A USING MuQ TO TACKLE FERMION SYSTEMS

Here, we show how to extend MuQ to support the analysis of the fermion system, starting with the extension of MuQ's types and semantics.

A.1 Modeling Fermion Particles

$$\text{Fermion Flag} \quad \aleph \qquad \text{Expression} \quad e ::= v : t^{[\aleph]}(n,m) \mid \alpha : \mathcal{F}^{\zeta}(t^{[\aleph]}(n,m)) \mid \ldots$$

$$t^{\aleph}(n,2) \simeq \aleph(n) \qquad t(\aleph(n)) \simeq \aleph(n) \qquad \text{T-Fem}\ \frac{m_j < 2}{\Gamma \vdash \bigotimes_{j=0}^{n} |m_j\rangle_j \triangleright (\aleph(n))}$$

S-Move

$$za_m^{[\dagger]} : \mathcal{F}^{\zeta}(\iota)\,(z' \bigotimes_{k=0}^{n-1} |j_k\rangle_k) \equiv (\mathcal{S}(\iota)(\bigotimes_{k=0}^{m-1} |j_k\rangle_k) * z * z') \bigotimes_{k=0}^{m-1} |j_k\rangle_k \otimes (a^{[\dagger]}\ |j_m\rangle) \otimes \bigotimes_{k=m+1}^{n-1} |j_k\rangle_k$$

S-TenF

$$\frac{v' = \alpha^{[\dagger]} : \mathcal{F}^{\zeta}(\iota)\, v}{(\alpha^{[\dagger]} : \mathcal{F}^{\zeta}(\iota) \otimes e)\,(v \otimes e') \equiv v' \otimes (\mathcal{S}(\iota)(v')\, e\, e')}$$

$$\mathcal{S}(\aleph(n))(\otimes_k |j_k\rangle) = (-1)^{\sum_k j_k} \qquad \mathcal{S}(t(n,m))(\otimes_k |j_k\rangle) = 1$$

Fig. 16. Extending MuQ Formalism to Fermion Systems. [$\aleph$] means either having or not having $\aleph$.

To extend MuQ for describing fermion particle behaviors, we extend the quantum state type to include a flag $\aleph$, where $t^{\aleph}(n,m)$ type refers to a fermion particle state, and $m = 2$ for any fermion, meaning that every spin only has two states. The anti-commutation property guarantees that every fermion spin is a two-state system. Therefore, we can abbreviate a fermion type $t^{\aleph}(n,2)$ as $\aleph(n)$. The biggest difference between fermions and boson-like particles is the anti-commutation property of fermion quantum states. The concept is that any quantum fermion state ψ can be rewritten to the application of a second quantization formula, containing creators and annihilators, to a $|0\rangle^{\otimes n}$ state. Then, in the second quantization formula, if there are two α_1 and α_2 where $\alpha_1 \neq \alpha_2$, then $\alpha_1\,\alpha_2\,(v : \aleph(n)) = (-1)\alpha_2\,\alpha_1\,(v : \aleph(n))$.

To enforce fermion anti-commutation, we maintain a quantum state in a certain structure by multiplying the correct -1 by a basis-ket. For a quantum state ψ, with many particle sites, each of which contains many spins, we can impose an order to every site in the while state, e.g., a state is arranged as $w_0 \otimes \ldots \otimes w_n$, where each w_k is a basis-ket, and a superposition quantum state can be expanded through the + operation. To apply a matrix operation to v_j, we count the number (m) of $|1\rangle$ vectors for all v_k, such that $k < j-1$, and apply $(-1)^m$ to the state.

To enforce the above counting mechanism, we rewrite semantic rules S-TenF and S-Move to include a function $\mathcal{S}$. The functional implementation of $\mathcal{S}$ shows the polymorphism of the MuQ system and maintains special commutation properties for different kinds of particles, such as boson-like particles and fermions, depending on the types of the particles. For boson-like particles (type $t(n,m)$), the function produces an identity 1, while for fermions (type $\aleph(n)$), the $\mathcal{S}$ function in Figure 16 performs the above counting mechanism. Here, we also need to track the right position of placing j, i.e., imposing the order we manage on the quantum state, to ensure the right counts

can be achieved. To do so, we use rules S-Move and S-TenF to track the right positions for placing a $\mathcal{S}$ function with the right counts.

$$a_\sigma(j)\, z_0\, |m_0\rangle \otimes ... \otimes z_j\, |m_j\rangle \otimes ... \otimes z_n\, |m_n\rangle \equiv (-1)^{\sum_{k=0}^{j-1} m_k} z_0\, |m_0\rangle \otimes ... \otimes z_j (a_\sigma\ |m_j\rangle) \otimes ... \otimes z_n\, |m_n\rangle$$

In the above example, with all sites being $\aleph(1)$ type, the application $a_\sigma(j)$ results in the blue part amplitude sign above, where we compute $\sum_{k=0}^{j-1} m_k$. To apply a_σ to a spin in a single particle basis-ket, we also need to perform such sign manipulation as the $\mathcal{S}$ function in S-Move. The functional implementation of $\mathcal{S}$ permits the polymorphism of the MuQ system, depending on the types of quantum states, i.e., when the type is $t(n, m)$, $\mathcal{S}$ outputs an identity 1. To properly type fermion particles, we need to include the type rule T-Fem to ensure that every spin of a $\aleph(n)$ typed basis-ket is within the range $[0, 1]$.

