We describe OpenFCI, an open source implementation of the full configuration-interaction method (FCI) for two-dimensional quantum dots with optional use of effective renormalized interactions. The code is written in C++ and is available under the Gnu General Public License. The code and core libraries are well documented and structured in a way such that customizations and generalizations to other systems and numerical methods are easy tasks. As examples we provide a matrix element tabulation program and an implementation of a simple model from nuclear physics, in addition to the quantum dot application itself.

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I. INTRODUCTION

Quantum dots, nanometre-scale semiconductor devices confining a varying number of electrons, have been studied intensely in the last two decades. Quantum dots are fabricated using essentially macroscopic tools, for example etching techniques, but the resulting confinement allows for quantum mechanical behaviour of the electrons. Many of the parameters are directly controllable, thereby justifying the term “artificial atoms” or “designer atoms”. These considerations explain the immense research activity on these systems. For a general introduction, see Ref. [1] and references therein.

A very common model is that of a parabolic quantum dot, in which $N$ electrons are confined in an isotropic harmonic oscillator potential in $d$ spatial dimensions, where $d$ is determined by the semiconductor environment. Electronic structure calculations on the parabolic dot and similar systems are often carried out using the full configuration-interaction method (FCI), also called exact diagonalization [1]. The Hamiltonian is then projected onto a finite-dimensional subspace of the $N$-electron Hilbert space and diagonalized. Care is taken in order to exploit dynamical and discrete symmetries of the exact problem, such as conservation of angular momentum and total electron spin, in order to block-diagonalize the Hamiltonian matrix and reduce the computational complexity.

In this article, we describe OpenFCI, a recently developed open source C++ code implementing the FCI method for quantum dots [2]. The code has a generic framework in the shape of library functions, thereby allowing easy customization and extension to other systems and methods, e.g., three-dimensional quantum dots or the nuclear no-core shell model.

OpenFCI implements a renormalization of the two-body interactions, a technique widely used in nuclear no-core shell model calculations. This allows for accelerated convergence with respect to Slater determinant basis size [3, 4]. To the author’s knowledge, no other available code provides such effective interactions for quantum dot systems. The code can be easily modified to create effective interactions for almost many-body problem using a harmonic oscillator basis.

The code is developed in a Linux environment using Gnu C++, and is readily portable to other environments and compilers. The Fortran 77 libraries LAPACK and ARPACK are required, but as these are available on a wide range of platforms, portability should not be affected. OpenFCI is released under the Gnu General Public License (Gnu GPL) [5] and is documented using Doxygen [6]. As an open source project, the code can freely be used and modified.

The article is organized as follows: In Section II the FCI method is introduced in the context of the parabolic quantum dot, where we also discuss the reduction of the Hamiltonian matrix by means of commuting operators and configurational state functions. In Section III we discuss the effective two-body interaction. As the technique is likely to be unfamiliar to most readers outside the nuclear physics community, this is done in some detail. In Section IV we discuss the organization and use of OpenFCI. We also give some results from example runs, and in particular an analytically solvable non-trivial model due to Johnson and Payne is considered [7], where the only modification of the parabolic quantum dot is the interaction. Finally, we conclude our article in Section V.

Two appendices have been provided, Appendix A detailing the heavily-used centre-of-mass transformation and Appendix B discussing the exact numerical solution of the two-electron quantum dot needed for the effective interaction scheme.
II. FCI METHOD

A. Hamiltonian in occupation number formalism

We consider \( N \) electrons trapped in an isotropic harmonic oscillator potential in \( d \) spatial dimensions. The electrons interact via the Coulomb potential given by \( U(r_{ij}) = \lambda/r_{ij} \), where \( r_{ij} = \| \vec{r}_i - \vec{r}_j \| \) is the inter-particle distance and \( \lambda \) is a constant. The quantum dot Hamiltonian then reads

\[
H := \sum_{i=1}^{N} H_0(i) + \sum_{i<j}^{N} U(r_{ij}),
\]

where the second sum runs over all pairs \( 1 \leq i < j \leq N \), and where \( H_0(i) \) is the one-body Hamiltonian defined by

\[
H_0(i) := -\frac{1}{2} \nabla_i^2 + \frac{1}{2} \| \vec{r}_i \|^2.
\]

The interaction strength \( \lambda \) is given by

\[
\lambda = \sqrt{\frac{m^*}{\omega \hbar^3}} \epsilon^2 / 4 \pi \epsilon_0,
\]

where \( \epsilon \) is the dielectric constant of the semiconductor bulk, \( \epsilon^2/4\pi\epsilon_0 \approx 1.440 \text{ eV}\cdot\text{nm} \), and \( \omega = \hbar/m^* a^2 \), \( a \) being the trap size and length unit, and \( m^* \) being the effective electron mass. Typical values for GaAs quantum dots are \( \epsilon = 12.3 \), \( m^* = 0.067 \) electron masses, and \( a = 20 \) nm, yielding \( \lambda = 2.059 \). The energy unit is \( \hbar \omega \), in this case \( \hbar \omega = 2.84 \text{ meV} \).

Choosing a complete set \( \{ \phi_\alpha(x) \}_{\alpha \in A} \) of single-particle orbitals (where \( x = (\vec{r}, s) \) denotes both spatial and spin degrees of freedom, and \( \alpha = (a, \sigma) \) denotes both generic spatial quantum numbers \( a \) and spin projection quantum numbers \( \sigma = \pm 1 \) ), \( H \) can be written in occupation number form as

\[
H = \sum_{a,b,\sigma} \sum_{\sigma'} \sum_{\gamma} \sum_{\tau} h_0^{ab,\sigma\sigma'} \phi^{\tau\gamma}_{a,s} a_{b,\sigma}^\dagger a_{b,\sigma'}^\dagger + \sum_{abcd\sigma\tau} u_{abcd}^{ab,\sigma\tau} a_{a,\sigma}^\dagger a_{b,\sigma'}^\dagger a_{d,\tau}^\dagger a_{c,\tau}^\dagger,
\]

where \( a_{\alpha}^\dagger \) (\( a_{\alpha} \)) creates (destroys) a particle in the orbital \( \phi_\alpha(x) \). These operators obey the usual anti-commutation relations

\[
\{ a_{\alpha}, a_{\beta}^\dagger \} = \delta_{\alpha,\beta}, \quad \{ a_{\alpha}, a_{\beta} \} = 0.
\]

For a review of second quantization and occupation number formalism, see for example Ref. [8]. The single-particle orbitals are chosen on the form

\[
\phi_{(a,\sigma)}(x) := \varphi_a(\vec{r}) \chi_\sigma(s),
\]

where \( \{ \varphi_a(\vec{r}) \} \) are spinless orbitals and \( \chi_\sigma(s) = \delta_{\sigma,s} \) are spinor basis functions corresponding to the eigenstates of the spin-projection operator \( S_z \) with eigenvalues \( \sigma/2 \).

It is important, that since the single-particle orbitals \( \{ \varphi_a(\vec{r}) \}_{a \in A} \) are denumerable, we may choose an ordering on the set \( A \), such that \( A \) can in fact be identified with a range of integers, \( A \cong \{ 0, 1, 2, \cdots, L/2 \} \). In most \textit{ab initio} systems \( L \) is infinite, since the Hilbert space is infinite-dimensional. Similarly, \( \alpha = (a, +1) \) is identified with even integers, and \( \alpha = (a, -1) \) with odd integers, creating an ordering of the single-particle orbitals \( \phi_\alpha(x) \), and \( \alpha \) is identified with an integer \( 0 \leq I(\alpha) \leq L \).

