between the Heisenberg model and the Hubbard model in the large-coupling limit, we use very accurate results for the CCM applied to the Heisenberg and its generalisation, the *XXZ* model, to determine CCM coefficients with the correct properties. Using the same approach we then study the 2D Hubbard model on a square and a honeycomb lattice, both of which can be thought of as simplified models of real 2D materials. We analyse the charge and spin excitations, and show that with care we can obtain good results.

© 2017 Elsevier Inc. All rights reserved.

1. Introduction

The Hubbard model [1] and its variations have been widely applied to investigate the electronic correlations of interacting electrons in low-dimensional systems. The simple form of the model not only provides an excellent test ground for bench-marking theoretical tools, but also has important

* Corresponding author.
E-mail address: Niels.Walet@manchester.ac.uk (N.R. Walet).

http://dx.doi.org/10.1016/j.aop.2017.01.018
0003-4916/© 2017 Elsevier Inc. All rights reserved.

applications in describing experimental data. The model has played an important role in our understanding of the high-T_c superconductors over the last few decades, see, e.g., Ref. [2], and has been extensively studied using many microscopic methods, see, e.g., Refs. [3,4] for recent reviews.

The Hubbard model consists of only two terms: a nearest-neighbour electron hopping term with strength t and an on-site electronic repulsion with strength U. In two dimensions on a square lattice when half the available electronic states are filled, the on-site repulsion causes a Mott transition from a paramagnetic conductor to an antiferromagnetic insulator for any non-zero value of U [2]. However, the model on a honeycomb lattice shows a different picture: the paramagnetic state is stable for small U, and the Mott transition occurs at a non-zero value of the interaction $U = U_c$, which has a value of about $U_c/t \approx 4.5$ (see e.g., Ref. [5]). This quantum phase transition has attracted strong theoretical interests since the discovery of graphene and other two-dimensional materials such as silicene and Boron Nitride [6] due to their hexagonal structures. Of course, the application of the Hubbard model to graphene and sister materials may be questioned and is a subject of ongoing debate; most theoretical studies of interaction effects in graphene employ the full long-range Coulomb interaction [7]. Nevertheless, the Hubbard model with local interactions (the on-site and nearest neighbour interactions) has been used to investigate the electronic correlations in graphene such as the possible edge magnetism of narrow ribbons and formation of local magnetic moments (see references in [7]). Furthermore, there is also some theoretical discussion of possible spin-liquid phase between the metallic phase and the ordered antiferromagnetic insulating phase on a honeycomb lattice. Sorella et al. [8] report, using a numerically exact Monte Carlo method, that there is little or no indication of such a phase transition to a spin liquid in clusters of 2592 atoms. Both Sorella et al. and He et al. [5] argue for a spin-liquid state below U_c, with a semi-metallic state only at $U = 0$, with evidence for a first order Mott phase transition. Yang et al. [9] apply an effective Hamiltonian approach, and also find weak or no evidence for a quantum spin liquid. In the work of Lin et al. [10], a slightly modified version of the Hubbard model is studied.

One of the important methods to systematically study electronic correlations of interacting electron systems is the coupled-cluster method (CCM) [11]. The key advantages of the CCM are its avoidance of unphysical divergences in the thermodynamic limit and its ability to be taken to high accuracy through systematic inclusion of high-order correlations. The price to pay is that the method does not provide a variational bound to the ground state energy, and that the wave function is not Hermitian. Nevertheless, convergence of CCM calculation has been found to be rapid. Therefore, the CCM is the method of choice for state-of-the-art calculations for atomic and molecular systems in quantum chemistry, where it is used, amongst others, to calculate correlation energies, to an accuracy of less than one millihartree (1 mH) [12]. The CCM has been successfully applied to a wide range of other physical systems, including problems in nuclear physics, both for finite and infinite nuclear matter, the electron gas and liquids, as well as various integrable and nonintegrable models, and various relativistic quantum field theories. In most such cases the numerical results are either the best or among the best available. A classical example is the electron gas, where the coupled cluster results for the correlation energy agree over the entire metallic density range to within less than 1 millihartree (or less than 1%) with the essentially exact Green's function Monte Carlo results [11]. Most relevant to our present work, over the last two decades the CCM has also been successfully applied to describe quantum spin lattice systems accurately, providing some of the best numerical results for the ground state energy, the sub-lattice magnetisation, and spin-wave excitation spectra (for a recent example see, e.g., Ref. [13]). In such applications, the power of the systematic improvements attainable by the inclusion of higher order calculations through the use of computer algebra has helped understanding of the physical properties of the quantum phase transitions in spin systems.

The CCM shares quite a few of its roots with classic many-body techniques based on many-body perturbation theory, see Refs. [3,4] for some modern examples. The result of CCM calculations look much like a resummation of the perturbation series, and indeed do not diverge where perturbation theory fails to converge. It is a pure method: normally one works directly with the full complement of quasi-particles relative to a generalised vacuum – usually called reference – state. There is a similarity with dynamical mean-field theory. The lowest order of CCM is like mean-field theory, and one can include higher order RPA-like correlations. In the standard formulation applied here it lacks the full power of the normal mean-field, which is included in the dynamical mean-field method, but including

Download English Version:

https://daneshyari.com/en/article/5495920

Download Persian Version:

https://daneshyari.com/article/5495920

Daneshyari.com