A.2 Jordan-Wigner Transformation for Fermions

The above section discusses the language features of having fermions. To analyze fermions in a quantum computer, we need to transform the $\aleph(n)$ typed particle system to a $t(1, 2)$ typed system; such compilation is done by Jordan-Wigner transformation. The Jordan-Wigner transformation is a critical tool in quantum mechanics and condensed matter physics. It allows for the mapping between Pauli systems (X, Y, Z) and fermionic/bosonic systems. This transformation is particularly useful in the study of lattice models, as it enables the analysis of spin chains in the language of fermions and facilitates the application of methods and insights from fermionic systems to solve spin-based problems. The Jordan-Wigner transformation is a mapping that allows the transformation of spin operators into fermionic creation and annihilation operators, while the inverse equations are useful to transform creators and annihilators into quantum computers based on Pauli systems.

Jordan-Wigner Transformation for a single lattice site. The Pauli matrices X, Y, and Z form the basis for the spin-$\frac{1}{2}$ operators. These matrices satisfy the commutation and anti-commutation relations.

The identity matrix $\mathbb{I}$ and the zero matrix (O, matrix format: $\left(\begin{smallmatrix} 0 & 0 \\ 0 & 0 \end{smallmatrix}\right)$) are used to represent the unit operator and the null operator, respectively. We now define the anti-commutation relation of the Pauli matrices:

$$\{M, N\} = 2\delta^{MN} I, \quad M, N \in \{X, Y, Z\}$$

Here, δ^{MN} is the Kronecker delta, which is 1 when M and N coincide and 0 otherwise, indicates that the square of each Pauli matrix is the identity matrix $M^2 = I$. In describing the Jordan-Wigner Transformation, much literature describes the raising and lowering operators, which are essentially the $t(1, 2)$ typed creators and annihilators, and their relations with respect to the Pauli operations are given in Section 6.2, as we restate below.

$$a^\dagger : \mathcal{F}^{\mathsf{p}}(t(1,2)) = \frac{1}{2}(X + iY) \qquad a : \mathcal{F}^{\mathsf{p}}(t(1,2)) = \frac{1}{2}(X - iY)$$

The inverse equations above can be used to define $t(1, 2)$ typed Pauli bases X, Y, and Z.

$$\begin{aligned} X &= a^\dagger : \mathcal{F}^{\mathsf{p}}(t(1,2)) + a : \mathcal{F}^{\mathsf{p}}(t(1,2)) \\ Y &= i(a : \mathcal{F}^{\mathsf{p}}(t(1,2)) - a^\dagger : \mathcal{F}^{\mathsf{p}}(t(1,2))) \\ Z &= 2a^\dagger : \mathcal{F}^{\mathsf{p}}(t(1,2))\, a : \mathcal{F}^{\mathsf{p}}(t(1,2)) - I \end{aligned}$$

Jordan-Wigner Transformation for a Particle Site with Many Spins. As we mentioned in Figure 3, a particle could have many spins, forming a chain. Compiling a fermion with n different spins is to compile a $\aleph(n) = t^{\aleph}(n, 2)$ typed system to a $t(1, 2)$ typed Pauli system. We show below the

compilation of a $\aleph(2)$ typed system, but the compilation of a $\aleph(2)$ typed system can be generalized based on the $\aleph(2)$ typed compilation.

$$a_0^\dagger : \mathcal{F}^{\mathsf{p}}(\aleph(2)) = a^\dagger : \mathcal{F}^{\mathsf{p}}(t(1,2)) \otimes I \qquad a_0 : \mathcal{F}^{\mathsf{p}}(\aleph(2)) = a : \mathcal{F}^{\mathsf{p}}(t(1,2)) \otimes I$$

$$a_1^\dagger : \mathcal{F}^{\mathsf{p}}(\aleph(2)) = Z \otimes a^\dagger : \mathcal{F}^{\mathsf{p}}(t(1,2)) \qquad a_1 : \mathcal{F}^{\mathsf{p}}(\aleph(2)) = Z \otimes a : \mathcal{F}^{\mathsf{p}}(t(1,2))$$

The above compilation results satisfy the anti-commutation relations expected of fermionic operators.

$$\{a_0 : \mathcal{F}^{\mathsf{p}}(\aleph(2)), a_0^\dagger : \mathcal{F}^{\mathsf{p}}(\aleph(2))\} = I \qquad \{a_1 : \mathcal{F}^{\mathsf{p}}(\aleph(2)), a_1^\dagger : \mathcal{F}^{\mathsf{p}}(\aleph(2))\} = I$$