The single-particle matrix elements \( h_0^{ab} \) and the two-particle elements \( u_{abcd}^{ab} \) are defined by

\[
h_0^{ab} := \langle \varphi_a | H_0 | \varphi_b \rangle = \int \varphi_a(\vec{r}) H_0 \varphi_b(\vec{r}) \, d^d r,
\]

and

\[
u_{abcd}^{ab} := \langle \varphi_a \varphi_b | U(\vec{r}_{12}) | \varphi_c \varphi_d \rangle
\]

\[
= \lambda \int \varphi_a(\vec{r}_1) \varphi_b(\vec{r}_2) \varphi_c(\vec{r}_3) \varphi_d(\vec{r}_4) \, d^d r_1 \, d^d r_2
\]

respectively.

The spatial orbitals \( \varphi_a(\vec{r}) \) are usually chosen as eigenfunctions of \( H_0 \), so that \( h_0^{ab} = \delta_{ab} \epsilon_a \).

The basis functions for \( N \)-particle Hilbert space are Slater determinants \( \{ \Phi_{\alpha_1, \alpha_2, \cdots, \alpha_N} \} \) defined by

\[
| \Phi_{\alpha_1, \cdots, \alpha_N} \rangle := a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \cdots a_{\alpha_N}^\dagger | - \rangle,
\]

where \( | - \rangle \) is the zero-particle vacuum. In terms of single-particle orbitals, the spatial representation is

\[
\Phi_{\alpha_1, \cdots, \alpha_N}(x_1, \cdots, x_N) = \frac{1}{\sqrt{N!}} \sum_{p \in S_N} (-1)^{|p|} \prod_{i=1}^{N} \phi_{\alpha_{p(i)}}(x_i),
\]

where \( S_N \) is the group of permutations of \( N \) symbols. The Slater determinants are anti-symmetric with respect to permutations of both \( x_i \) and \( \alpha_i \), so that the orbital numbers \( \alpha_i \) all must be distinct to give a nonzero function. Each orbital is then occupied by at most one particle. Moreover, for a given set \( \{ \alpha_i \}_{i=1}^{N} \) of orbitals, one can create \( N! \) distinct Slater determinants that are linearly dependent. In order to remove this ambiguity, we choose only orbital numbers such that \( I(\alpha_i) < I(\alpha_j) \) whenever \( i < j \).

It follows, that there is a natural one-to-one correspondence between Slater determinants with \( N \) particles and integers \( b \) whose binary representations have \( N \) bits set. (If \( |A| = L < \infty \), the integers are limited to \( 0 \leq b < 2^L \).) Each bit position \( k \) corresponds to an orbital \( \phi_\alpha(x) \) through \( k = I(\alpha) \), and the bit is set if the orbital is occupied. Creating and destroying particles in \( | \Phi_{\alpha_1, \cdots, \alpha_N} \rangle \) simply amounts to setting or clearing bits (possibly obtaining the zero-vector if a particle is destroyed or created twice in the same orbital), keeping track of the possible sign change arising from bringing the set \( \{ \alpha_i \} \) on ordered form using Eqn. [11]. Note that the vacuum \( | - \rangle \) corresponds to \( b = 0 \), which is not the zero vector, but the single state with zero particles.
The single-particle orbitals are illustrated in Fig. 1.

\[ H_0 |\Phi_n\rangle = \varepsilon_n |\Phi_n\rangle \]

These may be given on several equivalent forms, but it is convenient to utilize rotational symmetry of angular momentum \( L \) of \( \varepsilon_n \). All eigenfunctions with the same quantum number \( n \) and \( m \) span a single-particle shell. The diagonalization of Hamiltonian (3) also commutes with total electron spin projection \( S_z \), viz,

\[ S_z := \sum_{a \sigma} \sigma a^\dagger a \sigma \]

The Slater determinants are eigenvectors of both \( L_z \) and \( S_z \) with eigenvalues \( M \) and \( s_z \), respectively. We obtain a natural splitting of the model space \( \mathcal{P} \) into subspaces with constant angular momentum \( M \) and spin projection \( s_z \), viz,

\[ \mathcal{P} = \bigoplus_{M, s_z} \mathcal{P}_{M, s_z}, \quad \mathcal{P} = \sum_{M, s_z} \mathcal{P}_{M, s_z}. \]

B. Model spaces

The FCI calculations are done in a finite-dimensional subspace \( \mathcal{P} \) of the \( N \)-particle Hilbert space, called the model space. The model space has a basis of Slater determinants, and \( \mathcal{P} \) has the orthogonal projector \( P \) given by

\[ P := \sum_{|\Phi_b\rangle \in \mathcal{B}} \langle \Phi_b | \langle \Phi_b |. \quad (6) \]

The configuration-interaction method in general now amounts to diagonalizing (in the sense of finding a few of the lowest eigenvalues of) the, in general, large and sparse matrix \( PHP \). The only approximation we have made is the truncation of the \( N \)-particle Hilbert space.

The model space \( \mathcal{P} \) is seen to be a function of the single particle orbitals \( \varphi_n \), whom we choose to be the eigenfunctions of \( H_0 \), i.e., harmonic oscillator eigenfunctions. These may be given on several equivalent forms, but it is convenient to utilize rotational symmetry of \( H_0 \) to create eigenfunctions of the projection of the angular momentum \( L_z \). In \( d = 2 \) dimensions we obtain the Fock-Darwin orbitals defined in polar coordinates by

\[ \varphi_{n, m}(r, \theta) = \frac{1}{\sqrt{\pi}} e^{im\theta} r^{|m|} L_n^{|m|} (r^2) e^{-r^2/2}, \quad (7) \]

Here \( L_n^m(x) \) is the normalized generalized Laguerre polynomial. The factor \((-1)^n\) is for convenience, see Appendix A. The harmonic oscillator energy is \( 2n + |m| + 1 \) and the eigenvalue of \( L_z = -i\partial/\partial \theta \) is \( m \). All eigenfunctions with the same energy \( 2n + |m| + 1 \) span a single-particle shell. The single-particle orbitals are illustrated in Fig. 1.

For a Slater determinant \( |\Phi_{\alpha_1, \ldots, \alpha_N}\rangle \), we have

\[ \sum_{i=1}^{N} H_0(i) |\Phi_{\alpha_1, \ldots, \alpha_N}\rangle = E_{\alpha_1, \ldots, \alpha_N}^0 |\Phi_{\alpha_1, \ldots, \alpha_N}\rangle \]

with

\[ E_{\alpha_1, \ldots, \alpha_N}^0 := \sum_{i=1}^{N} (R_i + 1), \]

where \( R_i = 2n_i + |m_i|, \) and

\[ \sum_{i=1}^{N} L_z(i) |\Phi_{\alpha_1, \ldots, \alpha_N}\rangle = M |\Phi_{\alpha_1, \ldots, \alpha_N}\rangle, \]

where \( M = \sum_{i=1}^{N} m_i \).

To complete our definition of \( \mathcal{P} \), we let

\[ \mathcal{B} = \mathcal{B}_R = \left\{ |\Phi_{\alpha_1, \ldots, \alpha_N}\rangle : \sum_{i=1}^{N} R_i \leq R \right\}, \quad (8) \]

where \( R \) is called the energy cut, for obvious reasons. As \( R \to \infty \), the whole Hilbert space is spanned, and the eigenpairs of \( PHP \) converge to those of \( H \).

