Ab initio computation of circular quantum dots

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We perform coupled-cluster and diffusion Monte Carlo calculations of the energies of circular quantum dots up to 20 electrons. The coupled-cluster calculations include triples corrections and a renormalized Coulomb interaction defined for a given number of low-lying oscillator shells. Using such a renormalized Coulomb interaction brings the coupled-cluster calculations with triples correlations in excellent agreement with the diffusion Monte Carlo calculations. This opens up perspectives for doing ab initio calculations for much larger systems of electrons.

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I. INTRODUCTION

Strongly confined electrons offer a wide variety of complex and subtle phenomena which pose severe challenges to existing many-body methods. Quantum dots in particular, that is, electrons confined in semiconducting heterostructures, exhibit, due to their small size, discrete quantum levels. The ground states of, for example, circular dots show similar shell structures and magic numbers as seen for atoms and nuclei. These structures are particularly evident in measurements of the change in electrochemical potential due to the addition of one extra electron, \( \Delta N = \mu(N + 1) - \mu(N) \). Here \( N \) is the number of electrons in the quantum dot, and \( \mu(N) = E(N) - E(N - 1) \) is the electrochemical potential of the system. Theoretical predictions of \( \Delta N \) and the excitation energy spectrum require accurate calculations of ground-state and of excited-state energies.

The above-mentioned quantum mechanical levels can, in turn, be tuned by means of, for example, the application of various external fields. The spins of the electrons in quantum dots provide a natural basis for representing so-called qubits. The capability to manipulate and study such states is evidenced by several recent experiments (see, for example, Refs. [23]). Coupled quantum dots are particularly interesting since so-called two-qubit quantum gates can be realized by manipulating the exchange coupling which originates from the repulsive Coulomb interaction and the underlying Pauli principle. For such states, the exchange coupling splits singlet and triplet states, and depending on the shape of the confining potential and the applied magnetic field, one can allow for electrical or magnetic control of the exchange coupling. In particular, several recent experiments and theoretical investigations have analyzed the role of effective spin-orbit interactions in quantum dots and their influence on the exchange coupling.

A proper theoretical understanding of the exchange coupling, correlation energies, ground state energies of quantum dots, the role of spin-orbit interactions and other properties of quantum dots as well, requires the development of appropriate and reliable theoretical few- and many-body methods. Furthermore, for quantum dots with more than two electrons and/or specific values of the external fields, this implies the development of few- and many-body methods where uncertainty quantifications are provided. For most methods, this means providing an estimate of the error due to the truncation made in the single-particle basis and the truncation made in limiting the number of possible excitations. For systems with more than three or four electrons, ab initio methods that have been employed in studies of quantum dots are variational and diffusion Monte Carlo, path integral approaches, large-scale diagonalization, and coupled-cluster theory. Exact diagonalization studies are accurate for a very small number of electrons, but the number of basis functions needed to obtain a given accuracy and the computational cost grow very rapidly with electron number. In practice they have been used for up to eight electrons, but the accuracy is very limited for all except \( N \leq 3 \) (see, for example, Refs. [13–15,21]). Monte Carlo methods have been applied up to \( N = 24 \) electrons. Diffusion Monte Carlo, with statistical and systematic errors, provide, in principle, exact benchmark solutions to various properties of quantum dots. However, the computations start becoming rather time-consuming for larger systems. Hartree, restricted Hartree-Fock, spin- and/or space-unrestricted Hartree-Fock, and local spin-density, and current density functional methods give results that are satisfactory for a qualitative understanding of some systematic properties. However, comparisons with exact results show discrepancies in the energies that are substantial on the scale of energy differences.

Another many-body method with the potential of pro-
viding reliable error estimates and accurate results is coupled-cluster theory, with its various levels of truncations. Coupled-cluster theory is the method of choice in quantum chemistry, atomic and molecular physics, and has recently been applied with great success in nuclear physics as well (see, for example, Refs. 38–41). In nuclear physics, with our spherical basis codes, we expect now to be able to perform \textit{ab initio} calculations of nuclei up to $^{132}$Sn with more than 20 major oscillator shells. The latter implies dimensionalities of more than $10^{10}$ basis Slater determinants, well beyond the reach of the full configuration interaction approach. Coupled-cluster theory offers a many-body formalism which allows for systematic expansions and error estimates in terms of truncations in the basis of single-particle states. The cost of the calculations scale gently with the number of particles and single-particle states, and we expect to be able to study quantum dots up to 50 electrons without a spherical symmetry. The main advantage of the coupled-cluster method over, say, full configuration approaches relies on the fact that it offers an attractive truncation scheme at a much lower computational cost. It preserves, at the same time, important features such as size extensivity.

The aim of this work is to apply coupled-cluster theory with the inclusion of triples excitations through the highly accurate and efficient \textit{A}-CCSD(T) approach for circular quantum dots up to $N = 20$ electrons, employing different strengths of the applied magnetic field. The results from these calculations are compared in turn with, in principle, exact diffusion Monte Carlo calculations. Moreover, this work introduces a technique widely applied in the nuclear many-body problem, namely that of a renormalized two-body Coulomb interaction. Instead of using the free Coulomb interaction in an oscillator basis, we diagonalize the two-electron problem exactly using a tailor-made basis in the centre-of-mass frame. The obtained eigenvectors and eigenvalues are used, in turn, to obtain, via a similarity transformation, an effective interaction defined for the lowest $10 - 20$ oscillator shells. These shells define our effective Hilbert space where the coupled-cluster calculations are performed. This technique has been used with great success in the nuclear many-body problem, in particular since the strong repulsion at short interparticle distances of the nuclear interactions requires a renormalization of the short-range part. With this renormalized two-body Coulomb interaction and coupled-cluster calculations with triples excitations included through the \textit{A}-CCSD(T) approach, we obtain results in close agreement with the diffusion Monte Carlo calculations. This opens up many interesting avenues for \textit{ab initio} studies of quantum dots, in particular for systems beyond the simple circular quantum dots.

This article is organized as follows. Section II introduces (i) the Hamiltonian and interaction for circular quantum dots, (ii) the basic ingredients for obtaining an effective interaction using a similarity-transformed Coulomb interaction, then (iii) a brief review of coupled-cluster theory and the \textit{A}-CCSD(T) approach, and finally (iv) the corresponding details behind the diffusion Monte Carlo calculations. In Section III, we present our results, whereas Section IV is devoted to our conclusions and perspectives for future work.

## II. COUPLED-CLUSTER THEORY AND DIFFUSION MONTE CARLO

In this section we present first our Hamiltonian in Subsection II A, thereafter we discuss how to obtain a renormalized two-body interaction in an effective Hilbert space. In Subsection II C we present our coupled-cluster approach, and finally in Subsection II D we briefly review our diffusion Monte Carlo approach.

### A. Physical systems and model Hamiltonian

We will assume that our problem can be described entirely by a non-relativistic many-electron Hamiltonian $\hat{H}$, resulting in the Schrödinger equation

$$\hat{H}|\Psi\rangle = E|\Psi\rangle,$$

with $|\Psi\rangle$ being the eigenstate and $E$ the eigenvalue. The many-electron Hamiltonian is normally written in terms of a non-interacting part $\hat{H}_0$ and and interacting part $\hat{V}$, namely

$$\hat{H} = \hat{H}_0 + \hat{V} = \sum_{i=1}^{N} \hat{h}_i + \sum_{i<j}^{N} \hat{v}_{ij},$$

where $\hat{H}_0$ is the (one-body) Hamiltonian of the non-interacting system, and $\hat{V}$ denotes the (two-body) Coulomb interaction. In general, the Schrödinger equation cannot be solved exactly.

We define the reference Slater determinant $|\Phi_0\rangle$ as the ground state of the non-interacting system by filling all the lowest-lying single-particle orbits. Since we will limit ourselves to systems with filled shells, this may be a good approximation, in particular if the single-particle field is the dominating contribution to the total energy. The non-interacting Schrödinger equation reads

$$\hat{H}_0|\Phi\rangle = e_0|\Phi_0\rangle,$$

where

$$\hat{H}_0 = \sum_{i=1}^{N} \hat{h}_i = \sum_{i=1}^{N} \left[ \hat{t}_i + \hat{v}_{\text{con}}(\mathbf{r}_i) \right].$$

The terms $\hat{t}_i$ and $\hat{v}_{\text{con}}(\mathbf{r}_i)$ are the kinetic-energy operator and the confining potential (from an external applied potential field) of electron $i$, respectively. The vector $\mathbf{r}_i$ represents the position in two dimensions of electron $i$. 

