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Coupled Cluster Wave Functions for Ground State Wave Function for Many Physical System

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ABSTRACT We have studied and found coupled cluster wave functions as important functions for a projection quantum Monte Carlo algorithm within the configuration interaction scheme. The ground state wave function of a configuration interaction Hamiltonian is filtered out by propagating the amplitudes of an initial arbitrary wave function via a random walk in the many body Hilbert space spanned by a basis of Slater determinants. The coupled cluster wave functions are used to guide this random walk via importance sampling in order to circumvent the sign problem. This approach has provided upper bounds to the ground state energy whose tightness can be systematically improved by including higher order excitations in the coupled cluster wave function. We have applied three dimensional homogenous electron gas in momentum space. The electron gas was studied for large single particle basis sizes. We found that coupled cluster wave functions are very accurate and good approximation for ground state wave function for many physical systems. The obtained results were in good agreement with previously obtained results.

KEYWORDS Coupled, Cluster, Monte Carlo Algorithm, Configuration Interaction, Hamiltonian, Random Walk, Hilbert Space, Excitations.

INTRODUCTION

The spectacular success of the fixed node Quantum Monte Carlo is largely of the development of high quality importance functions. Most of these importance functions have forms that are convenient for calculations in co-ordinate space only. The lack of accurate and computationally efficient importance functions has precluded a wide exploration of the fixed node Quantum Monte Carlo method within the configuration interaction Scheme[1]. Recently it was sparked by the demonstration that even within the configuration interaction scheme it is possible to apply stochastic projection to systems much larger than that would be possible using conventional matrix diagonalization[2-4]. The development of an efficient ground state Quantum Monte Carlo algorithm within the configuration interaction or momentum space would be of great interest for physics. The most of the modern interactions are written in nonlocal forms[5] and in electronic structure calculations with non local pseudopotentials[6]. Quantum Monte Carlo methods have become presently standard tools for accurate computations of ground state properties in a wide variety of strongly correlated systems[7] ranging from quantum chemistry[8-9] to condensed matter[10-11] and nuclear physics[12]. In fermionic systems Quantum Monte Carlo methods are plagued by the sign problem. The sign problem is circumvented in the fixed node

approximation with the help of importance sampling with a trial ground state wave function or importance function[13]. The obtained results were compared with previously obtained results.

METHOD

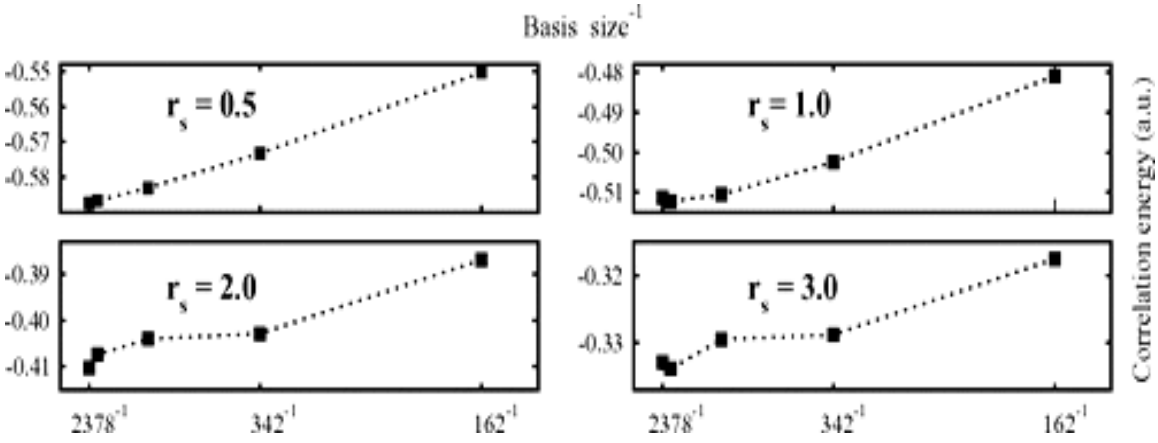
We have considered a general second quantized fermionic configuration interaction Hamiltonian which included only two body interactions.