C. Configurational state functions and block diagonality

In order to reduce the complexity of the calculations, we need to exploit symmetries of \( H \). First of all, \( [H, L_z] = 0 \), and it is obvious that also \( [H, S_z] = 0 \), where the spin projection operator \( S_z \) is given by

\[ S_z := \frac{1}{2} \sum_{a \sigma} \sigma a^\dagger a \sigma. \]

The Slater determinants are eigenvectors of both \( L_z \) and \( S_z \) with eigenvalues \( M \) and \( s_z \), respectively. We obtain a natural splitting of the model space \( \mathcal{P} \) into subspaces with constant angular momentum \( M \) and spin projection \( s_z \), viz,

\[ \mathcal{P} = \bigoplus_{M, s_z} \mathcal{P}_{M, s_z}, \quad \mathcal{P} = \sum_{M, s_z} \mathcal{P}_{M, s_z}. \]

The diagonalization of \( H \) can thus be done within each space \( \mathcal{P}_{M, s_z} \), separately, amounting to diagonalizing individual blocks \( P_{M, s_z} H P_{M, s_z} \).

The Hamiltonian \( H \) also commutes with total electron spin \( S^2 \), \( [S^2, S_z] = 0 \), given by

\[ S^2 := S_z^2 + \frac{1}{2} (S_+ S_- + S_- S_+), \]

with

\[ S_{\pm} := \sum_{a} a^\dagger_a a_{a \pm}, \]

so that a common basis for \( S_z \) and \( S^2 \) would lead to even smaller matrix blocks.

The eigenvalues of \( S^2 \) are on the form \( s(s + 1) \), where \( 0 \leq 2s \leq N \) is an odd (even) integer for odd (even)
N. For a joint eigenfunction of \( S_z \) and \( S^2 \), called a configurational state function (CSF), \( |s_z| \leq s \). The Slater determinants are, however, not eigenfunctions of \( S^2 \), but such can be constructed by taking linear combinations of a small number Slater determinants. For details on this algorithm, see Ref. [9]. Suffice it to say here, that \( S^2 \) only couples Slater determinants with identical sets of doubly occupied orbitals (meaning that \( \phi(a,+) \) and \( \phi(a,-) \) are both occupied, as in Figure 1) and singly occupied orbitals (meaning that only one of \( \phi(a,+) \) and \( \phi(a,-) \) are occupied). It is easy to see that \( S^2 \) does not couple Slater determinants in \( \mathcal{P}_{M,s_z} \) to another \( \mathcal{P}_{M',s_z'} \). Thus, we obtain the splitting

\[
\mathcal{P}_{M,s_z} = \bigoplus_s \mathcal{P}_{M,s_z,s}.
\]

We stress that all the mentioned operators commute with each other, viz,

\[
[H, \Omega_i] = [\Omega_i, \Omega_j] = 0,
\]

with \( \Omega_i \in \{L_z, S_z, S^2\} \). If a modified problem breaks, say, rotational symmetry, such that \( [H, L_z] \neq 0 \), we may still split the model space into to the eigenstates of \( S_z \) and \( S^2 \).

### D. Matrix elements of Coulomb interaction

The remaining ingredient in the FCI method is the Coulomb matrix elements \( u_{cd}^{ab} \) defined in Eqn. (5). These can be calculated by first expanding \( L_n^k(x) \) in powers of \( x \) using

\[
L_n^k(x) = \sum_{m=0}^{n} (-1)^m \frac{(n + k)!}{(n - m)!(k + m)!m!} x^m,
\]

and evaluating the resulting integral term-by-term by analytical methods [10]. The resulting expression is a seven-fold nested sum, which can be quite time-consuming, especially if a large number of Fock-Darwin orbitals occurs in the basis \( \mathcal{B} \). Moreover, the terms are fractions of factorials with alternating signs, which is a potential source of loss of numerical precision.

We therefore opt for a more indirect approach, giving a procedure applicable to a wide range of potentials \( U(r_{12}) \) in addition to the Coulomb potential. Moreover, it can be generalized to arbitrary spatial dimensions \( d \). The approach is based on directly transforming the product functions \( \varphi_n(r_1)\varphi_0(r_2) \) to the centre-of-mass system, where the interaction \( U(r_{12}) \) only acts on the relative coordinate, and then transforming back to the lab system. This reduces the computational cost to a doubly nested sum, as well as the pre-computation of the centre-of-mass transformation and the relative coordinate interaction matrix. Both can be done exactly using Gaussian quadrature. The transformations to and from the centre of mass frame are unitary transformations, which are stable and will not magnify round-off errors.

In Appendix A we provide the details of the centre-of-mass transformation. One then obtains the following expression for the interaction matrix elements \( u_{cd}^{ab} \): Let \( a = (\mu_1, \nu_1) \), \( b = (\nu_2, \nu_2) \), \( c = (\mu_3, \nu_3) \), and \( d = (\mu_4, \nu_4) \) be the circular quantum number equivalents of the usual polar coordinate quantum numbers \( n_i \) and \( m_i \).

Due to conservation of angular momentum, we assume \( m_1 + m_2 = m_3 + m_4 \); otherwise, the matrix element \( u_{cd}^{ab} = 0 \). Define \( M = \mu_1 + \mu_2, M' = \mu_3 + \mu_4, N = \nu_1 + \nu_2, \) and \( N' = \nu_3 + \nu_4 \). Since \( u_{cd}^{ab} \) is linear in \( \lambda \), we set \( \lambda = 1 \) without loss of generality. Now,

\[
u_{cd}^{ab} = \sum_{p=p_0}^{M} T_2^{(M)} T_2^{(M')} \sum_{q=q_0}^{N} T_2^{(N)} T_2^{(N')} C_{n,n+}, \quad (9)
\]

where \( n = \min(p, q), s = M' - M, p' = p + M' - M, \) \( q' = q + N' - N \). Moreover, \( p_0 = \max(M' - M, 0) \) and \( q_0 = \max(N' - N, 0) \).

Here, \( T_2^{(N)} \) are centre-of-mass transformation coefficients defined in Appendix A while the relative coordinate interaction matrix elements \( C_{n,n'}^{(m)} \), \( n, n' \geq 0 \), are defined by

\[
C_{n,n'}^{(m)} := \langle \varphi_n, m(r, \theta) | U(\sqrt{2}r) | \varphi_{n'}, m(r, \theta) \rangle
= 2 \int_0^\infty \int_0^{2\pi} |\tilde{L}_n^m(\rho^2)\tilde{L}_{n'}^m(\rho^2)| U(\sqrt{2}r) e^{-r^2} r d\theta d\rho
\]

Depending on \( U(r_{12}) \), the integral is best computed using generalized half-range Hermite quadrature (see Appendix B and Ref. [11]) or Gauss-Hermite quadrature. Weights and abscissa for quadratures are conveniently computed using the Golub-Welsch algorithm [12], which only depends on the ability to compute the coefficients of the three-term recursion relation for the polynomial class in question, as well as diagonalizing a symmetric tri-diagonal matrix.

Let \( p(r) \) be a polynomial, and let \( \alpha < 2 \) and \( \beta \) be non-negative constants. Then

\[
U(r_{12}) = r_{12}^{\alpha} p(r_{12}) e^{-\beta r_{12}} \quad (11)
\]

admit exact evaluations using generalized half-range Gauss-Hermite quadrature. The Coulomb potential, Gaussian potentials, and the parabolic interaction \( -\lambda r_{12}^2/2 \) of the analytically solvable model treated in Sec. [IV.C] belong to this class of potentials.

