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Coupled-cluster theory for bosons in rings and optical lattices

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Dedicated to Prof. D. Mukherjee on the occasion of his 60th birthday.

Abstract

Bosons in optical lattices and rings are attractive and active fields of research in cold-atom physics. Here, we apply our recently developed coupled-cluster approach for bosons in external traps to these systems, and extend it to the lowest-in-energy excited states with total quasi- or angular-momentum k. In the coupled-cluster approach the exact many-boson ground state is obtained by applying an exponential operator $\exp\{T\}$, $T=\sum_{n=1}^{N} T_n$ to the ground configuration, which is (usually) the state where the bosons occupy a single orbital. For excited states, a second exponential operator $\exp\{T^{(k)}\}$, $T^{(k)}=\sum_{n=1}^{N} T_n^{(k)}$ is employed to accommodate the remaining excitations from the unperturbed excited configuration. Due to the conservation of momentum, T_1 and $T_1^{(k)}$ can vanish. Working equations for coupled-cluster (singles) doubles (CCD) are provided and their implications are briefly discussed.

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1. Introduction

Following the experimental demonstrations of Bose–Einstein condensates in dilute gases [1,2], the problem of many bosonic atoms interacting in a trap potential has attracted an accelerated interest by the scientific community, see [3,4] and references therein. Nowadays, one of the most active subjects in cold-atom physics is the study of bosons in optical lattices, see, e.g. Refs. [5–10] and the recent review [11] and references therein. The problem of bosons in a ring, which dates back at least to the 1960s [12], has attracted its own attention in the context of cold-atom research [13–18].

There are many phenomena trapped bosons exhibit that can be described quite well by the standard mean-field approach, namely Gross–Pitaevskii (GP) theory [19], see [3,4] and reference therein. Side-by-side, the necessity to go beyond mean-field and describe many-body facets of trapped bosons, e.g. the superfluid to Mott-insulator transition in optical lattices [5,6], has become well-accepted and pursued by the community, see the reviews [20] and [21], and references therein.

The many-boson problem is difficult to tackle. Consider, for instance, the standard configuration-interaction (CI) approach, which employs a basis set expansion. When the interaction between the N bosons is substantial and/or many of them are present, the number of configurations necessary to properly describe the correlated wavefunction quickly increases beyond computational reach and truncations become a must. When truncations of the CI expansion are made, there are hints and evidences to slow convergence of the CI expansion, see, e.g. [15,22]. Evidently, development of other many-body methods, which truncate the full configuration space in a different manner are of high relevance and actuality. Such methods are reviewed in [20] and [21], the latter being devoted to the extensively studied homogeneous Bose gas problem.

Coupled-cluster theory was first formulated in nuclear physics by Coester [23] and Coester and Kümmel [24], and soon after was introduced to electron-structure theory by Čižek [25] and Čižek and Paldus [26]. Coupled-cluster theory has since proven to be a very valuable and accurate approach in the many-fermion problem, see [27–29] and references therein. For atomic and molecular systems, coupled-cluster theory is currently considered to be one of the if not the most powerful

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many-body tool for calculating electron-correlation energies [27–29], also in relativistic systems [30]. In the coupled-cluster approach the exact many-body wavefunction is obtained by applying an exponential operator $\exp\{T\}$ to the ground configuration $|\phi_0\rangle$. In practice, one truncates of course the operator T. For fermions, it is widely known that truncated coupled-cluster expansions are size consistent, which is another advantage the coupled-cluster approach possesses in comparison to truncated CI expansions, which are not size consistent [31].

Recently, we derived a coupled-cluster theory for bosons with emphasis on systems of interacting indistinguishable bosons in traps with up to many particles [32]. In Ref. [32], aspects like size consistency and what to use as the initial ground configuration $|\phi_0\rangle$ were investigated in detail. We have shown that, in contrast to the familiar situation for fermions for which coupled-cluster expansions are size consistent, for bosons the answer to this question depends on the choice of the ground configuration. In the present work, we would like to apply our recently developed coupled-cluster approach of Ref. [32] to the correlated ground-state of bosons in optical lattices and rings, making use of the high spatial symmetry of these systems. Furthermore, we extend our coupled-cluster approach to the lowest-in-energy excited states with total quasi- or angular-momentum k of bosons in optical lattices and rings. Finally, we would like to mention that coupled-cluster approaches for molecular vibrations [33], 'bosonic nuclei' [34], the spin-boson model [35], and within bosonization of many-electron systems [36] have been studied in the literature, but are very different from our work.