In addition, they commute with each other:

$$\{a_0^\dagger : \mathcal{F}^{\mathsf{p}}(\aleph(2)), a_1 : \mathcal{F}^{\mathsf{p}}(\aleph(2))\} = O, \quad \{a_1^\dagger : \mathcal{F}^{\mathsf{p}}(\aleph(2)), a_0 : \mathcal{F}^{\mathsf{p}}(\aleph(2))\} = O$$

The above compilation corresponds to the use of the $\mathcal{S}$ function in our semantics to guarantee the anti-commutation of fermions above, where we first fix the order of particle sites in a one-dimensional ($1D$) plane, and then we multiply -1 to a basis-ket state depending on the counts of the number of occupied spins. In Pauli group representation, multiplication refers to adding Z terms. For systems with more than two spins, the transformation extends to include additional spins.

$$a_0^\dagger : \mathcal{F}^{\mathsf{p}}(\aleph(3)) = a^\dagger : \mathcal{F}^{\mathsf{p}}(t(1,2)) \otimes I \otimes I \qquad a_0 : \mathcal{F}^{\mathsf{p}}(\aleph(3)) = a : \mathcal{F}^{\mathsf{p}}(t(1,2)) \otimes I \otimes I$$

$$a_1^\dagger : \mathcal{F}^{\mathsf{p}}(\aleph(3)) = Z \otimes a^\dagger : \mathcal{F}^{\mathsf{p}}(t(1,2)) \otimes I \qquad a_1 : \mathcal{F}^{\mathsf{p}}(\aleph(3)) = Z \otimes a : \mathcal{F}^{\mathsf{p}}(t(1,2)) \otimes I$$

$$a_2^\dagger : \mathcal{F}^{\mathsf{p}}(\aleph(3)) = Z \otimes Z \otimes a^\dagger : \mathcal{F}^{\mathsf{p}}(t(1,2)) \qquad a_2 : \mathcal{F}^{\mathsf{p}}(\aleph(3)) = Z \otimes Z \otimes a : \mathcal{F}^{\mathsf{p}}(t(1,2))$$

This extension allows the representation of spin interactions in longer quantum chains of particle spins. This compilation pattern is general to define the case for n particle site, e.g., to compile a $\aleph(1)$ system with n particle sites, we perform the following transformation $\gg^1$:

$$a_j : \mathcal{F}^{\mathsf{p}}(\aleph(1)) \gg^1 \bigotimes_{k=0}^{j-1} Z \otimes a : \mathcal{F}^{\mathsf{p}}(t(1,2)) \otimes \bigotimes_{k=j+1}^{n-1} \qquad a_j^\dagger : \mathcal{F}^{\mathsf{p}}(\aleph(1)) \gg^1 \bigotimes_{k=0}^{j-1} Z \otimes a^\dagger : \mathcal{F}^{\mathsf{p}}(t(1,2)) \otimes \bigotimes_{k=j+1}^{n-1}$$

Based on the above analysis, to define the Jordan-Wigner Transformation for an m fermion system as a function $\gg$ in MuQ, as $\gg$: $\mathcal{F}^{\zeta}(\bigotimes^m \aleph(n)) \to \mathcal{F}^{\zeta}(\bigotimes^m t(1,2))$, the function is a two-step function. The first step is a function $\gg^n$ to rearrange the particle spins, each of which is viewed as an individual particle site after the transformation, i.e., we compile a $\aleph(n)$ to $\aleph(1)$ typed system. To do so, we utilize the same methodology in Section 6.2 to turn the one-dimensional particle chain into a two-dimensional and then flatten the two-dimensional system to one-dimensional by enlarging the particle site size, e.g., the transformation produces a $m * n$ size participle system. For any operation j-th operation $op(j)$ in the original $\aleph(n)$, we transform to operations indexed as s $(j,0)...(j,n)$, as $op'_0(j,0)...op'_n(j,n)$; we then flatten the $2D$ system to one dimensional through index reordering. After the transformation, we can simply utilize the $\gg^1$ transformation function to transform the $\alpha(1)$ typed system to $t(1,2)$ type. Thus, the $\gg$ transformation can be defined as $\gg^1$ ($\gg^n$), the composition of $\gg^n$ and $\gg^1$.

B A HUBBARD MODEL FOR HYDROGEN CHAINS

The Hubbard model (system) describes the interactions between elementary particles, specifically focusing on the electrons having fermion behaviors. Here, we focus on the one-dimensional Hydrogen chain, one of the most quintessential systems described using the Hubbard system, which consists of many sites of $\aleph(2)$ typed Hydrogen atoms (fermions). Equation (3.2.2) describes the Hamiltonian for this system.

There are two terms in the Hamiltonian. The first accounts for the energy due to the movement (hopping) of electrons, whereas the second term accumulates the energy due to electron repulsion. As the atoms are arranged in a one-dimensional array, the electrons can only move (hop) to the neighboring adjacent atoms, such as moving from j-th to j+1-th site, in this system.