In the case of \( \alpha = 1 \) and \( p(r) = q(r^2) \) (i.e., an even polynomial), the integral is more convenient to evaluate using standard Gauss-Hermite quadrature. The Coulomb interaction falls into this class.

Of course, one may let \( p(r) \) be a non-polynomial function as well and still obtain very good results, as long as \( p(r) \) is well approximated with a polynomial, e.g., is smooth.
III. EFFECTIVE INTERACTIONS

A. Motivation

The FCI calculations converge relatively slowly as function of the model space parameter $R$, as the error $\Delta E$ in the eigenvalue behaves like $o(R^{-k})$ in general, where $k = O(1)$. This behaviour comes from the singular nature of the Coulomb interaction.

In Ref. 3, numerical results using an effective interaction were presented. This method is widely used in no-core shell model calculations in nuclear physics, where the nucleon-nucleon interaction is basically unknown but highly singular 4. This so-called sub-cluster effective interaction scheme replaces the Coulomb interaction (or another interaction) $U(r_{ij}) = \lambda/r_{ij}$ with a renormalized interaction $\tilde{U}(i,j)$ obtained by a unitary transformation of the two-body Hamiltonian that decouples the model space to first order in the interaction 16, 17. Such a generic unitary transformation to decouple the model space to first order in the interaction $\tilde{U}(i,j)$ obtained by a unitary transformation of the two-body Hamiltonian $H$ (i.e., Eqn. (1) or (3) with $\lambda$ being a parameter) that de-couples $P$ and its complement 13. Therefore, the two-body problem becomes exact in a finite number of harmonic oscillator shells. Loosely speaking, the effective interaction incorporates information about the interaction’s action outside the model space. In general, $\tilde{U}(i,j)$ is non-linear in $\lambda$ and not a local potential.

Using the renormalized $\tilde{U}(i,j)$, the many-body system does not become exact, of course, but $\tilde{U}(i,j)$ will perform better than the bare interaction in this setting as well. To the author’s knowledge, there exists no rigorous mathematical treatment with respect to this, but it has nevertheless enjoyed great success in the nuclear physics community 4, 14, 15, and our numerical experiments unambiguously demonstrate that the convergence of the FCI method is indeed improved drastically 3, especially for $N \leq 4$ particles. We stress that the cost of producing $\tilde{U}(i,j)$ is very small compared to the remaining calculations.

B. Unitary transformation of two-body Hamiltonian

We now describe the unitary transformation of the two-body Hamiltonian (i.e., Eqn. (1) or (3) with $N = 2$) that de-couples $P$ and its complement. This approach dates back as far as 1929, when Van Vleck introduced such a generic unitary transformation to de-couple the model space to first order in the interaction 16, 17.

Let $P$ be given by Eqn. (3), and let $D = \dim(\mathcal{P})$. The idea is to find a unitary transformation $\mathcal{H} = Z^\dagger HZ$ of $H$ such that

$$(1 - P)\mathcal{H}P = 0,$$

i.e., $\mathcal{H}$ is block diagonal. This implies that $H_{\text{eff}}$ defined by

$$H_{\text{eff}} := P\mathcal{H}P$$

has eigenvalues identical to $D$ of those of the full operator $H$. Since $D$ is finite, $H_{\text{eff}}$ is called an effective Hamiltonian.

Selecting $Z$ is equivalent to selecting a set of effective eigenpairs $\{(E_k, |\Psi_k\rangle)\}_{k=1}^D$, where $E_k$ is an eigenvalue of $H$ and $\{|\Psi_k\rangle\}_{k=1}^D \subset \mathcal{P}$ are the effective eigenvectors; an orthonormal basis for $\mathcal{P}$. It is clear that $Z$ is not unique, since there are many ways to pick $D$ eigenvalues of $H$, and for each such selection any unitary $D \times D$ matrix would yield an eigenvector set.

However, some choices are more natural than others, since the eigenvectors and eigenvalues are usually continuous functions of $\lambda$. We then select the $D$ eigenvalues $E_k(\lambda)$ that develop adiabatically from $\lambda = 0$. For the corresponding effective eigenvectors $|\Psi_k\rangle$, we choose the orthonormal set that minimizes the distance to the exact eigenvectors $\{|\Psi_k\rangle\}_{k=1}^D$, i.e.,

$$_{\{\Psi_k\}}_{D=1}^D := \arg\min_{\{\Psi_k\}} \sum_{k=1}^D ||\Psi_k - |\Psi_k\rangle||^2, \quad (12)$$

where the minimization is taken over orthonormal sets only. The effective eigenvectors also turn out to be continuous functions of $\lambda$, so $H_{\text{eff}}$ will also be continuous.

Let $U$ is the $D \times D$ matrix whose columns contain $P|\Psi_k\rangle$ in the chosen basis, and let $V$ be the corresponding matrix containing $|\Psi_k\rangle$. Clearly, $V$ is unitary, while $U$ only approximately so. Equation (12) can then be written

$$V := \arg\min_{U} \text{trace}[(U - U')(U - U')^\dagger], \quad (13)$$

where the minimum is taken over all unitary matrices. If $U$ has singular value decomposition given by

$$U = X\Sigma Y^\dagger, \quad (14)$$

the solution $V$ is given by

$$V := XY^\dagger. \quad (15)$$

If $E = \text{diag}(E_1, \cdots, E_D)$ is the diagonal matrix whose elements are the chosen eigenvalues, we have

$$H_{\text{eff}} = V EV^\dagger.$$

See Ref. 13 for a thorough discussion of the above prescription for $H_{\text{eff}}$.

Having computed the two-body $H_{\text{eff}}$, we define the effective interaction $\tilde{U}(1,2)$ by

$$\tilde{U}(1,2) := H_{\text{eff}} - \sum_{i=1}^2 H_0(i)P,$$

which gives meaning solely in the model space. In second quantization,

$$\tilde{U}(1,2) := \frac{1}{2} \sum_{ab\sigma\tau} C_d^a C_{\sigma\tau}^b a_{\sigma\tau} a_d a_{\sigma\tau},$$
and the $N$-body $H_{\text{eff}}$ becomes (cf. Eqn. 11)

$$H_{\text{eff}} = \sum_{i=1}^{N} H_{0}(i) + \sum_{i<j}^{N} \hat{U}(i,j),$$

with occupation number formalism form (cf. Eqn. 9)

$$H_{\text{eff}} = \sum_{a,b} \sum_{\sigma} h_a^a a^\dagger_a \sigma a^\sigma + \frac{1}{2} \sum_{abcd} \sum_{\sigma \tau} \tilde{u}_{cd}^{ab} a^\dagger_a \sigma a^\sigma b^\dagger_b \tau a^\tau c^\tau a^\tau c^\tau. \tag{16}$$

Now, $H_{\text{eff}}$ is well-defined in the space of $N$-body Slater determinants where no pairs of occupied orbitals constitute a two-body state outside the two-particle model space, since then the matrix element $\tilde{u}_{cd}^{ab}$ would be undefined. A little thought shows us that if $\hat{U}(1,2)$ was computed in a two-body energy cut space with parameter $R$, $H_{\text{eff}}$ is well-defined on the many-body model space with the same cut $R$.

C. A comment concerning the choice of model space

The two-body problem is classically integrable, i.e., there exists $2d - 1$ constants of motion $\Omega_i$, such that their quantum mechanical observables commute with $H$ and each other, viz,

$$[H, \Omega_i] = [\Omega_i, \Omega_j] = 0, \quad \text{for all } i,j.$$ 

Indeed, the centre-of-mass harmonic oscillator $H_C$ defined in Eqn. 18 below and the corresponding centre-of-mass angular momentum provides two constants, while total angular momentum $L_z$ provides a third.

