Institute of Computer Science
University of Augsburg

Bachelor's Thesis

Automatized Eigensolver for General One-body Potentials

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Date:	August 9, 2024

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Abstract

With quantum dots being a popular research topic following the 2023 Nobel Prize in Chemistry, the need to solve the Schrödinger equation for quantum dots has become increasingly important. Due to the variety of shapes and sizes of quantum dots, the potential is often complex and highly dependent on their properties. With this variety, it is difficult to find a sparse set of basis functions that can efficiently represent all quantum dots. For this reason, an adaptive real-space approach based on multiwavelets is used. This allows the dynamic generation of basis functions based on the given potential of the quantum dot. A method for the automatic generation of system-adapted initial guesses is developed and integrated into the automatized eigensolver for general one-body potentials. This automatized eigensolver is written using MADNESS, which ensures a high level of performance and accuracy.

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1 Introduction

2 Quantum dots and the Usage of Basis Sets

2.1 Quantum Dots

2.2 Second Quantization

In this chapter, the concept of second quantization is introduced and explained. To provide a better understanding of the second quantization, the necessary background knowledge about quantum field theory is presented. The chapter begins with an overview of the Fock Space, a mathematical structure used to describe quantum many-body systems. Following this, the creation and annihilation operators are introduced. These operators are essential for representing quantum many-body systems in the second quantization. Finally, the last section demonstrates how quantum many-body systems can be represented in the second quantized form using these operations.

2.2.1 Fock Space

The Fock space provides the fundamental structure for quantum many-body theory. Since this thesis focuses on electrons in a many-body system, the Fock space described here is the fermionic Fock space. Fermions, such as electrons, are particles that obey the Pauli exclusion principle, which states that two or more fermions cannot occupy the same quantum state [2]. This principle results in fermions having antisymmetric wavefunctions.

To describe an N-electron system, the Slater determinant is used. The Slater determinant is the determinant of a matrix whose rows are the single-particle wavefunctions of the electrons and fulfills the anti-symmetry requirement. Let $\{\phi_P(\mathbf{x})\}$ be a set of N orthonormal single-particle wavefunctions where $\mathbf{x}_l$ represents the coordinates of the l-th electron consisting of the spatial and spin coordinates [3]. The Slater determinant for an N-electron system is defined as:

$$\Psi(\phi_{P_1}, \phi_{P_2}, ..., \phi_{P_N}) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{P_1}(\mathbf{x_1}) & \phi_{P_2}(\mathbf{x_1}) & \cdots & \phi_{P_N}(\mathbf{x_1}) \\ \phi_{P_1}(\mathbf{x_2}) & \phi_{P_2}(\mathbf{x_2}) & \cdots & \phi_{P_N}(\mathbf{x_2}) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{P_1}(\mathbf{x_N}) & \phi_{P_2}(\mathbf{x_N}) & \cdots & \phi_{P_N}(\mathbf{x_N}) \end{vmatrix} = |\phi_{P_1}, \phi_{P_2}, ..., \phi_{P_N}| \tag{2.1}$$

With this definition of the Slater determinant, the Fock space can be explained. The Fock space $\mathcal{F}$ is an abstract linear vector space in which the Slater determinant is represented by an occupation-number vector $|\mathbf{k}\rangle$, defined as:

$$|\mathbf{k}\rangle = |k_1, k_2, \ldots, k_N\rangle, \quad k_P = \begin{cases} 1, & \text{if } \phi_P \text{ is occupied} \\ 0, & \text{if } \phi_P \text{ is unoccupied} \end{cases} \tag{2.2}$$

[3]. The occupation-number vectors form an orthonormal basis for the Fock space $\mathcal{F}^N$, where $\sum_{P=1}^N k_P = N$. Each state $|\Psi\rangle$ in the Fock space can be represented as a linear combination of these basis vectors:

$$|\Psi\rangle = \sum_{\mathbf{k}} c_{\mathbf{k}} |\mathbf{k}\rangle = \sum_{P=1}^{N} c_{k_1}, c_{k_2}, \ldots, c_{k_N} |k_1, k_2, \ldots, k_N\rangle \tag{2.3}$$