The obtained eigenvectors and eigenvalues are

$$|\Phi\rangle = |\Phi_0\rangle + \sum_{n=1}^{\infty} |\Phi_n\rangle$$

with $|\Phi_n\rangle$ being the $n$th excited state. 

The expectation values of the Hamiltonian are

$$\langle \Phi | \hat{H} | \Phi \rangle = \langle \Phi_0 | \hat{H}_0 | \Phi_0 \rangle + \sum_{n=1}^{\infty} \langle \Phi_n | \hat{V} | \Phi_n \rangle.$$
Due to the identical and fermionic nature of electrons, the eigenstates of Eq. (2) are Slater determinants, with the general form
\[ |\Phi_i\rangle = |ijk...m\rangle = \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k^\dagger ... \hat{a}_m^\dagger |0\rangle, \]
with \( \hat{a}^\dagger \) being standard fermion creation operators (and \( \hat{a} \) being annihilation operators). The single-particle eigenstates \( |i\rangle = \hat{a}_i^\dagger |0\rangle \) and eigenenergies \( \epsilon_i \) are given by the solutions of the one-particle Schrödinger equation governed by the operator \( \hat{h}_i \). Since the total energy of the non-interacting system is given by the sum of single-particle energies \( \epsilon_i \), we have
\[ \epsilon_0 = \sum_{i=1}^{N} \epsilon_i, \]
the reference determinant \( |\Phi_0\rangle \) is obviously the Slater determinant constructed from those orbitals with single-particle energies that yield the lowest total energy. In the particle-hole formalism, orbitals in the occupied space are referred to as hole states, while orbitals in the virtual space are denoted particle states. In principle, any complete and orthogonal single-particle basis can be used. However, since our coupled-cluster approach involves solution of a set of non-linear equations, it is preferable to start from a basis that produces a mean-field solution not too far away from the “exact” and fully correlated many-body solution. Therefore our main results will be obtained using the Hartree-Fock basis as a starting point for our coupled-cluster calculations. The Hartree-Fock basis is obtained from a linear expansion of harmonic oscillator basis functions, such that the expectation value of the Hamiltonian is minimized.

For the diffusion Monte Carlo calculations, it is also necessary to start from a model wavefunction that is used as importance function in the sampling, as we will discuss later. The Slater determinant part, in this case, is built starting from the self-consistent orbitals generated in a Local Density Approximation calculation, in order to include as much information as possible about both exchange and correlation effects at the one-body level. Explicit two-body correlations are then included as an elaborate Jastrow factor; see Subsection II D for further details.

Our model Hamiltonian for a quantum dot consists of a two-dimensional system of \( N \) electrons moving in the \( z = 0 \) plane, confined by a parabolic lateral confining potential \( V_{\text{con}}(r) \). The Hamiltonian is
\[ \hat{H} = \sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m_e} \nabla_i^2 + V_{\text{con}}(r_i) \right) + \frac{e^2}{\epsilon} \sum_{i<j}^{N} \frac{1}{|r_i - r_j|}. \]
In the above equation, \( m^* \) is a parameter relating the bare electron mass to an effective mass, and \( \epsilon \) is the dielectric constant of the semiconductor. In the following (if not explicitly specified otherwise), we will use effective atomic units, defined by \( \hbar = e^2/\epsilon = m_e m^* = 1 \). In this system of units, the length unit is the Bohr radius \( a_0 \) times \( \epsilon/m^* \), and the energy has units of Hartrees times \( m^*/\epsilon^2 \). As an example, for the GaAs quantum dots, typical values are \( \epsilon = 12.4 \) and \( m^* = 0.067 \). The effective Bohr radius \( a_0^* \) and effective Hartree \( \text{H}^* \) are \( \approx 97.93 \, \text{Å} \) and \( \approx 11.86 \, \text{meV} \), respectively. In this work we will consider circular dots only with \( N = 2, 6, 12, 20 \) electrons confined by a parabolic potential \( V_{\text{con}}(r) = m_e m^* \omega^2 r^2 / 2 \). The numbers \( N = 2, 6, 12, \) and \( N = 20 \) are so-called magic numbers corresponding to systems with closed harmonic oscillator shells, and hopefully a single-reference Slater determinant yields a good starting point for our calculations.

The one-body part of our Hamiltonian becomes
\[ \hat{H}_0 = \sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m_e} \nabla_i^2 + \frac{\omega^2}{2} r_i^2 \right), \]
whereas the interacting part is
\[ \hat{V} = \sum_{i<j}^{N} \frac{1}{|r_i - r_j|}. \]

The unperturbed part of the Hamiltonian yields the single-particle energies
\[ \epsilon_i = \omega \left( 2n + |m| + 1 \right), \tag{3} \]
where \( n = 0, 1, 2, 3, \ldots \) and \( m = 0, \pm 1, \pm 2, \ldots \). The index \( i \) runs from 0, 1, 2, . . . . The shell-structure is clearly deduced from this expression. We define \( R \) as the shell index. We will denote the shell with the lowest energy as \( R = 1 \), the shell with the second lowest energy as \( R = 2 \), and so forth. Hence,
\[ R_i \equiv \frac{\epsilon_i - 1}{\omega} \quad (i = 1, 2, 3, \ldots). \tag{4} \]
In the calculations, we limit ourselves to values of \( \omega = 0.28 \, \text{a.u.} \) (atomic units), \( \omega = 0.5 \, \text{a.u.} \), and \( \omega = 1.0 \, \text{a.u.} \). For higher values of the oscillator frequency, the contribution to the energy from the single-particle part dominates over the correlation part. The value \( \omega = 1.0 \) is an intermediate case which also allows for comparison with Taut’s exact solution for \( N = 2 \), see Ref. [40] while \( \omega = 0.5 \) and 0.28 represent cases where correlations are stronger, due to the lower average electron density in the dot.

### B. Effective interaction

Whenever a single-particle basis is introduced in order to carry out a many-body calculation, it must be truncated. The harmonic oscillator basis is the de facto standard for quantum dots and nuclear structure calculations. In nuclei, the intrinsic Hamiltonian is most easily treated using this basis, and for quantum dots the confining potential is to a good approximation harmonic.
However, the discrete Hilbert space $\mathcal{H}$ obtained from such a truncation grows exponentially with the number of particles. For example, allowing $n$ single-particle states and $N$ particles,

$$\dim(\mathcal{H}) = \binom{n}{N}.$$  

As an example, if we distribute $N = 6$ electrons in the total number of single-particle states defined by 10 major oscillator shells, we have $n = 110$, resulting in $\dim(\mathcal{H}) \approx 2.3 \times 10^{113}$ Slater determinants. This number is already beyond the limit of present full configuration interaction approaches. In our coupled-cluster calculations we perform studies up to some 20 major shells. For 20 shells, the total number of single-particle states is $n = 420$, for which $\dim(\mathcal{H}) \approx 1.3 \times 10^{18}$, well beyond reach of standard diagonalization methods in the foreseeable future. For 20 electrons in 20 shells, the number of Slater determinants is much larger, $7.6 \times 10^{32}$ in total.

But even if we could run large configuration interaction calculations, the convergence of the computed energies as a function of the chosen single-particle basis is slow for a harmonic oscillator basis, mainly due to the fact that this basis does not properly take into account the cusp condition at $|r_i - r_j| = 0$ of the Coulomb interaction. In fact, the error $\Delta E$ in the energy for a quantum dot problem, when increasing the dimensionality to one further shell with a harmonic oscillator basis, behaves like

$$\Delta E \sim O(R_{ho}^{-k+\delta-1}).$$  

Here, $k$ is the number of times a given wave function $\Psi$ may be differentiated weakly, $\delta \in [0, 1)$ is a constant and $R_{ho}$ is the last oscillator shell. The derivation of the latter relation is detailed in Ref. [21], together with extensive discussions of the convergence properties of quantum dot systems. For the ground state of the two-electron quantum dot, we have precisely $k = 1$, while for higher electron numbers one observes $k = O(1)$. This kind of estimate tells us that an approximation using only a few HO eigenfunctions necessarily will give an error depending directly on the smoothness $k$.

Although the coupled-cluster method allows for the inclusion of much larger single-particle spaces, the slow convergence of the energy seen in full configuration interaction calculations applies to this method as well as it approximates the configuration-interaction solution using the same set of single-particle functions. For an overview of coupled cluster error analysis, see Refs. [15, 21, 50].