Using the model space $\mathcal{P}$ defined by an energy cut, we have

$$[P, \Omega_i] = 0$$

as well, which is equivalent to

$$[H_{\text{eff}}, \Omega_i] = 0,$$ 

so that $H_{\text{eff}}$ is integrable as well. In particular, $\hat{U}(1,2)$ is block-diagonal with respect to $\Omega_i$.

If we consider the commonly encountered model space $\mathcal{P}'$ defined by the Slater determinant basis $\mathcal{B}'$ given by

$$\mathcal{B}' := \{ |\Phi_{s_1, \ldots, s_N} \rangle : \max(R_i) \leq R \}$$

instead of Eqn. 9, we will have

$$[P', H_C] \neq 0,$$

as is easily verified. Indeed, $\mathcal{P}'$ is not an invariant subspace of the centre-of-mass transformation $T$ defined in Appendix A. Thus, $[H_{\text{eff}}, H_C] \neq 0$, so that the centre-of-mass energy no longer is a constant of motion! The symmetry-breaking of the effective Hamiltonian in this case is problematic, since in the limit $\lambda \to 0$, the exact eigenfunctions that develop adiabatically are not all either in the model space or in the complement. The adiabatic continuation of the eigenpairs starting out in $\mathcal{P}$ is thus not well-defined.

We comment, that the model space $\mathcal{P}'$ is often used in both no-core shell model calculations and quantum dot calculations, but the effective interaction becomes, in fact, ill-behaved in this case.

D. Solution of the two-body problem

What remains for the effective interaction, is the computation of the exact eigenpairs $\{(E_k, |\Psi_k\rangle)\}_{k=1}^{P}$. We must also solve the problem of following eigenpairs adiabatically from $\lambda = 0$.

For the two-body Coulomb problem, analytical solutions are available only for very special values for $\lambda$ [18]. These are useless for our purpose, so we must use numerical methods.

A direct application of the FCI method using Fock-Darwin orbitals with a large $R' > R$ will converge slowly, and there is no device in the method for following eigenvalues adiabatically. As the eigenvalues may cross, selecting, e.g., the lowest eigenvalues will not work in general.

For the two-body problem, the Pauli principle leads to a symmetric spatial wave function for the singlet $s = 0$ spin state, and an anti-symmetric wave function for the triplet $s = 1$ spin states. For the spatial part, we exploit the integrability of the system as follows. Define centre-of-mass coordinates by

$$\vec{R} := \frac{1}{\sqrt{2}}(\vec{r}_1 + \vec{r}_2)$$

and

$$\vec{r} := \frac{1}{\sqrt{2}}(\vec{r}_1 - \vec{r}_2).$$

Using these coordinates, the two-body Hamiltonian becomes

$$H = H_0(\vec{R}) + \left[ H_0(\vec{r}) + U(\sqrt{2}r; \lambda) \right]$$

$$=: H_C + H_{\text{rel}} \tag{18}$$

where $r_{12} = \sqrt{2}r := \sqrt{2}||\vec{r}|$. We have introduced the parameter $\lambda$ explicitly in the potential in this equation. $H$ is clearly separable, and the centre-of-mass coordinate Hamiltonian $H_C$ is a trivial harmonic oscillator, while the relative coordinate Hamiltonian can be written as

$$H_{\text{rel}} := -\frac{1}{2} \nabla^2 + \frac{1}{2r^2} + U(\sqrt{2}r; \lambda),$$

where in polar coordinates $\vec{r} = (r \cos \theta, r \sin \theta)$ we have

$$\nabla^2 = \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{\partial^2}{\partial \theta^2}. $$
Applying separation of variables again, the eigenfunctions of $H_{\text{rel}}$ can be written

$$\psi_{n,m}(\vec{r}) := \frac{e^{im\theta}}{\sqrt{2\pi}} u_{n,m}(r)$$

where $n$ is the nodal quantum number. $u_{n,m}(r)$ satisfies

$$K_{[m]} u_{n,m}(r) = \mu_{n,m} u_{n,m}(r)$$  \hspace{2cm} (19)

where

$$K_{[m]} := -\frac{1}{2r} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{m^2}{2r^2} + \frac{1}{2} r^2 + U(\sqrt{2r}; \lambda).$$  \hspace{2cm} (20)

Equation (19) is an eigenvalue problem in the Hilbert space $L^2((0, \infty), dr)$, where the measure $dr$ is induced by the polar coordinate transformation. Although it is natural to try and solve the radial problem using Fock-Darwin orbitals, this will converge slowly. The solution to this problem is to use a radial basis of generalized half-range Hermite functions \[11\]. In Appendix B this is laid out in some detail.

Equation (19) is a one-dimensional equation, so there will be no degeneracy in the eigenvalues $\mu_{m,n}$ for fixed $m$. In particular, the eigenvalues as function of the interaction strength $\lambda$ will not cross, and will be continuous functions of $\lambda$. We thus have $\mu_{m,n} < \mu_{m,n+1}$ for all $n$, where $n$ is the nodal quantum number.

At $\lambda = 0$ we regain the harmonic oscillator eigenvalues $2n + |m| + 1$. Correspondingly, the eigenfunctions $\psi_{m,n}(r, \theta)$ approaches the Fock-Darwin orbitals $\varphi_{m,n}(r, \theta)$, i.e., the harmonic oscillator eigenfunctions. For the radial part,

$$\lim_{\lambda \to 0} u_{m,n}(r) = g_n^{[m]}(r) := \sqrt{2} g_n^{[m]} \tilde{L}_n^{[m]}(r^2) e^{-r^2/2}.$$

Reintroducing spin, the full eigenfunctions $\Psi = \Psi_{n_1,m_1,n_2,m_2}$ are on the form

$$\Psi(x_1, x_2) = \varphi_{n_1,m_1}(\vec{R}) \frac{e^{im_2\theta}}{\sqrt{2\pi}} u_{n_2,m_2}(r) \chi_{s,s_z},$$

where $s = 0$ for odd $m_2$, and $s = 1$ for even $m_2$, and $|s_z| \leq s$ is an integer.

Let $R_1 = 2n_1 + |m_1|$ be the shell numbers for the centre-of-mass coordinate and relative coordinate, respectively. The eigenvalue $E = E_{n_1,m_1,n_2,m_2}$ is

$$E = R_1 + 1 + \mu_{n_2,m_2},$$

with limit

$$E \xrightarrow{\lambda \to 0} R_1 + R_2 + 2,$$

which is the harmonic oscillator eigenvalue.

As the centre-of-mass coordinate transformation conserves harmonic oscillator energy, at $\lambda = 0$, the eigenfunctions that are in the model space are exactly those obeying $R_1 + R_2 \leq R$. Turning on the interaction adiabatically, the eigenpairs we must choose for the effective Hamiltonian at a given $\lambda$ are exactly those with $R_1 + R_2 \leq R$.

The model-space projection $P\Psi$ needed in Eqns. (12) and (13) is now given by

$$P\Psi(x_1, x_2) = \varphi_{n_1,m_1}(\vec{R}) \frac{e^{im_2\theta}}{\sqrt{2\pi}} \left[ \tilde{P}_R^{[m_2]} u_{n_2,m_2}(r) \right] \chi_{s,s_z},$$

where

$$\tilde{P}_R^{[m]} := \sum_{n=0}^{\tilde{n}} |g_n^{[m]}| \langle g_n^{[m]} |, \quad \tilde{n} = \left\lfloor \frac{R - |m|}{2} \right\rfloor,$$

where $[x]$ is the integer part of $x$. This operator thus projects onto the $\tilde{n} + 1$ first radial basis functions with given $|m|$.