The structure of the paper is as follows. In Section 2, we derive the coupled-cluster theory for the ground- and excited-states of bosons in rings and optical lattices. Working equations for the particular truncation of the coupled-cluster to (single) and double excitations (CCD) are derived in Section 3 for bosons in a ring. Finally, in Section 4, we discuss the present results and provide concluding remarks.

2. Ground and excited-state coupled-cluster Ansätze

2.1. Preliminaries

Consider a system of interacting N identical bosons in an one-dimensional (1D) optical lattice where a is the lattice constant. Periodic boundary conditions are assumed with L being the normalization 'volume'. The problem of N identical bosons in an 1D ring of perimeter L is equivalent to the former, when the optical-lattice potential vanishes. Therefore, we describe both systems by the same coordinate x and treat them hereafter simultaneously, as much as possible. For instance, we use the shorthand notion of momentum k to describe the bosons angular momentum in the ring and quasi-momentum in the *optical* lattice. Due to the presence of translational symmetry–continuous symmetry for the ring and discrete symmetry for the lattice—the momentum k is a good quantum number. Of course, for the ring k is unbounded, $k=2\pi n/L$ where n is any integer, whereas in optical lattices k can be restricted, say, to the first Brillouin zone, $-\pi/a<k\leq\pi/a$ ($\pm\pi/a$ correspond to equivalent points in reciprocal space). The many-boson ground state of the system has, of course, zero total momentum.

As usual, the Hamiltonian H of the system consists of an one-particle operator $\hat{h}(x)$ and a two-particle interaction $\hat{V}(|x-x'|)$. It is convenient to introduce one-body functions (orbitals), which are eigenfunctions of $\hat{h}(x)$ and of the translation operator, $\hat{h}(x)\varphi_k(x)=\varepsilon_k\varphi_k(x)$. Let us also introduce destruction and creation operators b_k and $b_k^\dagger$ corresponding to the orbitals $\varphi_k(x)$. These operators fulfill the usual commutation relations

$$[b_k,b_{k'}^\dagger]=\delta_{k,k'},\qquad [b_k,b_{k'}]=[b_k^\dagger,b_{k'}^\dagger]=0 \tag{1}$$

for bosons. Utilizing these operators, we define the ground configuration

$$|\phi_0\rangle=\frac{1}{\sqrt{N!}}\left(b_0^\dagger\right)^N|0\rangle\equiv|N_0\rangle,\qquad \langle\phi_0|\phi_0\rangle=1 \tag{2}$$

which is the ground state of the system in the absence of interaction between the bosons. $|0\rangle$ denotes the vacuum. Similarly, we define the lowest-in-energy excited configurations of definite momentum k, obtained by an excitation of a single boson from $\varphi_0(x)$ to $\varphi_k(x)$, as:

$$|\phi_k\rangle=\frac{1}{\sqrt{(N-1)!}}b_k^\dagger\left(b_0^\dagger\right)^{(N-1)}|0\rangle\equiv|(N-1)_0,1_k\rangle,\qquad \langle\phi_k|\phi_k\rangle=1. \tag{3}$$

Obviously, $|\phi_0\rangle$ and $|\phi_k\rangle$ are orthonormal configurations. Finally, expressed in second quantization notation H takes on the common appearance [37]

$$H=\sum_k h_{kk}b_k^\dagger b_k+\frac{1}{2}\sum_{kpq}V_{(p+q-k)kpq}b_{(p+q-k)}^\dagger b_k^\dagger b_p b_q \tag{4}$$

where:

$$h_{kk}=\int\varphi_k^*(x)\hat{h}\varphi_k(x)\mathrm{d}x=\varepsilon_k,$$

$$V_{(p+q-k)kpq}=\iint\varphi_{p+q-k}^*(x)\varphi_k^*(x')\hat{V}(|x-x'|)\varphi_p(x)\varphi_q(x')\mathrm{d}x\mathrm{d}x'. \tag{5}$$

Here, conservation of momentum has been assumed explicitly.

2.2. Coupled-cluster for the ground state

Let us begin by formulating our coupled-cluster theory for the bosons in the ground-state [32], making particular use of the translational symmetry of the systems under investigation. In the coupled-cluster approach, the exact ground wavefunction $|\Psi_0\rangle$ is obtained by applying an exponential operator to the ground configuration (2):

$$|\Psi_0\rangle=\mathrm{e}^T|\phi_0\rangle. \tag{6}$$