In simulating the Hubbard system, users typically try to manipulate different z_t and z_u values for using the Hubbard system to analyze different particle behaviors. In simulating the Hydrogen chain [Melo et al. 2021], we assign a constant to z_t and make z_u depending on the time periods. For a period of T. z_u will transit from the initial value z_{u0} at time $t = 0$ to the final value Z_{uf} at time $t = T$, and the equation looks like $z_u(t) = (1 - \frac{t}{T})z_{u0} + \frac{t}{T}z_{uf}$. The naive compilation of the Hubbard system is similar to the one described in Section 6.2, except that we also need to include Z terms by enforcing anti-commutation. To better compile the system, previous researchers [Melo et al. 2021] tried to use unconventional quantum state mapping from a $\aleph(2)$ typed state to a $t(1, 2)$ typed qubit state. For example, for a two-particle system, they utilize an optimized state mapping as follows.

$$|1\rangle_0 |1\rangle_1 \otimes |0\rangle_0 |0\rangle_1 \rightarrow |0\rangle |0\rangle \qquad |1\rangle_0 |0\rangle_1 \otimes |0\rangle_0 |1\rangle_1 \rightarrow |0\rangle |1\rangle$$
$$|0\rangle_0 |1\rangle_1 \otimes |1\rangle_0 |0\rangle_1 \rightarrow |1\rangle |0\rangle \qquad |0\rangle_0 |0\rangle_1 \otimes |1\rangle_0 |1\rangle_1 \rightarrow |1\rangle |1\rangle$$

They assume that the other basis-ket states do not exist. With the unconventional mapping, they can rewrite the Hubbard system to an Ising system as:

$$\hat{H_S} = -z_t(X \otimes I + I \otimes X) + z_u Z \otimes Z$$

The compilation of this new optimized system is similar to the one in Section 5.2, i.e., through Trotterization, the simulation of the system generates a series of X-axis rotation gate Rx as well as ZZ interaction gates.

Determining the Parameters z_t and z_u in Hubbard System. The parameters z_t and z_u in the Hubbard system are crucial for accurately describing the physical system. For a $1D$ chain of hydrogen atoms, these parameters can be determined as follows:

1. **Hopping Integral** z_t: The hopping integral z_t represents the kinetic energy associated with an electron hopping from one site to another. It can be estimated using the overlap integral of the atomic orbitals on neighboring sites. For hydrogen atoms, the 1s orbitals are used. The hopping integral can be calculated as:

$$z_t = \int \psi_{1s}^*(r - R_i)\hat{H}\psi_{1s}(r - R_j)\, dr$$

where $\psi_{1s}(r)$ is the 1s orbital wave function, $\hat{H}$ is the Hamiltonian of the system, and R_i and R_j are the positions of the neighboring atoms. In practice, this integral is often approximated using empirical or computational methods, such as density functional theory (DFT).

2. **On-Site Interaction** z_u: The on-site interaction z_u represents the Coulomb repulsion between two electrons occupying the same site. For hydrogen atoms, this can be approximated using the Coulomb integral:

$$z_u = \int \psi_{1s}^*(r_1)\psi_{1s}^*(r_2)\frac{e^2}{|r_1 - r_2|}\psi_{1s}(r_1)\psi_{1s}(r_2)\, dr_1\, dr_2$$

where e is the electron charge, and $\psi_{1s}(r)$ is the 1s orbital wave function. This integral can also be evaluated using computational techniques, providing an estimate of the electron repulsion energy at each site.

C QUANTUM MECHANICS

C.1 Hilbert Space $\mathcal{H}$

A complex vector space with an inner product satisfying:

- Conjugate Symmetry: $\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*$
- Linearity: $\langle\psi|a\phi + b\chi\rangle = a\langle\psi|\phi\rangle + b\langle\psi|\chi\rangle$, where a and b are complex numbers.
- Positive Definiteness: $\langle\psi|\psi\rangle \geq 0$ and the equality holds, if and only of $|\psi\rangle = 0$.

C.2 Completeness

Every Cauchy sequence $\{|\psi_n\rangle\}$ in $\mathcal{H}$ converges to an element in $\mathcal{H}$. A Cauchy sequence is defined where, for every $\epsilon > 0$, there exists an N such that $|\psi_n - \psi_m| < \epsilon$ for all $m, n > N$. (For finite-dimensional Hilbert spaces, the completeness requirement is trivially satisfied.)

C.3 Composite Systems

- Direct Sum ($\oplus$): Represents the combination of two independent quantum systems described by Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$. The direct sum space $\mathcal{H}_1 \oplus \mathcal{H}_2$ consists of all ordered pairs $|\psi_1\rangle, |\psi_2\rangle$ where $|\psi_1\rangle \in \mathcal{H}_1$ and $|\psi_2\rangle \in \mathcal{H}_2$. It represents scenarios where the systems do not interact or influence each other.
- Tensor Product ($\otimes$): Describes the space for composite quantum systems. The tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$ is formed by combining elements from $\mathcal{H}_1$ and $\mathcal{H}_2$ such that every pair of vectors $|\psi_1\rangle \in \mathcal{H}_1$ and $|\psi_2\rangle \in \mathcal{H}_2$ contributes a new vector $|\psi_1\rangle \otimes |\psi_2\rangle$ to $\mathcal{H}_1 \otimes \mathcal{H}_2$. This space encompasses all possible states of the combined system, including entangled states.