Due to Eqn. (17), the unitary operator $Z$ can be decomposed into its action on blocks defined by tuples of $n_1, m_1$, and $m_2, \tilde{n}$. The minimization (12) can then be applied on block-per-block basis as well. Each subproblem is equivalent to the calculation of an effective Hamiltonian $K_{\text{eff}}$ of the radial problem for a given $m_2$ and $\tilde{n}$.

To this end, let $\tilde{n}$ and $m = m_2$ be given. Let $U$ be the $(\tilde{n} + 1) \times (\tilde{n} + 1)$ matrix whose elements are given by

$$U_{n,k} = \langle g_n^{[m]} | u_{m,n} \rangle, \quad 0 \leq n, k \leq \tilde{n},$$

i.e., the model space projections of the exact eigenvectors with the lowest eigenvalues. Let $U = X\Sigma Y^\dagger$ be the singular value decomposition, and let $V = XY^\dagger$. Then,

$$K_{\text{eff}} = V \text{ diag}(E_0, \cdots, E_\tilde{n}) V^\dagger$$

and

$$C_n^{[m]} := K_{\text{eff}} - \text{ diag}(|m| + 1, 2 + |m| + 1, \cdots, 2\tilde{n} + |m| + 1)$$

is the $(n_1, m_1, m_2)$-block of the effective interaction. If we return to Eqn. (19), the effective interaction matrix elements $C_{n_1,n_2}^{[m]}$ are now given by replacing the matrix elements $C_{n_1,n_2}^{[m]}$ by the matrix elements $C_{n_1,n_2}^{[m]}$, where

$$\tilde{n} = \left\lfloor \frac{R - R_1 - |m|}{2} \right\rfloor, \quad R_1 = N + M - (p + q),$$

where $N, M, p$ and $q$ are defined immediately after Eqn. (19).

### IV. Code Organization and Use

#### A. Overview

The main program is called qdot, and processes a textual configuration file with problem parameters before proceeding with the diagonalization of the Hamiltonian. Eventually, it writes the resulting data to a MATLAB/GNU Octave compatible script for further processing.
As a C++ library as well as stand-alone application, OpenFCI is organized in several namespaces, which logically separate independent units. There are three main namespaces: manybody, gauss, and quantumdot. Put simply, manybody provides generic tools for manybody calculations, such as occupation number formalism, Slater determinants and CSFs, while gauss provides tools for orthogonal polynomials and Gaussian quadrature. These namespaces are independent of each other, and are in no way dependent on the particular quantum dot model. On the other hand, quantumdot synthesizes elements from the two former into a quantum dot FCI library. In qdot, the main work is thus processing of the configuration file.

Two other namespaces are also defined, being simple_sparse and simple_dense, which are, respectively, simple implementations of sparse and dense matrices suitable for our needs. We will not go into details in the present article.

It should be clear that extending and customizing qdot is a relatively easy task. The application qdot is provided as a tool with a minimum of functionality, and the interested will almost certainly desire to further develop this small application.

In order to help with getting started on such tasks, some stand-alone demonstration applications are provided, all based on the core classes and functions. These include an interaction matrix element tabulator tabulate, and a simple program pairing for studying the well-known pairing Hamiltonian \([19]\), which we will not discuss further here. Finally, there is a small interactive console-based Slater determinant demonstration program slater_demo as well. These applications will also serve as indicators of the flexibility of OpenFCI.

OpenFCI does not yet support parallel computation on clusters of computers, using for example the Message Passing Interface \([20]\). Future versions will almost certainly be parallelized, but the present version in fact competes with parallel implementations of the standard FCI method with respect to convergence due to the effective interaction implemented, see Sec. \([\text{IV.C}]\). The simple structure of OpenFCI also allows users with less resources to compile and run the code.

**B. Core functionality**

The manybody namespace currently contains four main classes: Slater, CsfMachine, NChooseKBitset, and MatrixMachine. These will probably form the backbone of any manybody computation with OpenFCI.

The class Slater provides Slater determinants, creation and annihilation operators, and so on. It is based on the standard template library’s (STL) bitset class, which provides generic bit set manipulations. The class NChooseKBitset provides means for generating sets of \(k\) objects out of \(n\) possible represented as bit-patterns, i.e., bit patterns corresponding to Slater determinants in the basis \(\mathcal{B}\) or \(\mathcal{B}'\). This results in a STL vector<Slater> object, which represent Slater determinant bases in OpenFCI.

The class CsfMachine is a tool for converting a basis of Slater determinants into a basis of configurational state functions. These are represented as vector<csf_block> objects, where csf_block is a struct containing a few CSFs associated with the same set of Slater determinants \([9]\).

A CSF basis is again input for the class MatrixMachine, which is a template class, and generates a sparse matrix \(PAP\) of an operator \(A\), where \(P\) projects onto the basis. It also handles bases of pure Slater determinants as they are trivially dealt with in the CSF framework. The template parameter to MatrixMachine is a class that should provide the matrix elements \(h_{\alpha\beta}^\gamma, u_{\alpha\beta}^\gamma\delta\), etc, of the generic operator given by

\[
A = \sum_{\alpha\beta} h_{\alpha\beta} a_\alpha^\dagger a_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} u_{\alpha\beta\gamma\delta} a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta + \frac{1}{3!} \sum_{\alpha\beta\gamma\delta\epsilon\zeta} v_{\alpha\beta\gamma\delta\epsilon\zeta} a_\alpha^\dagger a_\beta^\dagger a_\gamma^\dagger a_\delta^\dagger a_\epsilon a_\zeta.
\]

Notice, that the indices are generic orbitals, and not assumed to be on the form \((a, \sigma)\) as in Eqn. \([9]\).

Currently, only one-, two-, and three-body operators are implemented. The reason is, that the matrix elements are not computed by directly applying the sum of creation- and annihilation operators to Slater determinants, since this approach, however natural, is very inefficient. Instead, we apply Wick’s theorem directly \([8]\) on the matrix elements known to be not identically zero.

In the gauss namespace, several functions are defined which computes sequences of orthogonal polynomials via recurrence relations and weights and abscissa for Gaussian quadratures based on these. The latter is done using the Golub-Welsh algorithm, which only depends on being able to compute the coefficients of the recurrence relation \([12]\). The most important functions are perhaps computeLaguerrePolys() and computeGenHalfGaussHermite(), which computes a sequence of generalized Laguerre polynomials evaluated at a given set of points and quadrature rules for generalized half-range Hermite functions, respectively.