[1]. The Fock space $\mathcal{F}^N$ can be represented as a direct sum of the subspaces:

$$\mathcal{F}^N = \mathcal{F}^0 \oplus \mathcal{F}^1 \oplus \mathcal{F}^2 \oplus \ldots \oplus \mathcal{F}^N \tag{2.4}$$

where $\mathcal{F}^i$ is the subspace of all occupation-number vectors $|\mathbf{k}\rangle$ for which $\sum_{P=1}^N k_P = i$. The subspace $\mathcal{F}^0$ is the vacuum state in which no single-particle wavefunction is occupied. This subspace contains only the vacuum state $|0\rangle$.

With the Fock space $\mathcal{F}^N$ now defined, the particles in a many-body system can be manipulated using the creation and annihilation operators, which are introduced in the next section.

2.2.2 Creation and Annihilation Operators

The following section introduces the creation and annihilation operators, which are used for creating and destroying particles in the Fock space.

First, the creation operator $a_P^\dagger$ is defined as

$$a_P^\dagger |k_1, k_2, \ldots, 0_P, \ldots, k_N\rangle = \xi_P^{\mathbf{k}} |k_1, k_2, \ldots, 1_P, \ldots, k_N\rangle \tag{2.5}$$

$$a_P^\dagger |k_1, k_2, \ldots, 1_P, \ldots, k_N\rangle = 0 \tag{2.6}$$

where

$$\xi_P^{\mathbf{k}} = \prod_{Q=1}^{P-1} (-1)^{k_Q} \tag{2.7}$$

[1, 3]. The factor $\xi_P^{\mathbf{k}}$ is 1 if the number of occupied states before P is even and -1 if it is odd. The creation operator $a_P^\dagger$ creates a particle in the state ϕ_P if it is unoccupied (2.5) and annihilates the particle if it is already occupied (2.6). This behavior is consistent with the Pauli exclusion principle, which states that if a particle appears twice in the same state, the wavefunction, and thus the Slater determinant, vanishes.

With this definition, every basis state of the Fock space $\mathcal{F}$ can be generated by applying the operator $a_P^\dagger$ repeatedly to the vacuum state $|0\rangle$:

$$|\mathbf{k}\rangle = \prod_{P=1}^{N} (a_P^\dagger)^{k_P} |0\rangle \tag{2.8}$$

Therefore, the operator is called creation operator, as it creates particles in the Fock space by applying it to the vacuum state.

The equations (2.5) and (2.6) can be summarized as:

$$a_P^\dagger |\mathbf{k}\rangle = \delta_{k_P,0} \xi_P^{\mathbf{k}} |k_1, k_2, \ldots, 1_P, \ldots, k_N\rangle \tag{2.9}$$

where $\delta_{k_P,0}$ is the Kronecker delta function, which is 1 if $k_P = 0$ and 0 otherwise.

By applying $a_P^\dagger$ twice on an occupation-number vector, the result is:

$$a_P^\dagger a_P^\dagger |k_1, k_2, \ldots, k_P, \ldots, k_N\rangle = a_P^\dagger \delta_{k_P,0} \xi_P^{\mathbf{k}} |k_1, k_2, \ldots, 1_P, \ldots, k_N\rangle = 0 \tag{2.10}$$

It follows from the equation that the creation operator $a_P^\dagger$ is nilpotent, meaning that applied twice, it results in zero:

$$(a_P^\dagger)^2 = a_P^\dagger a_P^\dagger = 0. \tag{2.11}$$

The order in which the operators are applied is important because the operators do not commute. For $P \neq Q$ and $P < Q$ the following holds:

$$\begin{aligned} a_P^\dagger a_Q^\dagger |\ldots, k_P, \ldots, k_Q, \ldots\rangle &= a_P^\dagger \left(\delta_{k_Q,0} \xi_Q^{\mathbf{k}} |\ldots, k_P, \ldots, 1_Q, \ldots\rangle\right) \\ &= \delta_{k_P,0} \xi_P^{\mathbf{k}} \left(\delta_{k_Q,0} \xi_Q^{\mathbf{k}} |\ldots, 1_P, \ldots, 1_Q, \ldots\rangle\right) \end{aligned} \tag{2.12}$$