One way to circumvent the dimensionality problem is to introduce a renormalized Coulomb interaction $\tilde{V}_{eff}$ defined for a limited number of low-lying oscillator shells. Such techniques have been widely used in nuclear many-body problems (see, for example, Refs. [15, 17, 48]). For quantum dots, this was first applied to a configuration interaction calculation by Navratil et al. [48], albeit for a different quantum dot model. But the potential of this method has not been explored fully, except for recent preliminary studies in Refs. [15, 21, 50], which demonstrate a significant improvement of the eigenvalues. Furthermore, we expect that the potential of this method is of even greater interest when linked up with an efficient many-body method like the coupled-cluster approach.

The recipe for obtaining such an effective interaction is detailed in several works (see, for example, Refs. [15, 48, 50]). Here we give only a brief overview.

The Hilbert space $\mathcal{H}$ is divided into two parts $PH$ and $Q\mathcal{H}$, where $P$ is the orthogonal projector onto the smaller, effective model space, and $Q = 1 - P$. Note here, that $PH$ will be the space in which we do our many-body computations, and $\mathcal{H}$ is, in principle, the whole untruncated Hilbert space. The interaction operator $\hat{V}$ is considered a perturbation, and we introduce a convenient complex parameter $z$ and study $\hat{H}(z) = \hat{H}_0 + z \hat{V}$. Setting $z = 1$ recovers the original Hamiltonian.

Consider a similarity transformation of $\hat{H}(z)$ defined by

$$\hat{H}(z) \equiv e^{-X(z)} \hat{H}(z) e^{X(z)}$$  

where the operator $X(z)$ is such that the property

$$Q \hat{H}(z) P = 0$$  

holds. Equation (6) must not be confused with equations from coupled-cluster theory. The idea is that $X(z)$ should be determined from perturbation theory, which gives an analytic operator function with $X(0) = 0$.

The most important consequences of these equations are that (i) $\hat{H}$ have identical eigenvalues with $\hat{H}$, (ii) that there are $D = \dim(\mathcal{H})$ eigenvalues whose eigenvectors are entirely in the model space $PH$. Thus, the effective Hamiltonian defined by

$$\hat{H}_{eff}(z) \equiv P \hat{H}(z) P$$  

is a model-space operator with $D$ exact eigenvalues. At $z = 0$ these are the unperturbed eigenvalues, and these are continued analytically as $z$ approaches $z = 1$.

Equations (6) and (7) are not sufficient to determine $X(z)$ uniquely. The order-by-order-expansion of $X(z)$ must be supplied with side conditions. One of the most popular conditions is that $X(z)^\dagger = -X(z)$ such that $\hat{H}(z)$ is Hermitian, and additionally that the effective eigenvectors are as close as possible to the exact eigenvectors, i.e., that the quantity $\Delta$ defined by

$$\Delta \equiv \sum_{k=1}^{D} \| \langle \Psi_k | - \langle \Psi_{eff,k} | \|^2$$  

is minimized, where $|\Psi_{eff,k}\rangle$ are the eigenvectors of $\hat{H}_{eff}$, see Ref. [15]. One can obtain a formula for $X(z)$ in this case, namely

$$X = \text{artanh}(\omega - \omega^\dagger),$$

where $\omega = Q\omega P$ is the operator such that $\exp(\omega) P|\Psi_k\rangle = |\Psi_k\rangle$. 
Order-by-order expansion of $\tilde{H}(z)$ reveals that it contains $m$-body terms for all $m \leq N$, even though $V$ only contains two-body interactions. However, the many-body terms can be shown to be of lower order in $z$. By truncating $\tilde{H}(z)$ at terms at the two-body level we obtain the so-called sub-cluster approximation to the effective Hamiltonian. This can be computed by exact diagonalization of the two-body problem; a simple task for the quantum dot problem.

The one-body part of $\tilde{H}$ is always $H_0$, so it is natural to define the effective interaction by

$$H_{\text{eff}} = H_0 + V_{\text{eff}}.$$  

The reader should, however, keep in mind that the sub-cluster approximation always produces missing many-body correlations when inserted in a many-body context. The size of this source of error can only be quantified a posteriori, either by comparison with experiment and/or exact calculations (see, for example, Ref. [53]) for a discussion on missing many-body physics and the nuclear many-body problem.

C. Coupled-cluster method

The single-reference coupled-cluster theory is based on the exponential ansatz for the ground-state wave function of the $N$-electron system,

$$|\Psi_0\rangle = e^T|\Phi_0\rangle,$$

where $T$ is the cluster operator (an $N$-particle-$N$-hole excitation operator) and $|\Phi_0\rangle$ is the corresponding reference determinant (defining our chosen closed-shell system or vacuum) obtained by performing some mean-field calculation or by simply filling the $N$ lowest-energy single-electron states in two dimensions.

The operator $T$ is a simple many-body excitation operator, which in all standard coupled-cluster approximations is truncated at a given (usually low) $M$-particle-$M$-hole excitation level $M < N$, with $N$ being the number of electrons. If all excitations are included up to the $N$-particle-$N$-hole set of Slater determinants, one ends up with solving the full problem. The general form of the truncated cluster operator, defining a standard single-reference coupled-cluster approximation characterized by the chosen excitation level $M$, is

$$T = T_1 + T_2 + T_3 + \cdots + T_M,$$

where

$$T_k = \frac{1}{(k!)^2} \sum_{i_1, \ldots, i_k, a_1, \ldots, a_k} t_{a_1 \cdots a_k}^{a_1 \cdots a_k} \hat{a}_{a_1} \cdots \hat{a}_{a_k} \hat{a}_{i_1} \cdots \hat{a}_{i_k}.$$  

Here and in the following, the indices $i, j, k, \ldots$ label occupied single-particle orbitals while $a, b, c, \ldots$ label unoccupied orbitals. The unknown amplitudes $t_{ij}^a$ and $t_{ab}^{ij}$ etc in the last equation are determined from the solution of the coupled-cluster equations discussed below. For a truncated $T$ operator, we will use the notation $T(M)$, where $M$ refers to highest possible particle-hole excitations.

As an example, we list here the expressions for one-particle-one-hole, two-particle-two-hole, and three-particle-three-hole operators, labeled $T_1$, $T_2$, and $T_3$, respectively,

$$T_1 = \sum_{i<\varepsilon_f} \sum_{a<\varepsilon_f} t_{ia}^a \hat{a}_a \hat{a}_i$$

and

$$T_2 = \frac{1}{4} \sum_{i<j<\varepsilon_f} \sum_{ab<\varepsilon_f} t_{ijab}^{ab} \hat{a}_a \hat{a}_b \hat{a}_j \hat{a}_i,$$

and finally

$$T_3 = \frac{1}{36} \sum_{ijk<\varepsilon_f} \sum_{abc>\varepsilon_f} t_{ijkl}^{abc} \hat{a}_a \hat{a}_b \hat{a}_c \hat{a}_d \hat{a}_j \hat{a}_k \hat{a}_i.$$  

We will in this work limit ourselves to a single reference Slater determinant $\Phi_0$.

The cluster amplitudes $t_{i_1 \cdots i_n}^{a_1 \cdots a_n}$ are determined by solving a coupled system of nonlinear and energy-independent algebraic equations of the form

$$\langle \Phi_{i_1 \cdots i_n}^{a_1 \cdots a_n} | \tilde{H} | \Phi_0 \rangle = 0, \quad i_1 < \cdots < i_n, \quad a_1 < \cdots < a_n,$$

where $n = 1, \ldots, M$. Here,

$$\tilde{H} = e^{-T(M)} \tilde{H} e^{T(M)} = (\tilde{H} e^{T(M)})_C,$$

is the similarity-transformed Hamiltonian of the coupled-cluster theory truncated at $M$-particle-$M$-hole excitations and the subscript $C$ denotes the connected part of the corresponding operator expression, and $|\Phi_{i_1 \cdots i_n}^{a_1 \cdots a_n} \rangle \equiv a^{a_1} \cdots a^{a_n} a_{i_1} \cdots a_{i_n} |\Phi\rangle$ are the $n$-particle-$n$-hole or $n$-tuply excited determinants relative to reference determinant $|\Phi_0\rangle$. The Hamiltonians $\tilde{H}$ and $\tilde{H}$ are normal ordered.