C.4 Operators

- Direct Sum: For operators $\hat{A}, \hat{B}$, the direct sum $(\hat{A} \oplus \hat{B})$ acts on each component of the direct sum space independently: $(\hat{A} \oplus \hat{B})(|\psi_1\rangle, |\psi_2\rangle) = (\hat{A}|\psi_1\rangle, \hat{B}|\psi_2\rangle)$.
- Tensor Product: For operators $\hat{A}, \hat{B}$, the tensor product $(\hat{A} \otimes \hat{B})$ combines the actions of each operator on the respective Hilbert spaces: $(\hat{A} \otimes \hat{B})(|\psi_1\rangle \otimes |\psi_2\rangle) = (\hat{A}|\psi_1\rangle) \otimes (\hat{B}|\psi_2\rangle)$.
- Hermitian Operators: An operator $\hat{A}$ is Hermitian if it equals its own adjoint: $\hat{A} = \hat{A}^\dagger$. This means for all vectors $|\psi\rangle, |\phi\rangle$ in $\mathcal{H}$, we have $\langle\psi|\hat{A}|\phi\rangle = \langle\hat{A}\psi|\phi\rangle^*$. Hermitian operators represent observable quantities in quantum mechanics and have real eigenvalues.
- Unitary Operators: An operator $\hat{U}$ is Unitary if its inverse is its adjoint: $\hat{U}^{-1} = \hat{U}^\dagger$. This implies $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \hat{I}$, where $\hat{I}$ is the identity operator. Unitary operators preserve the inner product and are used to describe the time evolution and symmetries in quantum systems.
- Projection Operators: A Projection operator $\hat{P}$ satisfies $\hat{P}^2 = \hat{P}$ and $\hat{P} = \hat{P}^\dagger$. These operators project vectors onto a subspace of the Hilbert space. If $|\phi\rangle$ is a vector in the space, then $\hat{P}|\phi\rangle$ is the projection of $|\phi\rangle$ onto the subspace defined by $\hat{P}$.

C.5 Fundamental Postulates of Quantum Mechanics

(1) State Postulate: Every quantum system is completely described by its state vector, which is a unit vector in a complex Hilbert space $\mathcal{H}$. The state vector is represented as $|\psi\rangle$. In mathematical terms: $|\psi\rangle \in \mathcal{H}$, with $\langle\psi|\psi\rangle = 1$.

(2) Observable Postulate: Physical observables in quantum mechanics are represented by Hermitian operators (denoted as $\hat{A}, \hat{B}, \hat{C}, \ldots$) acting on the Hilbert space $\mathcal{H}$. The possible measurement outcomes of an observable correspond to the eigenvalues of its associated Hermitian operator. Mathematically, if $\hat{A}$ is an observable, and λ is a measurement outcome, then: $\hat{A}|a\rangle = \lambda|a\rangle$, where $|a\rangle \in \mathcal{H}$.

(3) Measurement Postulate: If an observable $\hat{A}$ with non-degenerate eigenvalues is measured in a system in state $|\psi\rangle$, the probability of obtaining eigenvalue λ is given by $|\langle a|\psi\rangle|^2$, where $|a\rangle$ is the eigenvector of $\hat{A}$ associated with λ. After the measurement, the state of the system collapses to $|a\rangle$. For a normalized state, this is expressed as: $P(\lambda) = |\langle a|\psi\rangle|^2$, Post-measurement state: $|\psi'\rangle = \frac{\hat{P}_a|\psi\rangle}{\sqrt{\langle\psi|\hat{P}_a|\psi\rangle}}$ where $\hat{P}_a = |a\rangle\langle a|$ is the projection operator onto the state $|a\rangle$.

(4) Evolution Postulate: The time evolution of a quantum state is governed by the Schrödinger equation. If $|\psi(t)\rangle$ describes the state of the system at time t, then its time evolution is given by: $i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$ where $\hat{H}$ is the Hamiltonian operator of the system, which corresponds to the total energy observable.

For further details, see [Dirac 1958; Eisberg and Resnick 1985; Griffiths 2005].

D QUANTUM MECHANICS REPRESENTATIONS

D.1 Position Representation

In the position representation, states are expressed as wave functions $\psi(x)$ in real space, where x denotes the position. The wave function gives the probability amplitude for finding a particle at position x. The position operator $\hat{x}$ and the momentum operator $\hat{p}$ are represented as:

$$\hat{x}\psi(x) = x\psi(x), \tag{1}$$

$$\hat{p}\psi(x) = -i\hbar\frac{d}{dx}\psi(x). \tag{2}$$

D.2 Momentum Representation

In the momentum representation, states are described as wave functions $\phi(p)$ in momentum space. The operators are represented as:

$$\hat{p}\phi(p) = p\phi(p), \tag{3}$$

$$\hat{x}\phi(p) = i\hbar\frac{d}{dp}\phi(p). \tag{4}$$

D.3 Energy Representation

In systems with a well-defined Hamiltonian, states can be represented in terms of energy eigenstates. This representation is particularly useful for solving the Schrödinger equation.