Finally, the quantumdot namespace defines classes and functions that combined define the quantum dot problem. The class RadialPotential encapsulates potentials on the form \([11]\). It also computes effective interaction blocks \(C^{\alpha[m]}\). The class QdotHilbertSpace provides means for generating the bases \(\mathcal{B}\) and \(\mathcal{B}'\), utilizing conservation of angular momentum, using a fast, custom made algorithm independent of NChooseKBitset. The class QdotFci sews everything together and is basically a complete solver for the FCI method with effective interactions.
# ** Simple configuration file for qdot **

# -- model space parameters --
A = 4  # number of particles
M = 0  # angular momentum
S = 0  # total spin * 2
R = 15 # cut of model space

# -- interaction parameters --
lambda = 1.0  # interaction strength

# -- computational parameters --
nev = 50   # no. eigenpairs
use_energy_cut = yes
use_veff = no
matlab_output = results.m

FIG. 2: Simple configuration file for qdot

TABLE I: Some ground state eigenvalues produced by qdot for N = 3,4 electrons with \( \lambda = 2 \). Both the bare and the effective interaction are used

| R   | \( E_0 \)   | \( E_{0,\text{eff}} \) | \( E_0 \)   | \( E_{0,\text{eff}} \) |
|-----|------------|----------------|------------|----------------|
| 6   | 9.02370    | 8.96523        | 13.98824   | 13.88832       |
| 10  | 9.07698    | 8.95555        | 13.86113   | 13.83280       |
| 14  | 9.08800    | 8.95465        | 13.84491   | 13.82848       |
| 18  | 9.06411    | 8.95444        | 13.83923   | 13.82761       |
| 22  | 9.06191    | 8.95435        | 13.83626   | 13.82730       |
| 26  | 9.06049    | 8.95430        | 13.83626   | 13.82730       |
| 30  | 8.95950    | 8.95428        |            |                |

C. Sample runs

A basic configuration file for qdot is shown in Fig. 2. Varying the parameters \( \lambda \), \( R \), \( S \) and the number of particles \( A \), and running qdot each time, we produce a table of ground state energies, shown in Table II. By changing the parameter use_veff we turn on and off the effective interaction. The corresponding effective interaction ground states are also shown in the table. Notice, that with the effective interaction we obtain the same precision as the bare interaction, but with much smaller model spaces. This indicates that OpenFCI can produce results that in fact compete with parallel implementations of the standard FCI method, even in its present serial form.

In Table II we compare the ground state energies reported in Ref. [9] with the alternative model space \( \mathcal{P}' \) to the corresponding values produced by qdot, also using \( \mathcal{P}' \). This Table also appears in Ref. [3], and serves as a check of the validity of the calculations.

By uncommenting the lines following the definition of \( \lambda \), we override the default Coulomb interaction, and produce a configuration file for the analytically solvable model given by Johnson and Payne [3], where the Coulomb interaction is replaced by the parabolic interaction

\[
U(r_{12}) = -\frac{1}{2} \lambda r_{12}^2.
\]

If \( \lambda \) is sufficiently small, all the eigenvalues of this model are on the form

\[
E_{j,k} = 1 + j + (k + N - 1)\sqrt{1 - N\lambda}, \quad j, k \geq 0. \quad (22)
\]

Since the potential is smooth, the eigenfunctions are all smooth, implying exponential convergence with respect to \( R \). We therefore expect very accurate eigenvalues even with moderate \( R \). In Table III we show the first eigenvalues along with the error computed for \( N = 4 \) electrons with \( \lambda = 1/8 \). The computations are done in the \( M = s = s_z = 0 \) model space with \( R = 10 \) and \( R = 15 \). Some duplicates exist, and they are included for illustration purposes. It is evident, that the eigenvalues become very accurate with increasing \( R \); a clear indication of the correctness of the implementation.

V. CONCLUSION AND OUTLOOK

We have presented OpenFCI, an open source full configuration interaction implementation for quantum dots and similar systems. OpenFCI also implements a renormalized effective interaction widely used in nuclear non-core shell model calculations, and we demonstrated that such interactions are indeed useful in the quantum dot calculations as well.

OpenFCI is easy to extend and adapt. Possible applications are computations on systems with more general symmetry-breaking geometries and in \( d = 3 \) spatial dimensions. Also, a generalization of the CSF part of the code to handle isobaric spin would allow us to handle nuclear systems.

There is one more symmetry of the Hamiltonian \( H \) that can be exploited, namely that of conservation of centre-of-mass motion, which would further reduce the block sizes of the matrices. We exploited this symmetry for the effective interaction, but it is a fact that it is a symmetry for the full Hamiltonian as well. Using the energy cut model space \( \mathcal{P} \) we may take care of this symmetry in a way similar to the CSF treatment [21].

As mentioned, we have not parallelized the code at the time of writing, but it is not difficult to do so. A future version will almost certainly provide parallelized executables, for example using the Message Passing Interface [20].
\[ \lambda \quad M \quad 2n \quad \text{Current} \quad \text{Ref. 9} \quad \text{Current} \quad \text{Ref. 9} \quad \text{Current} \quad \text{Ref. 9} \\
\hline
2 \quad 1 \quad 0 \quad 0 \quad 3.013626 \quad \text{3.013626} \quad 3.013626 \quad \text{3.013626} \quad 3.009296 \quad \text{3.009296} \\
2 \quad 2 \quad 0 \quad 0 \quad 3.733598 \quad 3.7338 \quad 3.731057 \quad 3.7312 \quad 3.729324 \quad 3.7295 \\
3 \quad 1 \quad 2 \quad 4.143592 \quad 4.1437 \quad 4.142946 \quad 4.1431 \quad 4.142581 \quad 4.1427 \\
3 \quad 2 \quad 1 \quad 1 \quad 8.175035 \quad 8.1755 \quad 8.169913 \quad 8.1678 \quad 8.1671 \\
4 \quad 1 \quad 1 \quad 11.04480 \quad 11.046 \quad 11.04338 \quad 11.0425 \quad 11.0432 \quad 11.043 \\
4 \quad 2 \quad 2 \quad 23.68944 \quad 23.691 \quad 23.65559 \quad 23.6483 \quad 23.650 \quad 23.65 \\
5 \quad 2 \quad 0 \quad 5 \quad 21.15093 \quad 21.15 \quad 21.13414 \quad 21.13 \quad 21.12992 \quad 21.13 \\
5 \quad 4 \quad 0 \quad 5 \quad 29.43528 \quad 29.44 \quad 29.30898 \quad 29.31 \quad 29.3025 \quad 29.30 \\
\hline
\]
Since $T$ maps eigenfunctions in the two frames onto each other, $T$ must be a unitary operator, and the invariance of $H_0$ under the coordinate transformation is the same as $[H_0, T] = 0$, i.e., that energy is conserved. This in turn means that $T$ is block diagonal with respect to each shell $R = n_1 + n_2$, viz,

$$T\Phi_{R-n_1,n_2} = \sum_{n=0}^{R} (\Phi_{R-n_1,n_2} \Phi_{R-n_1,n_2}) \Phi_{R-n_1,n_2}$$

$$= \sum_{n=0}^{R} T(R,n) \Phi_{R-n_1,n_2}, \quad (A8)$$

where $T(R)$ is the $(R+1) \times (R+1)$ transformation matrix within shell $R$. It is real, symmetric, and orthogonal. Numerically, the matrix elements are conveniently computed using two-dimensional Gauss-Hermite quadrature of sufficiently high order, producing exact matrix elements.

In a two-dimensional setting, the two-particle harmonic oscillator becomes a 4-dimensional oscillator. Let $r'_1 = (x_1, y_1)$, $i = 1, 2$, be the particles’ coordinates, and let $a = (m_1, n_2)$ and $b = (m_2, n_2)$ to compress the notation a little. An eigenfunction is now on the form

$$\Phi_{a,b}(\vec{r}_1, \vec{r}_2) := \Phi_{a}(\vec{r}_1) \Phi_{b}(\vec{r}_2) = CA^m_{n_1} A^n_{n_2} \Psi_{0,0}(\vec{r}_1, \vec{r}_2) \quad (A9)$$

where $C = (m_1!n_1!m_2!n_2)!^{-1/2}$.