If we limit ourselves to include only one-particle-one-hole and two-particle-two-hole excitations, what is known as coupled cluster of singles and doubles (CCSD), the method corresponds to $M = 2$, and the cluster operator $T(N)$ is approximated by

$$T(M) = T(2) = T_1 + T_2,$$

given by the operators of Eqs. (12) and (13).

The standard CCSD equations for the singly and doubly excited cluster amplitudes $t_{ij}^a$ and $t_{ab}^{ij}$, defining $T_1$ and $T_2$, respectively, can be written as

$$\langle \Phi_0^i | \tilde{H} (\text{CCSD}) | \Phi_0 \rangle = 0,$$

and

$$\langle \Phi_0^{ij} | \tilde{H} (\text{CCSD}) | \Phi \rangle = 0, \quad i < j, \quad a < b,$$
where

$$\hat{H}(\text{CCSD}) = \hat{H} = e^{-T(2)} \hat{H} e^{T(2)} = (\hat{H} e^{T(2)})_C$$  \hfill (20)$$

is the similarity-transformed Hamiltonian of the CCSD approach and the subscript $C$ stands for connected diagrams only.

The system of coupled-cluster equations is obtained in the following way. We first insert the coupled-cluster wave function $|\Psi_0\rangle$ into the $N$-body Schrödinger equation,

$$\hat{H}|\Psi_0\rangle = \Delta E_0|\Psi_0\rangle,$$  \hfill (21)$$

where

$$\Delta E_0 = E_0 - \langle \Psi_0 | \hat{H} | \Psi_0 \rangle$$

is the corresponding energy relative to the reference energy $\langle \Psi_0 | \hat{H} | \Psi_0 \rangle$, and premultiply both sides on the left by $e^{-T(5)}$ to obtain the connected-cluster form of the Schrödinger equation

$$\hat{H}|\Phi\rangle = \Delta E_0|\Phi\rangle,$$  \hfill (22)$$

where

$$\hat{H} = e^{-T(2)} \hat{H} e^{T(2)} = (\hat{H} e^{T(2)})_C$$  \hfill (23)$$

is the similarity-transformed Hamiltonian.

Next, we project Eq. (22), in which $T$ is replaced by its approximate form $T(M)$, Eq. (11), onto the excited determinants $|\Phi^{a_1...a_n}\rangle$, corresponding to the $M$-particle-$M$-hole excitations included in $T_M$. The excited determinants $|\Phi^{a_1...a_n}\rangle$ are orthogonal to the reference determinant $|\Phi_0\rangle$, so that we end up with nonlinear and energy-independent algebraic equations of the form of Eq. (15).

Once the system of equations, Eq. (15), is solved for $T_M$ or $T^{a_1...a_n}_{a_1...a_n}$ (or Eqs. (15) and (19)) are solved for $T_1$ and $T_2$ or $t_1^{a_1}$ and $t_2^{a_2}$), the ground-state coupled-cluster energy is calculated using the equation

$$E_0 = \langle \Phi_0 | \hat{H} | \Phi_0 \rangle + \Delta E_0 = \langle \Phi_0 | \hat{H} | \Phi_0 \rangle + \langle \Phi_0 | \hat{H} | \Phi_0 \rangle.$$  \hfill (24)$$

It can easily be shown that if $H$ contains only up to two-body interactions and $2 \leq M \leq N$, we can write

$$E_0 = \langle \Phi_0 | \hat{H} | \Phi_0 \rangle + \langle \Phi_0 | (\hat{H} (T_1 + T_2 + \frac{1}{2} T_1^2)) | \Phi_0 \rangle.$$  \hfill (25)$$

In other words, we only need $T_1$ and $T_2$ clusters to calculate the ground-state energy $E_0$ of the $N$-body ($N \geq 2$) system even if we solve for other cluster components $T_n$ with $n > 2$. As long as the Hamiltonian contains up to two-body interactions, the above energy expression is correct even in the exact case, when the cluster operator $T$ is not truncated (see, for example, Refs. 18, 32 for proof).

The nonlinear character of the system of coupled-cluster equations of the form of Eq. (15) does not mean that the resulting equations contain very high powers of $T_M$. For example, if the Hamiltonian $\hat{H}$ does not contain higher-than-pairwise interactions, the CCSD equations for the $T_1$ and $T_2$ clusters, or for the amplitudes $t^n_a$ and $t^{ij}_ab$ that represent these clusters, become

$$\langle \Phi^n_a | (\hat{H} (1 + T_1 + T_2 + \frac{1}{2} T_1^2 + T_1 T_2 + \frac{1}{6} T_1^3)) | \Phi \rangle = 0,$$  \hfill (26)$$

$$\langle \Phi^{ij}_{ab} | (\hat{H} (1 + T_1 + T_2 + \frac{1}{2} T_1^2 + T_1 T_2 + \frac{1}{6} T_1^3) + \frac{1}{2} T_2^2 + \frac{1}{2} T_1^2 T_2 + \frac{1}{24} T_2^3)) | \Phi \rangle = 0.$$  \hfill (27)$$

The explicitly connected form of the coupled-cluster equations, such as Eqs. (15) or (26) and (27), guarantees that the process of solving these equations leads to connected terms in cluster components of $T$ and connected terms in the energy $E_0$, independent of the truncation scheme $M$ used to define $T_M$. The absence of disconnected terms in $T_M$ and $E_0$ is essential to obtain the rigorously size-extensive results. It is easy to extend the above equations for the cluster amplitudes to include triples excitations, leading to the so-called CCSDT hierarchy of equations. Defining

$$f = \sum_{pq} f_{pq} \{a^+_pa_q\}$$

with $f_{pq}$ the Fock matrix elements and

$$W = \frac{1}{4} \sum_{pqrs} \langle pq||rs\rangle \{a^+_pa_q^+a_ra_s\}$$

where $\langle pq||rs\rangle$ are anti-symmetrized two-body matrix elements, the extension to triples gives the following equations for the amplitudes with one-particle-one-hole excitations

$$\langle \Phi^n_a | f (T_1 + f (T_2 + 1/2T_1^2) + WT_1 + W(T_2 + 1/2T_1^2) + W(T_1 T_2 + 1/6 T_1^3 + T_3)) | \Phi \rangle = 0,$$
\[
\langle \Phi_0^{ab} | [fT_3 + f(T_3T_1 + 1/2T_2^2) + WT_2 + W(T_3 + T_1T_2) + W(1/2T_2 + T_3T_1/2T_1^2 + T_1) \\
+ W(T_2T_3 + 1/2T_2^2T_1 + 1/2T_3T_1^2 + 1/6T_2T_1^3) ]_C | \Phi \rangle = 0.
\]

and with three-particle-three-hole excitations we end up with

\[
\langle \Phi_{ijk}^{abc} | [fT_3 + f(T_3T_1 + 1/2T_2^2) + WT_2 + W(T_3 + T_1T_2) + W(1/2T_2 + T_3T_1/2T_1^2 + T_1) \\
+ W(T_2T_3 + 1/2T_2^2T_1 + 1/2T_3T_1^2 + 1/6T_2T_1^3) ]_C | \Phi \rangle = 0.
\]

Different approximations to the solution of the triples equations yield different CCSDT approximations. The CCSD method scales (in terms of the most computationally expensive contribution) as \( n_o^3 n_u^4 \), where \( n_o \) represents the number of occupied orbitals and \( n_u \) the number of unoccupied single-particle states. The full CCSDT scales as \( n_o^3 n_u^5 \).