D.4 Second Quantization (Occupation Number Representation)

Second quantization, or the occupation number representation, describes systems with variable numbers of indistinguishable particles by the number of particles occupying each possible state, referred to as a mode. The state of a system can be represented as:

$$|n_1, n_2, n_3, \ldots\rangle \tag{5}$$

Creation ($\hat{a}_i^\dagger$) and annihilation ($\hat{a}_i$) operators, which satisfy commutation or anticommutation relations for bosons and fermions, respectively, are introduced to change the occupation numbers of the modes.

D.4.1 Commutation Properties and Actions of Creation and Annihilation Operators. The creation and annihilation operators play a crucial role in the framework of second quantization, with their actions and commutation or anticommutation relations defined based on the type of particles (bosons or fermions).

For Bosons:

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}, \tag{6}$$

$$[\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0. \tag{7}$$

For Fermions:

$$\{\hat{a}_i, \hat{a}_j^\dagger\} = \delta_{ij}, \tag{8}$$

$$\{\hat{a}_i, \hat{a}_j\} = \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0. \tag{9}$$

E MANY-PARTICLE QUANTUM MECHANICS

Many-particle quantum mechanics underpins the theoretical framework necessary for understanding phenomena across condensed matter physics, chemical systems, and nuclear physics. Traditional wave function approaches scale poorly with the number of particles due to the combinatorial explosion of configuration space. Second quantization addresses these complexities by focusing on occupation numbers and field operators rather than individual particle coordinates, thus offering a scalable approach to studying systems of identical particles.

E.1 Second Quantization in Many-Particle Quantum Mechanics

Second quantization transcends the limitations of first quantization by introducing a more abstract but immensely powerful framework, ideally suited for systems of identical particles, like electrons in a metal or photons in electromagnetic fields.

E.1.1 Creation and Annihilation Operators. Central to the formalism are the creation ($\hat{c}_{i,\sigma}^\dagger$) and annihilation ($\hat{c}_{i,\sigma}$) operators, which respectively add and remove particles from quantum states. These operators are defined for each quantum state labeled by index i and spin σ, following specific algebraic rules:

For fermions (e.g., electrons), the anticommutation relations are:

$$\{\hat{c}_{i,\sigma}, \hat{c}_{j,\sigma'}^\dagger\} = \delta_{ij}\delta_{\sigma\sigma'},$$

$$\{\hat{c}_{i,\sigma}, \hat{c}_{j,\sigma'}\} = \{\hat{c}_{i,\sigma}^\dagger, \hat{c}_{j,\sigma'}^\dagger\} = 0,$$

reflecting the Pauli exclusion principle, ensuring no two fermions can occupy the same quantum state.

For bosons, the commutation relations are:

$$[\hat{b}_i, \hat{b}_j^\dagger] = \delta_{ij},$$

$$[\hat{b}_i, \hat{b}_j] = [\hat{b}_i^\dagger, \hat{b}_j^\dagger] = 0,$$

allowing any number of bosons to occupy the same state.

E.1.2 Fock Space and Quantum States. Fock space, or the state space of many-body systems, is constructed from the vacuum state $|0\rangle$, which contains no particles. States with particles are built by applying creation operators to the vacuum:

$$|n_{1,\uparrow}, n_{1,\downarrow}, n_{2,\uparrow}, \ldots\rangle = \prod_i (\hat{c}_i^\dagger)^{n_i} |0\rangle,$$

Here, $n_{i,\sigma}$ are occupation numbers indicating how many particles occupy the state specified by i and σ. For fermions, $n_{i,\sigma}$ can be either 0 or 1, while for bosons, it can be any non-negative integer.

E.1.3 Operators in Fock Space. Within Fock space, physical observables are represented by operators constructed from the creation and annihilation operators. The number operator $\hat{n}_{i,\sigma} = \hat{c}^\dagger_{i,\sigma}\hat{c}_{i,\sigma}$ counts the number of particles in state (i, σ).

The total number operator for the system is:

$$\hat{N} = \sum_{i,\sigma} \hat{n}_{i,\sigma},$$

which sums the occupation numbers across all states.

The kinetic energy of particles hopping between lattice sites or states can be modeled as:

$$\hat{T} = \sum_{ij,\sigma} t_{ij}\hat{c}^\dagger_{i,\sigma}\hat{c}_{j,\sigma},$$

where t_{ij} represents the kinetic energy matrix elements, indicating the probability amplitude for a particle to hop from state j to state i.

Potential energy terms, often arising from external fields or intrinsic properties, are represented as:

$$\hat{V} = \sum_{i,\sigma} V_i \hat{n}_{i,\sigma},$$

where V_i denotes the potential energy associated with particles in state i.

Interaction terms, particularly relevant in electron systems for capturing Coulomb repulsion, take the form:

$$\hat{H}_{\text{int}} = \frac{1}{2}\sum_{ijkl}\sum_{\sigma,\sigma'} U_{ijkl}\hat{c}^\dagger_{i,\sigma}\hat{c}^\dagger_{j,\sigma'}\hat{c}_{l,\sigma'}\hat{c}_{k,\sigma},$$

where U_{ijkl} are the elements of the interaction matrix, encapsulating the strength and nature of particle-particle interactions within the many-body system.