The COM coordinate transformation now acts in the $x$ and $y$ directions separately, viz, $F$ acts on $x_i$ and $y_i$ to yield the COM coordinates $\xi_i$ and $\eta_i$: $[\xi_1, \xi_2]^T = F[x_1, x_2]^T$ and $[\eta_1, \eta_2]^T = F[y_1, y_2]^T$. The induced operator $T$ again conserves energy. Let $M = m_1 + m_2$ and $N = n_1 + n_2$. It is readily verifiable that the COM frame transformation becomes

$$T\Psi_{M-m_2, N-n_2, m_2, n_2} := \Psi'_{M-m_2, N-n_2, m_2, n_2}$$

$$= \sum_{p=0}^{M} \sum_{q=0}^{N} T(M,p) T(N,q) \Psi_{M-p, N-q, p, q}. \quad (A10)$$

Note that the shell number is $R = N + M$, which is conserved by $T$.

2. Centre of mass transformation for Fock-Darwin orbitals

Consider a Fock-Darwin orbital $\varphi_{n,m}(\vec{r})$ in shell $R = 2n + |m|$ with energy $R + 1$. It is straightforward but somewhat tedious to show that these can be written in terms of co-called circular raising operators $B_+$ and $B_-$ defined by

$$B_+ := \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & i \\ 1 & -i \end{bmatrix} A_x \quad \text{and} \quad B_- := \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & i \\ 1 & -i \end{bmatrix} A_y \quad (A11)$$

and similarly for $A_{\xi_1}$ in terms of $A_{\xi_2}$. In terms of the raising operators, the COM transformation becomes

$$\varphi'_{n_1,n_2,m_1,m_2} = C (A_{\xi_1} + A_{\xi_2})^m (A_{\eta_1} + A_{\eta_2})^n$$

$$\times (A_{\xi_1} - A_{\xi_2})^m (A_{\eta_1} - A_{\eta_2})^n \Psi_{n,m}(A16)$$

where

$$C = (2n_1! + n_2! + m_1! + m_2! + 1)!^{-1/2} \quad (A17)$$

and we have used Eqn. (A9), but in the analogous COM case. Expanding the powers using the binomial formula (and the fact that the raising operators commute), we obtain a linear combination of the individual eigenfunctions, which must be identical to Eqn. (A10).

Let the COM circular ladder operators be defined by

$$\begin{bmatrix} B_{+}^I \\ B_{-}^I \end{bmatrix} := \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & i \\ 1 & -i \end{bmatrix} \begin{bmatrix} A_{\xi_1} \\ A_{\eta_1} \end{bmatrix} \quad (A18)$$

Using Eqn. (A15), we obtain that the circular raising operators transform in the same way as the Cartesian operators when going to the COM frame, i.e.,

$$\begin{bmatrix} B_{+}^I \\ B_{-}^I \end{bmatrix} = F \begin{bmatrix} B_{+} \\ B_{-} \end{bmatrix} \quad (A19)$$
APPENDIX B: NUMERICAL TREATMENT OF RADIAL PROBLEM

We now briefly discuss the numerical method used for solving the radial problem \([19]\), i.e., the eigenvalue problem for the operator \(K_{|m|}\) defined in Eqn. (20). This is an eigenproblem in the Hilbert space \(L^2([0, \infty), rdr)\), where the measure \(rdr\) is induced by the polar coordinate transformation. The inner product on this space is thus given by

\[
\langle f | g \rangle = \int_0^\infty f(r)g(r)rdr. \tag{B1}
\]

Let the Fock-Darwin orbitals be given by

\[
\varphi_{n,m}(r, \theta) = \frac{e^{im\theta}}{\sqrt{2\pi}} g_n^{\!|m|}(r), \tag{B2}
\]

with radial part

\[
g_n^{\!|m|}(r) := \sqrt{2l_n^{\!|m|}(r^2)} r^{|m|} \exp(-r^2/2) \tag{B3}
\]

Thus,

\[
\langle g_n^{\!|m|} | g_n'^{\!|m'|} \rangle = \delta_{n,n'}, \tag{B4}
\]

gives the Fock-Darwin orbitals as a finite linear combination of the generalized half-range Hermite functions, while the converse is not possible.

Computing the matrix of \(K\) with respect to \(\{f_j(r)\}_{j=0}^\infty\) and diagonalizing will give eigenpairs converging exponentially fast with respect to increasing \(j\). The resulting eigenfunctions’ expansion in \(g_n^{\!|m|}\) are readily computed using Eqn. (B4), whose coefficients \(\langle f_j | g_n^{\!|m|} \rangle\) can be computed numerically exactly using Gaussian quadrature induced by \(P_j(r)\), for \(J\) sufficiently large.

The basis size \(j\) to use in the diagonalization depends on how many eigenfunctions \(n\) we desire. We adjust \(j\) semi-empirically, noting that \(2n + |m|\) is sufficient to resolve \(g_n^{\!|m|}\), and assuming that the exact eigenfunctions are dominated by the latter. We then add a fixed number \(j_0\) to get \(j = 2n + |m| + j_0\), and numerical experiments confirm that this produces eigenvalues that indeed have converged within desired precision.

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[1] S. M. Reimann and M. Manninen, Rev. Mod. Phys 74, 1283 (2002).
[2] The code can be downloaded at: http://folk.uio.no/simenkva/openfci.shtml
[3] S. Kvaal (2008), submitted to Phys. Rev. B., arXiv:0808.2145.
[4] P. Navrátíl, J. Vary, and B. Barrett, Phys. Rev. C 62, 054311 (2000).
[5] See http://www.gnu.org/.
[6] See http://www.doxygen.org/.
[7] N. F. Johnson and M. C. Payne, Phys. Rev. Lett. 67, 1157 (1991).
[8] S. Raines, Many-Electron Theory (North-Holland, 1972).
[9] M. Rontani, C. Cavazzoni, D. Belucci, and G. Goldoni, J. Chem. Phys. 124, 124102 (2006).
[10] E. Anisimovas and A. Matulis, Journal of Physics: Condensed Matter 10, 601 (1998).
[11] J. S. Ball, SIAM Journal on Numerical Analysis 40, 2311 (2003).
[12] G. H. Golub and J. H. Welsch, Math. Comp. 23, 221 (1969), ISSN 00255718.
[13] S. Kvaal (2008), to appear in Phys. Rev. C, arXiv:0808.1832.
[14] M. Hjorth-Jensen, T. Kuo, and E. Osnes, Phys. Rep. 261, 125 (1995).
[15] B. R. Barrett, I. Stetcu, P. Navrátil, and J. P. Vary, Journal of Physics A: Mathematical and General 39, 9983 (2006).
[16] J. Van Vleck, Phys. Rev. 33, 467 (1929).
[17] Kemble, The Fundamental Principles of Quantum Mechanics with Elementary Applications (McGraw Hill, 1937).
[18] M. Taut, Phys. Rev. A 48, 3561 (1993).
[19] I. S. Ball, SIAM Journal on Numerical Analysis 40, 2311 (2003).
[20] See http://www-unix.mcs.anl.gov/mpi/ for a description of the Message Passing Interface standard.
[21] A. Wensauer, M. Korkusinski, and P. Hawrylak, Solid State Communications 130, 115 (2004).
[22] R. Mota, V. D. Granados, A. Queijiro, and J. Garcia, J. Phys. A: Math. Gen. 36, 2979 (2002).
[23] In nuclear physics, it is common to denote by $A$ the number of particles, i.e., the atomic number. The choice of the variable name was chosen also partly because $N$ is used frequently for other purposes in the code.