Coupled-cluster theory with inclusion of full triples CCSDT is usually considered to be too computationally expensive in most many-body systems of considerable size. Therefore triples corrections are usually taken into account perturbatively using the non-iterative CCSD(T) approach described in Ref. 34. Recently, a more sophisticated way of including the full triples known as the \( \Lambda \)-CCSD(T) approach, has been developed by Taube et al.35–37. In the \( \Lambda \)-CCSD(T) approach, the left-eigenvector solution of the CCSD similarity-transformed Hamiltonian is utilized in the calculation of a non-iterative triples correction to the coupled-cluster ground-state energy. The left eigenvalue problem is given by

\[
\langle \Phi_0 | \Lambda \hat{H} = E \langle \Phi_0 | \Lambda, \quad (28)
\]

where \( \Lambda \) denotes the de-excitation cluster operator

\[
\Lambda = 1 + \Lambda_1 + \Lambda_2, \quad (29)
\]

with

\[
\Lambda_1 = \sum_{i,a} \lambda_a^i a_a^i, \quad (30)
\]

\[
\Lambda_2 = \frac{1}{4} \sum_{i,j,a,b} \lambda_{ab}^{ij} a_a^i a_b^j. \quad (31)
\]

The unknowns, \( \lambda_a^i \) and \( \lambda_{ab}^{ij} \), result from the ground-state solution of the left eigenvalue problem. Using a single-particle basis that diagonalizes the fock matrix \( f \) within the hole-hole and particle-particle blocks simultaneously, and utilizing the \( \lambda_a^i \) and \( \lambda_{ab}^{ij} \) de-excitation amplitudes together with the cluster amplitudes, \( t_i^a \) and \( t_{ij}^a \), we get the non-iterative \( \Lambda \)-CCSD(T) energy correction to the coupled-cluster correlation energy (see Ref. 35 for more details),

\[
\Delta E_3 = \frac{1}{(3!)^2} \sum_{ijkabc} \langle \Phi_0 | \Lambda (f_{hp} + W) \Lambda | \Phi_{ijk}^{abc} \rangle \\
\times \frac{1}{\gamma_{ijk}^{abc}} \langle \Phi_{ijk}^{abc} | (WN T_2)_C | \Phi_0 \rangle. \quad (32)
\]

Here, \( f_{hp} \) denotes the part of the normal-ordered one-body Hamiltonian that annihilates particles and creates holes, while

\[
\gamma_{ijk}^{abc} = f_{ii} + f_{jj} + f_{kk} - f_{aa} - f_{bb} - f_{cc} \quad (33)
\]

is expressed in terms of the diagonal matrix elements of the normal-ordered one-body Hamiltonian \( f \). In the case of Hartree-Fock orbitals, the one-body part of the Hamiltonian is diagonal and \( f_{hp} \) vanishes. The state \( | \Phi_{ijk}^{abc} \rangle \) is a three-particle-three-hole excitation of the reference state. For a further discussion of various approximations to the triples correlations, see, for example, the recent review by Bartlett and Musiališ.”

In this work we will focus on the CCSD, the CCSD(T), and the \( \Lambda \)-CCSD(T) approaches, using either a renormalized or an unrenormalized interaction. In order to avoid an iterative solution of the CCSD(T) and \( \Lambda \)-CCSD(T) equations, we start from a self-consistent Hartree-Fock basis such that the Fock matrix \( f \) is diagonal. Using such a basis, the computational cost of the CCSD(T) and \( \Lambda \)-CCSD(T) energy corrections is \( n_o^3 n_u^4 \) number of cycles, done only once. It is also important to keep in mind, in particular when linking our coupled-cluster theory with Monte Carlo approaches, that a wavefunction-based method like coupled-cluster theory is defined within a specific subset of the full Hilbert space. In our case, the Hilbert space will be defined by all possible many-body wave functions which can be constructed within a certain number of the lowest-lying single-particle states.
D. Diffusion Monte Carlo

The diffusion Monte Carlo method seeks the solution of the equation:

$$\partial_\tau |\Psi(R, \tau)\rangle = (\hat{H} - E_0) |\Psi(R, \tau)\rangle$$  \hspace{1cm} (34)

where $R$ collectively indicates the degrees of freedom of the system (the 3N electron coordinates, in this case). By expanding the state $|\Psi(R, \tau)\rangle$ on the basis of eigenstates $|\phi_n\rangle$ of $\hat{H}$, a formal solution of Eq. (34) is given by

$$|\Psi(R, \tau)\rangle = \frac{1}{\sqrt{Z}} \sum_n e^{-\frac{1}{2} \sum_{ij} b_{ij} r_{ij}} e^{-\gamma_{L,S}(\hat{H} - E_0)\tau} |\phi_n\rangle |\Psi(R, 0)\rangle$$  \hspace{1cm} (35)

from which it is evident that for $\tau \to \infty$ the only surviving component is the ground state of $\hat{H}$. Eq. (34) can be numerically solved by expanding the state to be evolved in eigenstates $|R_i\rangle$ of the position operator (called “walkers”), so that the evolution reads:

$$\sum_i \langle R_i | |\Psi(R, \tau)\rangle = \sum_i \langle R_i | e^{-(\hat{H} - E_0)\tau} |R_i'\rangle \langle R_i' | |\Psi(R, 0)\rangle.$$  \hspace{1cm} (36)

Formally, in terms the Green’s function solution of Eq. (34), the solution can be written as:

$$|\Psi(R, \tau)\rangle = \int G(R', R, \tau) |\Psi(R', 0)\rangle \ dR'.$$  \hspace{1cm} (37)

The Green’s function $G(R', R, \tau) = \langle R | \exp[-(\hat{H} - E_0)\tau] | R \rangle$ is in general unknown. However, in the limit $\Delta \tau \to 0$ it can be written in the following form:

$$G(R', R, \tau) \simeq \sqrt{\frac{m\epsilon}{2\pi i\hbar^2}} e^{\frac{i}{\hbar}} \int \frac{d\mathbf{r}}{\sqrt{2\pi m\epsilon}} e^{-|V(R') - V(R)|/\epsilon \Delta \tau},$$  \hspace{1cm} (38)

that is as the product of the free particle Green’s function, having the effect of displacing the $d$-dimensional walkers, and a factor containing the potential, which is interpreted as a weight for the estimators computed at the walker position, and a probability for the walker itself to generate one or more copies of itself in the next generation. Due to the divergence of the potential at the origin, it is necessary to modify the algorithm, introducing the so-called “importance sampling”. In practice, the sampled distribution is modified by multiplying by an approximate solution of the Schrödinger equation $\Psi_T(R)$, which is usually determined by a variational Monte Carlo calculation:

$$\Psi_T(R) |\Psi(R, \tau)\rangle = \int G(R', R, \tau) \frac{\Psi_T(R')}{\Psi_T(R')} \Psi_T(R') |\Psi(R', 0)\rangle \ dR'.$$  \hspace{1cm} (39)

A final important observation is the fact that the procedure described above is well defined only in the case of a totally symmetric ground state. For a many-Fermion system it would be necessary, in principle, to project on an excited state of the Hamiltonian, which leads to a severe instability of the variance on the energy estimation. This problem is usually treated by artificially imposing, as an artificial boundary condition, that the solution vanishes on the nodes of the trial function $\Psi_T$ (fixed-node approximation). Many other technical details enter the real calculation. A thorough description of the DMC algorithm, as implemented for the calculations of this paper, can be found in Ref. 52.

The fixed-node DMC calculations depend on the quality of the trial wavefunction $\Psi_T(R)$, which is usually built starting from a parametrized ansatz. The values of the parameters are computed by minimizing the expectation value of the Hamiltonian on $\Psi_T(R)$. The trial wavefunctions we use have the form:

$$\Psi(R)_{L,S} = \exp[\phi(R)] \sum a_i \Xi_{L,S}^i (R),$$  \hspace{1cm} (40)

where the $a_i$ are variational parameters. Because in this paper we are considering only closed–shell dots which have $L = 0$ and $S = 0$, the sum in Eq. (40) reduces to a single term:

$$\Xi_{L=0,S=0} = D^\uparrow D^\downarrow,$$  \hspace{1cm} (41)

where the $D^\uparrow$ are Slater determinants of spin-up and spin-down electrons, using orbitals from a local density approximation calculation with the same confining potential and the same number of electrons. The function $\exp[\phi]$ in Eq. (40) is a generalized Jastrow factor of the form:

$$\phi(R) = \sum_{i=1}^N \sum_{k=1}^6 \frac{\gamma_k J_0}{R_i} \left( \frac{k\pi r_{ij}}{R_i} \right) + \sum_{i<j} \frac{a_{ij} r_{ij}}{1 + b(r_{ij}) r_{ij}} + \frac{a_{ij} r_{ij}}{1 + b(r_{ij}) r_{ij}} + \frac{a_{ij} r_{ij}}{1 + b(r_{ij}) r_{ij}},$$  \hspace{1cm} (42)

where

$$b(r) = b_{0,1}^{ij} + b_{1,1}^{ij} \tan^{-1}[|r - R_c|^2/2R_c\Delta].$$  \hspace{1cm} (43)

It explicitly includes one- and two-body correlations and effective many-body correlations via the spacial dependence of $b(r)$. The quantity $R_c$ represents an “effective” radius of the dot, which is optimized in the variational procedure. The $b_0$ and $b_1$ parameters depend only on the relative spin configuration of the pair $ij$. The parameters $a_{ij}$ are fixed in order to satisfy the cusp conditions, that is, the condition of finiteness of the local energy $\hat{H} |\Psi/R$ for $r_{ij} \to 0$. For a two dimensional system, $a_{ij} = 1$ if the electron pair $ij$ has antiparallel spin, and $a_{ij} = 1/3$ otherwise. The dependence of $a_{ij}$ on the relative spin orientation of the electron pair introduces spin-contamination into the wavefunction. However, the magnitude of the spin contamination and its effect on the energy has been shown to be totally negligible in the case of well-optimized atomic wavefunctions and we expect that to be true here as well.
Also the coefficients $\gamma_k$ in the one–body term, the coefficients $\Delta$, $b_0$, and $b_1$ in the two–body term, and the coefficients $\alpha_i$ multiplying the configuration state functions are optimized by minimizing the variance of the local energy\textsuperscript{21}.