E.1.4 Quantum Statistics and Symmetry. The statistical properties of particles in quantum mechanics — Fermi-Dirac for fermions and Bose-Einstein for bosons — naturally emerge from the anticommutation and commutation relations of the creation and annihilation operators. This elegant unification underlies the power of second quantization, encapsulating the quantum statistics inherently without imposing them externally.

Moreover, the symmetries of physical systems, such as translational, rotational, and spin symmetries, can be systematically explored within this framework by examining the commutation relations of the Hamiltonian with relevant symmetry operators, leading to conservation laws and selection rules essential for understanding quantum dynamics and spectra.

E.2 Conclusion

The second quantization formalism provides a potent and versatile approach to describing and analyzing many-body quantum systems. By transcending the limitations of traditional wave function approaches, it lays the groundwork for a deeper understanding of complex quantum phenomena, from superfluidity and superconductivity to quantum magnetism and beyond. For further details, see [Altland and Simons 2010; Fetter and Walecka 2003; Negele and Orland 1998].

F OTHER PHYSICAL MODELS DEFINABLE IN MuQ

Here, we show many other systems that are definable in MuQ.

F.1 Ising Model

The Ising model is one of the simplest quantum spin lattice models. It considers spins that can be in one of two states (up or down) interacting with their nearest neighbors. The Hamiltonian for the quantum Ising model in a transverse field is given by:

$$H = -J \sum_{\langle i,j \rangle} Z(i)Z(j) - h \sum_{i} X(i) \tag{10}$$

where J represents the interaction strength between neighboring spins, h is the external magnetic field (which is a constant), and the sum $\langle i, j \rangle$ runs over all pairs of nearest neighbors.

F.2 Heisenberg Model

The Heisenberg model includes interaction in all three spin components. Its Hamiltonian is expressed as:

$$H = -J \sum_{\langle i,j \rangle} (X(i)X(j) + Y(i)Y(j) + Z(i)Z(j)) \tag{11}$$

In this model, J represents the interaction strength, and the S terms are spin-$\frac{1}{2}$ operators, allowing for complex spin interactions.

F.3 XY Model

The XY model restricts interactions to the X and Y axis components. Its Hamiltonian is:

$$H = -J \sum_{\langle i,j \rangle} (X(i)X(j) + Y(i)Y(j)) \tag{12}$$

The quantum spin lattice models are fundamental for understanding quantum phase transitions, magnetic properties, and many-body quantum phenomena. They provide a rich framework for exploring quantum correlations, entanglement, and the effects of quantum fluctuations on macroscopic systems.

F.4 t-J Model

The t-J model is a pivotal framework in condensed matter physics for exploring high-temperature superconductivity in cuprate materials. Originating from the Hubbard model in the limit of strong on-site Coulomb repulsion, it prohibits double occupancy of lattice sites, thereby allowing for a focused analysis of electron hopping and spin interactions. This approach is key to understanding superconductivity and magnetism in strongly correlated electron systems.

Hilbert Space. The Hilbert space $\mathcal{H}$ excludes states with double occupancy. Basis states $|s_1, s_2, ..., s_N\rangle$ represent each site as empty (0), occupied by an electron with spin up ($\uparrow$), or spin down ($\downarrow$). This space is formally defined as:

$$\mathcal{H} = \{|s_1, s_2, ..., s_N\rangle : s_i \in \{0, \uparrow, \downarrow\} \, \forall \, i\}$$

Hamiltonian. The Hamiltonian H includes terms for electron mobility and spin interactions:

$$H = -t \sum_{\langle ij \rangle, \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma}) + J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j)$$

Hopping Term ($-t$). Allows electrons to move between adjacent sites, governed by:

$$-t \sum_{\langle ij \rangle, \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma})$$

Spin-Spin Interaction Term (J). Models antiferromagnetic interactions:

$$J \sum_{\langle ij \rangle} (\mathrm{S}_i \cdot \mathrm{S}_j - \frac{1}{4} n_i n_j)$$

Operator Actions.

Creation and Annihilation Operators.

$$c_{i\sigma}^{\dagger}|0\rangle_i = |\sigma\rangle_i, \quad c_{i\sigma}|\sigma\rangle_i = |0\rangle_i$$

Number Operator (n_i).

$$n_i = n_{i\uparrow} + n_{i\downarrow} = c_{i\uparrow}^{\dagger} c_{i\uparrow} + c_{i\downarrow}^{\dagger} c_{i\downarrow}$$

Spin Operators and Pauli Matrices.

$$S_i^x = \frac{\hbar}{2}\sigma_x, \quad S_i^y = \frac{\hbar}{2}\sigma_y, \quad S_i^z = \frac{\hbar}{2}\sigma_z$$

For further details, see [Anderson 1997; Auerbach 1994; Sachdev 2011].