Whereas for $P > Q$, the result is:

$$\begin{aligned} a_Q^\dagger a_P^\dagger |\ldots, k_P, \ldots, k_Q, \ldots\rangle &= a_Q^\dagger \left[\delta_{k_P,0} \xi_P^{\mathbf{k}} |\ldots, 1_P, \ldots, k_Q, \ldots\rangle\right] \\ &= \delta_{k_Q,0} \left(-\xi_Q^{\mathbf{k}}\right) \left[\delta_{k_P,0} \xi_P^{\mathbf{k}} |\ldots, 1_P, \ldots, 1_Q, \ldots\rangle\right] \end{aligned} \tag{2.13}$$

The factor $-\xi_Q^{\mathbf{k}}$ results from the additional particle created by the operator $a_P^\dagger$, provided that the particle does not vanish. This is because $a_P^\dagger |\mathbf{k}\rangle$ contains one more particle than $|\mathbf{k}\rangle$ [3]. Altogether, the creation operators are anti-commutative and for all arbitrary occupation-number vectors $|\mathbf{k}\rangle$ and any pair of creation operators, the following holds:

$$a_P^\dagger a_Q^\dagger + a_Q^\dagger a_P^\dagger = \left[a_P^\dagger, a_Q^\dagger\right]_+ = 0. \tag{2.14}$$

[1, 3].

After introducing the creation operator $a_P^\dagger$, the annihilation operator a_P is defined as the adjoint of the creation operator. While the creation operator increases the number of particles in the Fock space, the annihilation operator decreases it. The annihilation operator a_P is defined by:

$$a_P |\mathbf{k}\rangle = \delta_{k_P,1} \xi_P^{\mathbf{k}} |k_1, k_2, \ldots, 0_P, \ldots, k_N\rangle , \tag{2.15}$$

where $\delta_{k_P,1}$ is 1 if $k_P = 1$ and 0 otherwise. The operator annihilates the particle in state ϕ_P if it is occupied and results in zero if the state is unoccupied. For this reason, the operator is called the annihilation operator. Applied to the vacuum state, the outcome is:

$$a_P |0\rangle = 0. \tag{2.16}$$

Since there is no particle to annihilate in the vacuum state, the result is zero. By taking the hermitian adjoint of the equation (2.14), the following relation is obtained:

$$a_P a_Q + a_Q a_P = [a_P, a_Q]_+ = 0. \tag{2.17}$$

Next, the commutation relations between creation and annihilation operators are established by applying these operators to an arbitrary occupation-number vector $|\mathbf{k}\rangle$.

In case the annihilation operator is applied before the creation operator on the same particle, the result is:

$$a_P^\dagger a_P |\mathbf{k}\rangle = \delta_{k_P,1} |\mathbf{k}\rangle . \tag{2.18}$$

This is because if $k_P = 0$, the annihilation operator results in 0 and the creation operator has no effect:

$$a_P^\dagger a_P |k_1, \ldots, 0_P, \ldots, k_N\rangle = a_P^\dagger 0 = 0 \tag{2.19}$$

If $k_P = 1$, the annihilation operator removes the particle and the creation operator then creates the particle again in the same state:

$$\begin{aligned} a_P^\dagger a_P |k_1, \ldots, 1_P, \ldots, k_N\rangle &= a_P^\dagger \left[\xi_P^{\mathbf{k}} |k_1, \ldots, 0_P, \ldots, k_N\rangle\right] \\ &= \left(\xi_P^{\mathbf{k}}\right)^2 |k_1, \ldots, 1_P, \ldots, k_N\rangle = |\mathbf{k}\rangle \end{aligned} \tag{2.20}$$