### III. RESULTS

We start our discussion with the results for the two-electron system, since these can, for certain values of the oscillator frequency, be compared with the exact results of Taut\textsuperscript{46}. These results are presented in the next subsection using both a renormalized two-body Coulomb interaction and the ‘bare’ Coulomb interaction. Thereafter we present coupled-cluster results with singles and doubles excitations for systems with $N = 6$ and $N = 12$ electrons with the bare Coulomb interaction. The slow convergence as a function of the number of oscillator shells with the bare interaction serves to motivate the introduction of an effective Coulomb interaction. In the main result section, we present CCSD, CCSD(T), and Λ-CCSD(T) results for $N = 6, 12$ and $N = 20$ electrons using an effective two-body Coulomb interaction and compare with diffusion Monte Carlo (DMC) calculations for the same systems.

#### A. Results for two electrons

In this subsection we limit our attention to the two-electron system and compare our DMC results with coupled-cluster calculations with CCSD correlations only. The results presented here serve to demonstrate the reliability of using an effective Coulomb interaction.

The CCSD approach gives the exact eigenvalues for the two-particle system. We have employed a standard harmonic oscillator basis using the frequencies $\omega = 0.5$ and $\omega = 1.0$ a.u. Our results are listed in Table I. The variable $R$ represents the number of oscillator shells in the effective two-body problem. The variable $\omega$ represents the number of oscillator shells $R$. For $\omega = 1.0$ a.u., Taut’s exact result from Ref.\textsuperscript{46} is reproduced. The non-interacting part of the Hamiltonian gives a contribution of 2 a.u. to the ground-state energy while the two-particle interaction results in 1 a.u.

We notice also that the DMC results agree perfectly (within six leading digits) with our CCSD-$V_{\text{eff}}$ calculations. The standard error in the DMC calculations is given in parentheses.

If we, on the other hand, use the bare Coulomb interaction, we see that the convergence of the CCSD-$V$ results as a function of $R$ is much slower and in line with the analysis of Ref.\textsuperscript{21} and our discussion in subsection II B. One needs at least some 16-20 major oscillator shells (between 272 and 420 single-particle states) in order to get a result within three to four leading digits close to the exact answer. The slow convergence of the bare interaction for the two-electron problem may be even more prevalent in a many-body system, in particular for small values of $\omega$, where correlations are expected to be more important. With more particles, we may expect even worse convergence. In Table II we present for the case of $\omega = 1.0$ a.u. CCSD results for $N = 6$ and $N = 12$ electrons. The bare Coulomb interaction in an oscillator basis is used. The diffusion Monte Carlo results are for $N = 6$ 20.1597(2) a.u. and for $N = 12$ 65.700(1) a.u. Using the bare interaction thus results in a slow convergence, as will be demonstrated in the next subsection. The result of 20.1742 a.u. obtained with an effective Coulomb at the

| $\omega$ | $R$ | CCSD-$V$ | CCSD-$V_{\text{eff}}$ | DMC |
|----------|-----|----------|----------------------|-----|
| 1.0      | 2   | 3.152329 | 3.000000             |     |
|          | 4   | 3.025323 | 3.000000             |     |
|          | 6   | 3.036273 | 3.000000             |     |
|          | 8   | 3.009237 | 3.000000             |     |
|          | 10  | 3.008955 | 3.000000             |     |
|          | 12  | 3.000654 | 3.000000             |     |
|          | 14  | 3.000505 | 3.000000             |     |
|          | 16  | 3.000406 | 3.000000             | 3.000000(3) |

TABLE I: Ground-state energies for two electrons in a circular quantum dot within the CCSD approach with (CCSD-$V_{\text{eff}}$) and without (CCSD-$V$) an effective Coulomb interaction. The diffusion Monte Carlo (DMC) results are also included. For $\omega = 1$ Taut’s exact result from Ref.\textsuperscript{46} is 3 a.u. All energies are in atomic units. There are no triples corrections for the two-body problem. The variable $R$ represents the number of oscillator shells.
CCSD level for \(N = 6\) and \(R = 10\) is much closer to the DMC result, as can be seen from Table III. These results serve the aim of motivating the introduction of an effective two-particle interaction. In the next subsection, we will make further comparisons between our results with and without an effective interaction. In particular, we will try to extract convergence criteria for both approaches and link our numerical results with the predictions made by Kvaal in Eq. 3.

### B. Results with an effective Coulomb interaction

We present here our final and most optimal results for \(N = 6\), \(N = 12\), and \(N = 20\) electrons using the CCSD, the CCSD(T), and the \(\Lambda\)-CCSD(T) approaches. We list the CCSD(T) triples results as well. This method has for a long time been considered as the calculational ‘gold standard’ in quantum chemistry due to its low computational cost and accuracy. We emphasize, however, that the \(\Lambda\)-CCSD(T) approach is an improvement of the standard CCSD(T) approach, and should therefore be considered as our best and most accurate coupled-cluster calculation in this work. In all calculations we employ an effective Coulomb interaction and a self-consistent Hartree-Fock basis for different values of the oscillator frequency \(\omega\) and the model space \(R\). The results are compared with diffusion Monte Carlo calculations (DMC).

In addition to the values of \(\omega = 1.0\) and \(\omega = 0.5\), which serve more as a reference for earlier calculations, we present results for \(\omega = 0.28\) a.u., which corresponds to 3.32 eV, a frequency which should approximate the experimental situation in Ref. 22. The role of correlations is also more important for smaller values of \(\omega\), allowing us therefore to test the reliability of our single-reference CCSD and \(\Lambda\)-CCSD(T) calculations. As the system becomes more and more correlated, contributions from clusters beyond the \(T(3)\) (beyond three-particle-three-hole correlations) level might become non-negligible. For values of \(\omega > 1\), the single-particle part of the Hamiltonian dominates and correlations play a less prominent role.

Our results for \(N = 6\), \(N = 12\), and \(N = 20\) electrons are displayed in Tables III, IV, and V respectively. We present also the mean-field energies (that is, the Hartree-Fock ground-state energies). These are labeled as \(E_0\) in the Tables. For all values of \(\omega\) with \(R = 20\) major oscillator shells, our best coupled-cluster results, the \(\Lambda\)-CCSD(T) calculations, are very close to the diffusion Monte Carlo calculations. Even for 10 major shells, the results are close to the DMC calculations, suggesting thereby that the usage of an effective interaction provides a better starting point for many-body calculations. The convergence of the coupled-cluster calculation in terms of the number of major oscillator shells is also better than the results shown in Table III with the bare Coulomb interaction. This discussion will be further elaborated at the end of this section.