$$H = \sum_{i \in S} \varepsilon_i a_i^\dagger a_i + \sum_{abij \in S} V_{ij}^{ab} a_a^\dagger a_b^\dagger a_i a_j$$

where $a_i^\dagger$ creates a particle in the single particle state labeled *i*. The set S of single particle state is assumed to be finite and size N_s. The V_{ij}^{ab} are general two body interaction matrix elements. For homogeneous systems we have assumed the plane wave state which defines momentum and space as the single particle basis set. The single particle energies are $\varepsilon_i = \frac{k_i^2}{2m}$ where $\boldsymbol{k}_i$ is the momentum of the *i*-state and *m* is the fermion mass. We have included single particle *i* with $k_i^2 \le k_{\max}^2$. The cutoff independent results have been obtained by performing successive calculations with increasing $k_{\max}$ and then extrapolating to $k_{\max} \to \infty$. In three dimensional electron gas the interaction matrix elements are $V_{ij}^{ab} = \left(1 - \delta_{k_a - k_i, 0}\right) \delta_{k_i + k_j, k_a + k_b} \frac{4\pi}{\Omega} \frac{1}{\left(k_a - k_i\right)^2}$. The volume Ω of the simulation box was determined by the density and the number of particles N in the simulation. The ground state wave function of $H, \left|\Psi_{gs}\right|$ was projected out with the power method, $\left|\Psi_{gs}\right| = \lim_{M \to \infty} P^M \left|\Psi_0\right\rangle$, where the propagator $P = 1 - \Delta\tau\left(H - E_T\right)$ or a more efficient variation. The $\Delta\tau$ is a small number in inverse energy units and E_T is and energy shift used to fix the norm of the wave function. In quantum Monte Carlo, the power method is applied stochastically. For a generic configuration interaction Hamiltonian the matrix elements of the propagator P are not non negative. This leaded a sign problem in quantum Monte Carlo.

RESULTS AND DISCUSSION

Graph (1) shows the configuration interaction Monte Carlo ground state energy estimated for $N = 14$ and $r_s = 0.5, 1.0, 2.0 \text{ and } 3.02$ for some large basis size calculations. Previously it was suggested for the three dimensional electron gas that is might be possible to extrapolate to the $N_s \to \infty$ by exploiting a linear $\frac{1}{N_s}$ dependence of the correlation energy for large but finite N_s. For r_s=0.5 and N = 14 such a linear trend in the correlation energy is visible for other values of r_s shown in the graph, no such trend is evident. The situation is similar for calculations with N = 32 and 54. We found that at least upto largest basis size $N_s = 2378$. The ground state energy of different r_s and N for the largest N_s was calculated. The energies were calculated in finite configuration interaction like basis set using the initiator full configuration interaction quantum Monte Carlo method. The $N_s \to \infty$ results were obtained by using the so called single point extrapolation from much smaller values of N_s than our obtained values. The finite basis set results were found in good agreement with previous results.



Graph: 1 Correlation energies for N=14 and rs =0.5, 1.0, 2.0, and 3.0 as a function of the single particle basis size from CIMC with the CCD (1) importance function.

CONCLUSION

We have found that three dimensional electron gas described by a simple Hamiltonian nevertheless encapsulated many of the difficulties associated with modern many body theories. It has both the weakly and strongly correlated regimes which can be accessed via single tunable density parameter, the Wigner-Seitz radius r_s provided an ideal system for bench making many body theories. We also found that coupled cluster wave functions introduced as importance functions in a Monte Carlo method designed for the configuration interaction framework to provide upper bounds to the ground state energy. The obtained results were found in good agreement with previously obtained theoretical and experimental works..

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