When the creation operator is applied before the annihilation operator, the result is:

$$a_P a_P^\dagger |\mathbf{k}\rangle = \delta_{k_P,0} |\mathbf{k}\rangle . \tag{2.21}$$

Here, the creation operator results in 0 and the annihilation operator has no effect if $k_P = 1$ and for $k_P = 0$, the creation operator creates a particle and the annihilation operator removes it, resulting in the original state $|\mathbf{k}\rangle$.

With these equations (2.18) and (2.21), the following expression for an arbitrary occupation-number vector $|\mathbf{k}\rangle$ is obtained:

$$(a_P^\dagger a_P + a_P a_P^\dagger)\,|\mathbf{k}\rangle = (\delta_{k_P,1} + \delta_{k_P,0})\,|\mathbf{k}\rangle = |\mathbf{k}\rangle \tag{2.22}$$

with

$$a_P^\dagger a_P + a_P a_P^\dagger = 1. \tag{2.23}$$

After applying the creation and annihilation operators to the same particle of an arbitrary occupation-number vector $|\mathbf{k}\rangle$, the application to different particles is considered. For $P \neq Q$ and $P < Q$, the outcomes are:

$$a_P^\dagger a_Q\,|\ldots, k_P, \ldots, k_Q, \ldots\rangle = \delta_{k_P,0}\xi_P^{\mathbf{k}}\left[\delta_{k_Q,1}\xi_Q^{\mathbf{k}}\,|\ldots, 1_P, \ldots, 0_Q, \ldots\rangle\right] \tag{2.24}$$

$$a_Q a_P^\dagger\,|\ldots, k_P, \ldots, k_Q, \ldots\rangle = \delta_{k_Q,1}\left(-\xi_Q^{\mathbf{k}}\right)\left[\delta_{k_P,0}\xi_P^{\mathbf{k}}\,|\ldots, 1_P, \ldots, 0_Q, \ldots\rangle\right]. \tag{2.25}$$

The factor $-\xi_Q^{\mathbf{k}}$ results from the additional particle created by the operator $a_P^\dagger$, provided that the particle does not vanish. Altogether, for $P < Q$, the following commutation relation holds:

$$a_P^\dagger a_Q + a_Q a_P^\dagger = 0. \tag{2.26}$$

For $P > Q$, the result can be obtained by taking the Hermitian conjugate of (2.25) and renaming the indices. Finally, the commutation relations between the creation and annihilation operators are summarized as:

$$a_P^\dagger a_Q + a_Q a_P^\dagger = \left[a_P^\dagger, a_Q\right]_+ = \delta_{P,Q} \tag{2.27}$$

$$a_P^\dagger a_Q^\dagger + a_Q^\dagger a_P^\dagger = \left[a_P^\dagger, a_Q^\dagger\right]_+ = 0 \tag{2.28}$$

$$a_P a_Q + a_Q a_P = \left[a_P, a_Q\right]_+ = 0 \tag{2.29}$$

After introducing the creation and annihilation operators with their commutation relations, the next section demonstrates how quantum many-body systems can be represented in the second quantized form using these operators.

2.2.3 Second Quantized Representation

The second quantization is a formalism to describe and analyze quantum many-body systems. [1]

3 Eigensolver for General One-body Potentials

Bei ihrer Abschlussarbeit handelt es sich um eine wissenschaftliche Arbeit, die auch entsprechenden Qualit"atsanspr"uchen gen"ugen muss.

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3.1 Methods for Eigensolver

3.2 Approaches to Generate Initial Guess Functions

3.3 Basis Functions for Harmonic Oscillator

3.4 Basis Functions for General Potentials

3.4.1 General Basis Functions

3.4.2 Examples

4 Hartree Fock Approximation

5 Results

6 Conclusion

Bibliography

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