### TABLE II: Ground-state energies for \(N = 6\) and \(N = 12\) electrons in a circular quantum dot within the CCSD approach using the bare Coulomb interaction. All energies are in atomic units. There are no triples corrections. Results are presented for an oscillator frequency \(\omega = 1.0\) a.u. The variable \(R\) represents the number of oscillator shells. For \(N = 12\) the first three shells are filled and there are no results for two shells only.

| \(R\) | \(N = 6\) | \(N = 12\) |
|------|---------|----------|
| 2    | 22.219813 |          |
| 3    | 21.419889 | 73.765549 |
| 4    | 20.421325 | 70.297531 |
| 5    | 20.310716 | 66.989912 |
| 6    | 20.260893 | 66.452006 |
| 7    | 20.236760 | 65.971686 |
| 8    | 20.221750 | 65.889324 |
| 9    | 20.211590 | 65.838932 |
| 10   | 20.204345 | 65.806539 |

### TABLE III: Ground-state energies for \(N = 6\) electrons in a circular quantum dot within various coupled-cluster approximations utilizing an effective Coulomb interaction and the diffusion Monte Carlo (DMC) approach. The coupled-cluster results have been obtained with an effective two-body interaction using a self-consistent Hartree-Fock basis and the CCSD, the CCSD(T), and the \(\Lambda\)-CCSD(T) approaches discussed in the text. \(E_0\) is the Hartree-Fock energy while \(R\) stands for the number of major oscillator shells. All energies are in atomic units.

| \(\omega\) | \(R\) | \(E_0\) | CCSD | CCSD(T) | \(\Lambda\)-CCSD(T) | DMC |
|-----------|------|--------|------|--------|------------------|-----|
| 0.28      | 10   | 7.9504 | 7.6241 | 7.6032 | 7.6064           |     |
|           | 12   | 7.9632 | 7.6245 | 7.6023 | 7.6057           |     |
|           | 14   | 7.9720 | 7.6247 | 7.6016 | 7.6052           |     |
|           | 16   | 7.9785 | 7.6249 | 7.6012 | 7.6048           |     |
|           | 18   | 7.9834 | 7.6251 | 7.6008 | 7.6046           |     |
|           | 20   | 7.9872 | 7.6252 | 7.6006 | 7.6044           | 7.6001(1) |
| 0.5       | 10   | 12.1927| 11.8057| 11.7871| 11.7892          |     |
|           | 12   | 12.2073| 11.8055| 11.7858| 11.7880          |     |
|           | 14   | 12.2173| 11.8055| 11.7850| 11.7873          |     |
|           | 16   | 12.2246| 11.8055| 11.7845| 11.7868          |     |
|           | 18   | 12.2302| 11.8055| 11.7841| 11.7864          |     |
|           | 20   | 12.2346| 11.8055| 11.7837| 11.7862          | 11.7888(2) |
| 1.0       | 10   | 20.6295| 20.1766| 20.1623| 20.1633          |     |
|           | 12   | 20.6461| 20.1753| 20.1602| 20.1612          |     |
|           | 14   | 20.6576| 20.1746| 20.1589| 20.1600          |     |
|           | 16   | 20.6659| 20.1742| 20.1580| 20.1592          |     |
|           | 18   | 20.6723| 20.1739| 20.1574| 20.1586          |     |
|           | 20   | 20.6773| 20.1737| 20.1570| 20.1582          | 20.1597(2) |
changing the set of single-particle orbitals show that differences are of the order of one millihartrees or less. The optimization of the Jastrow factor only influences the variance of the energy, which is typically of the order of 0.5% of the total energy. Therefore, for circular quantum dots, we can conclude, assuming that the DMC calculations are as close as possible to the exact energies, that with an effective two-body interaction, a finite basis set of \( R = 20 \) major oscillator shells, and at most three-particle-three-hole correlations in the cluster amplitude, the remaining many-body effects are almost negligible as we are within 99-100% of the full correlation energy.

| \( \omega \) | \( R \) | \( E_0 \) | CCSD | CCSD(T) | \( \Lambda \text{-CCSD(T)} \) | DMC |
|---|---|---|---|---|---|---|
| 0.28 | 10 | 26.3556 | 25.7069 | 25.6445 | 25.6540 |
| 12 | 26.3950 | 25.7066 | 25.6388 | 25.6491 |
| 14 | 26.4221 | 25.7074 | 25.6363 | 25.6470 |
| 16 | 26.4410 | 25.7081 | 25.6346 | 25.6456 |
| 18 | 26.4551 | 25.7085 | 25.6334 | 25.6446 |
| 20 | 26.4659 | 25.7089 | 25.6324 | 25.6439 |
| 0.5 | 10 | 39.9948 | 39.2218 | 39.1659 | 39.1721 |
| 12 | 40.0409 | 39.2203 | 39.1599 | 39.1667 |
| 14 | 40.0709 | 39.2197 | 39.1565 | 39.1635 |
| 16 | 40.0922 | 39.2195 | 39.1543 | 39.1615 |
| 18 | 40.1080 | 39.2194 | 39.1527 | 39.1601 |
| 20 | 40.1292 | 39.2194 | 39.1516 | 39.1591 |
| 1.0 | 10 | 66.6596 | 65.7552 | 65.7118 | 65.7149 |
| 12 | 66.7106 | 65.7484 | 65.7017 | 65.7051 |
| 14 | 66.7445 | 65.7449 | 65.6961 | 65.6996 |
| 16 | 66.7686 | 65.7430 | 65.6926 | 65.6963 |
| 18 | 66.7867 | 65.7417 | 65.6903 | 65.6941 |
| 20 | 66.8006 | 65.7409 | 65.6886 | 65.6924 |

TABLE IV: Same caption as in Table III except the results are for \( N = 12 \) electrons.

In order to study the role of correlations as a function of the oscillator frequency \( \omega \) and the number of electrons, we define the relative energy

\[
\epsilon = \left| \frac{E_{\text{DMC}} - \langle \hat{H}_0 \rangle}{E_{\text{DMC}}} \right|
\]

where \( \langle \hat{H}_0 \rangle \) is the expectation value of the one-body operator, the so-called unperturbed part of the Hamiltonian. For \( N = 6 \) this corresponds to an expectation value \( \langle \hat{H}_0 \rangle = 10 \omega \) for the one-body part of the Hamiltonian, while for \( N = 12 \) and \( N = 20 \) the corresponding numbers are \( \langle \hat{H}_0 \rangle = 28 \omega \) and \( \langle \hat{H}_0 \rangle = 60 \omega \), respectively. Assuming that the diffusion Monte Carlo results are as close as possible to the true eigenvalues, the quantity \( \epsilon \) measures the role of the two-body interaction and correlations caused by this part of the Hamiltonian as functions of \( \omega \) and \( N \), the number of electrons. The results for \( \epsilon \) are shown in Fig. 11. Results for \( N = 2 \) are also included.
TABLE VI: Percentage of correlation energy at the CCSD level ($\Delta E_2$) and at the $\Lambda$-CCSD(T) level ($\Delta E_3$), for different numbers of electrons $N$ and values of the confining harmonic potential $\omega$. All numbers are for $R = 20$.

| $\omega$ | $E_0$ | CCSD | CCSD(T) | $\Lambda$-CCSD(T) | DMC |
|----------|-------|-------|---------|-------------------|-----|
| 0.28     | 63.5788 | 62.8251 | 62.1802 | 62.1946 |
| 0.50     | 95.5072 | 94.0870 | 93.9864 | 93.9971 |
| 1.00     | 157.4356 | 156.0128 | 155.9324 | 155.9381 |

TABLE V: Same caption as in Table III except the results are for $N = 20$ electrons.

| $\omega$ | $\Delta E_2$ | $\Delta E_3$ | $\Delta E_3^\omega$ | $\Delta E_3^\Lambda$ | $\Delta E_3^\Lambda$ |
|----------|---------------|---------------|---------------------|---------------------|---------------------|
| 0.28     | 94%           | 99%           | 96%                 | 100%                | 97%                 |
| 0.50     | 94%           | 99%           | 96%                 | 100%                | 97%                 |
| 1.00     | 94%           | 99%           | 96%                 | 100%                | 97%                 |

We see from this figure that the effect of the two-body interaction becomes increasingly important as we increase the number of particles. Moreover, the interaction is more important for the smaller values of the oscillator frequency $\omega$. This is expected since the contribution from the one-body operator is reduced due to smaller values of $\omega$. Including more electrons obviously increases the contribution from the two-body interaction. Since our optimal coupled-cluster results are very close to the DMC results, almost identical results are obtained if we replace the DMC results with the $\Lambda$–CCSD(T) results.

We can also study the role of correlations beyond the Hartree-Fock energy $E_0$. In order to do this, we relate the Hartree-Fock energy $E_0$ in Tables III to the optimal coupled-cluster calculation, namely the $\Lambda$-CCSD(T) results. The relative difference between these quantities conveys thereby information about correlations beyond the mean-field approximation. This relative measure is defined as

$$\chi = \frac{|E_{\text{CCSD(T)}} - E_0|}{E_{\text{DMC}}}.$$  \hspace{1cm} (45)

The results are shown in Fig. 2 for $N = 6$, $N = 12$, and $N = 20$.