t-J Model in MuQ. The program definition for the t-J model Hamiltonian in MuQ is as follows:

$$-c_t \textstyle\sum_{i,\sigma\in\{\uparrow,\downarrow\}} [a_\sigma^*(i)a_\sigma(i+1) + a_\sigma^*(i+1)a_\sigma(i)] +$$
$$c_J \textstyle\sum_i [\frac{1}{2}\sigma_\uparrow^*(i)\sigma_\uparrow(i)\sigma_\downarrow^*(i+1)\sigma_\downarrow(i+1) - \frac{1}{4}(a_{i\uparrow}^* a_{i\uparrow} + a_{i\downarrow}^* a_{i\downarrow}) \cdot (a_{i+1\uparrow}^* a_{i+1\uparrow} + a_{i+1\downarrow}^* a_{i+1\downarrow})]$$

The t-J model's hopping (t) term is the same as the one of the Hubbard model. c_t and c_J are some constant numbers [7]. The i index in an operator, e.g., $a_\sigma^*(i)$, is also a syntactic sugar of the tensor composition ($\otimes$) of identities $\mathbb{1}$. Matrix multiplications and Summations function the same as we mentioned in the overview with the Hubbard model example.

Transformed t-J Model. The Jordan-Wigner transformation allows us to map the fermionic operators in the t-J model into spin operators. Below is the transformed t-J model for a one-dimensional lattice system.

Hopping Term. The fermionic hopping terms in the t-J model are transformed as follows:

$$-t \sum_{\langle i,j \rangle} \left(\exp\left(i\pi \sum_{l=i}^{j-1} n_l \right) S_i^+ S_j^- + \text{h.c.} \right), \tag{13}$$

where S_i^+ and S_j^- are spin raising and lowering operators at sites i and j, respectively. The term $n_l = \frac{1}{2}(1 - \sigma_l^z)$ corresponds to the number operator after transformation, and the exponential term arises due to the non-local string of σ^z operators, ensuring the preservation of fermionic anticommutation relations.

Spin-Spin Interaction Term. The exchange interaction term, crucial in the t-J model, transforms into:

$$J \sum_{\langle i,j \rangle} \left(\frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) + S_i^z S_j^z \right), \tag{14}$$

where the terms now involve combinations of the spin raising, lowering, and z-component operators, indicative of the transformed spin interactions.

[7] c_t represents hopping integral and c_u represents electron repulsion

G BRAVYI-KITAEV TRANSFORMATION

The Bravyi-Kitaev transformation offers an alternative to the Jordan-Wigner transformation, providing a more efficient mapping of fermionic operators to qubits for certain quantum simulation tasks. This transformation is particularly beneficial for quantum computation, where it can lead to reduced gate counts in quantum algorithms.

G.1 Fundamentals of the Bravyi-Kitaev Transformation

The Bravyi-Kitaev transformation redefines fermionic creation and annihilation operators in terms of Pauli operators, in a manner that maintains the anticommutation relations while optimizing the locality of terms. For a system of N fermionic modes, the transformation can be expressed as:

$$\hat{c}_j \to \frac{1}{2}(\hat{Q}_j\hat{X}_j + i\hat{Q}_j\hat{Y}_j), \quad \hat{c}_j^\dagger \to \frac{1}{2}(\hat{Q}_j\hat{X}_j - i\hat{Q}_j\hat{Y}_j),$$

where $\hat{X}_j$, $\hat{Y}_j$, and $\hat{Q}_j$ are products of Pauli matrices that encode the fermionic anticommutation relations into qubit operations. The exact form of $\hat{Q}_j$ depends on the specific fermionic mode j and the chosen encoding.

G.2 Transformed t-J Model

In the context of the t-J model, the Bravyi-Kitaev transformation enables the efficient simulation of electron dynamics and spin interactions on a quantum computer. The transformed Hamiltonian in the Bravyi-Kitaev framework for the t-J model takes the form:

$$H_{\text{t-J}}^{\text{BK}} = -t \sum_{\langle i,j\rangle,\sigma} \left(\frac{1}{2}(\hat{Q}_i\hat{X}_i - i\hat{Q}_i\hat{Y}_i)\frac{1}{2}(\hat{Q}_j\hat{X}_j + i\hat{Q}_j\hat{Y}_j) + \text{h.c.} \right) + J \sum_{\langle i,j\rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right),$$

where $\mathbf{S}_i$ and n_i are expressed in terms of qubit operators using the Bravyi-Kitaev encoding. The hopping terms (t) and the spin-spin interaction terms (J) now involve the manipulation of qubits instead of fermions, which is more natural for quantum computational frameworks.

The Bravyi-Kitaev transformation offers improved scaling of quantum resources compared to the Jordan-Wigner transformation and can be crucial for implementing quantum simulations of condensed matter systems in practice.

The Bravyi-Kitaev transformation provides a significant advantage in quantum simulation by mapping fermionic algebra to qubit operations more efficiently than the Jordan-Wigner transformation. It is especially useful in the context of quantum computing, where it enables more effective resource utilization and can potentially lead to faster quantum algorithms for simulating many-particle systems in condensed matter physics.