We see from this figure that correlations beyond the Hartree-Fock level are important for few particles and low values of $\omega$. Increasing the number of electrons in the circular dot decreases the role of correlations beyond the mean-field approximation, a feature which can be understood from the fact that for larger systems, multi-particle excitations across the Fermi level decrease in importance. This is due to the fact that the single-particle wave function for many states around the Fermi level have more than one node, resulting in normally smaller matrix elements. Stated differently, with an increasing number of electrons, the particles close to the Fermi level are more apart from each other, in particular for those particles which occupy states around and above the Fermi level. The consequence of this is that correlations beyond the Hartree-Fock level decrease in importance when we add more and more particles. This means in turn that for larger systems, mean-field methods are rather good approximations to systems of many interacting electrons in quantum dots. Similar features are seen in nuclei. For light nuclei, correlations beyond the mean field are very important for ground-state properties, whereas for heavy nuclei like $^{208}$Pb mean-field approaches provide a very good starting point for studying several observables.

The reader should, however, note that here we have limited our attention to ground-state energies only. Whether our conclusions about the role of correlations pertain to quantities like say spectroscopic factors remains to be studied.

We conclude this section by studying in more detail the convergence properties of our coupled-cluster approaches, in particular, we will relate our $\Lambda$-CCSD(T) and CCSD results with the diffusion Monte Carlo results and study the dependence on $R$. This analysis will be performed with and without an effective Coulomb interaction. The reason for doing this is that we wish to study whether the convergence criterion of Eq. 13, derived for a full configuration interaction analysis, applies to various coupled-cluster truncations as well. Furthermore, we wish to see whether our calculations with an effective interaction converge faster as a function of $R$ compared to a calculation with the bare interaction.

We compute the following quantities

$$\log_{10} \epsilon_{\text{CCSD}}(R) = \log_{10} \left| \frac{E_{\text{CCSD}}(R) - E_{\text{DMC}}}{E_{\text{DMC}}} \right|,$$  \hspace{1cm} (46)

and

$$\log_{10} \epsilon_{\text{A–CCSD(T)}}(R) = \log_{10} \left| \frac{E_{\text{A–CCSD(T)}}(R) - E_{\text{DMC}}}{E_{\text{DMC}}} \right|.$$  \hspace{1cm} (47)
In Fig. 3 we plot the results for $N = 20$ electrons and $\omega = 0.5$. We have chosen these values since they represent one of the cases where the $\Lambda$-CCSD(T) results are always above the DMC results and we have no crossing between these two sets of calculations. The CCSD results on the other hand are always, for all cases reported here, above the DMC results. This means that the trend seen in Fig. 3 for the CCSD calculations applies to all cases listed in Tables III and IV, while for the $\Lambda$-CCSD(T) calculations, these results are similar for all cases except for $N = 6$ and $\omega = 0.5$ and $\omega = 1.0$, $N = 12$, and $\omega = 1.0$, and $N = 20$ and $\omega = 1.0$. In these cases the results at $R = 20$ are slightly below the DMC results. However, the agreement is still excellent.

The interesting feature to note in Fig. 3 is that the CCSD results change marginally after $R = 12$ for $N = 20$, and there is essentially very little to gain beyond twenty major shells. With the present accuracy of the DMC results, we can conclude that the CCSD results reach at most a relative error of approximately $10^{-3}$ and that it stays almost stable from $R = 12$ shells. The relative error with respect to the Monte Carlo results does not change much. This applies to all CCSD results. This tells us clearly that there are important correlations beyond two-particle-two-hole excitations and that these correlations do not stabilize after some few shells. Furthermore, the slope of the $\Lambda$-CCSD(T) calculations is much more interesting and resembles the slope of the configuration interaction analysis of Ref. 21 with an effective interaction. For the ground states of three to five electrons, Kvaal found in Ref. 21 a slope of approximately $\alpha = -4$ for $\alpha = -5$ for a parameterization

$$\log_{10} \epsilon \approx c + \alpha \log_{10} R,$$

for the ground-state energies of various $N$-electron quantum dots. The variable $c$ is a constant. Our slopes vary between $\alpha = -4$ and $\alpha = -6$, resulting in a relative error of approximately $10^{-5}$ at $R = 20$ for the results in Fig. 3. The slope of the $\Lambda$-CCSD(T) result is $\alpha = -4.93$. The reader should note that the DMC results cannot reach a higher precision. The slope of the CCSD calculation with an effective interaction is $\alpha = -0.67$ after $R = 12$.

In the same figure, we plot also the $\Lambda$-CCSD(T) results obtained without an effective Coulomb interaction, that is, with the bare interaction only. These results are labelled as $\log_{10} \epsilon_{\Lambda-CCSD(T)}(R)$—bare. A Hartree-Fock basis was used in this case as well in order to obtain converged solutions for the $\Lambda$-CCSD(T) equations. We see in this case that the convergence is much slower, resulting in a slope given by $\alpha = -2.58$, a result not far from the analysis of Ref. 21 for the bare interaction. Figure 4 exhibits a similar trend, except that here we present results for $N = 12$ electrons and $\omega = 0.5$. The slope of the $\Lambda$-CCSD(T) results is now $\alpha = -6.38$ with an effective interaction and $\alpha = -1.81$ with a bare Coulomb interaction. We notice again that the CCSD results saturate around $R = 12$ major shells.

These results are very interesting as they show that the usage of an effective interaction can really speed up the convergence of the energy as a function of the number of shells. Furthermore, these results tell us also that correlations beyond the singles and doubles approach are simply necessary. The convergence behavior of the $\Lambda$-CCSD(T) results resembles, to a large extent, those of a full configuration interaction approach with and without an effective interaction. Although we can extract similar convergence behaviors as those predicted in Ref. 21 as functions of a truncation in the single-particle basis, the challenge is to provide more rigid mathematical convergence criteria for truncations in the number of particle-hole excitations. Here we can only justify a posteriori that triples corrections are necessary. Work along these lines is in progress.

**IV. CONCLUSIONS AND PERSPECTIVES**

We have shown in this work that coupled-cluster calculations that employ an effective Coulomb interaction and a self-consistent Hartree-Fock single-particle basis reproduce excellently diffusion Monte Carlo calculations, even for very low oscillator frequencies. This opens up many interesting perspectives, in particular since our coupled-cluster calculations are rather inexpensive from a high-performance computing standpoint. Properties like addition spectra and excited states can be extracted using equation-of-motion-based techniques (see, for example, Refs. 18,40,41). Furthermore, since our codes run in an uncoupled basis, one can also study other trapping potentials than the standard harmonic oscillator potential. A time-dependent formulation of coupled-cluster theory may even allow for studies of temporal properties of quantum dots such as the effect of a time-dependent perturbation.

For circular dots, we found that with the inclusion of triples correlations, there are, for all systems studied, indications that many-body correlations beyond three-particle-three-hole excitations in the coupled-cluster amplitude $T$, are negligible. We observe also that for systems with more particles, correlations beyond the Hartree-Fock level tend to decrease. Thus, although we are able to extend $ab\ ini	ext{tio}$ coupled-cluster calculations of quantum dots to systems up to 50 electrons, a mean-field description will probably convey most of the interesting physics.

With two popular and reliable many-body techniques like coupled-cluster theory and diffusion Monte Carlo resulting in practically the same energies, one is in the position where one can extract almost exact density functionals for quantum dot systems. This allows for important comparisons with available density functionals for quantum dots. Finally, we have also noted that triples correlations are necessary in order to obtain correct results. The convergence pattern of our calculations resemble to a large extent those seen in full configuration interaction calculations.
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FIG. 1: Relative correlation energy $\epsilon$ defined in Eq. (44) for different values of $\hbar \omega$ and number of electrons. The DMC numbers are obtained from Tables II and III-V using $R = 20$.

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FIG. 2: Relative correlation energy $\chi$ defined in Eq. (45) for different values of $\hbar\omega$ and number of electrons. The numbers are obtained from Tables III-V using $R = 20$.

FIG. 3: Relative correlation energy $\epsilon$ defined in Eqs. (46) and (47) for different values of $R$. The values displayed here are for $N = 20$ and $\omega = 0.5$. The numbers are obtained from Table VI. We include also the $\Lambda$-CCSD(T) results obtained with the bare interaction.
FIG. 4: Relative correlation energy $\epsilon$ defined in Eqs. (16) and (17) for different values of $R$. The values displayed here are for $N = 12$ and $\omega = 0.5$. The numbers are obtained from Table IV. We include also the Λ-CCSD(T) results obtained with the bare interaction.