1 Rewriting Creation and Annihilation Operators in a New Basis

Recall that any state $|\tilde{\lambda}\rangle$ can be rewritten in another basis $|\lambda\rangle$ as:

$$|\tilde{\lambda}\rangle = \sum_{\lambda} \langle \lambda | \tilde{\lambda} \rangle |\lambda\rangle$$

In second quantization such a state can be written as:

$$|\tilde{\lambda}\rangle = a^{\dagger}_{\tilde{\lambda}}|0\rangle = \sum_{\lambda} \langle \lambda | \tilde{\lambda} \rangle a^{\dagger}_{\lambda}|\lambda\rangle$$

Where we only used that states are built from the vacuum. From this we may read off how creation operators transform:

$$a^{\dagger}_{\tilde{\lambda}} = \langle \lambda | \tilde{\lambda} \rangle a^{\dagger}_{\lambda}; \quad a_{\tilde{\lambda}} = \langle \tilde{\lambda} | \lambda \rangle a_{\lambda}$$

In the exact same way we find that for fermions:

$$c^{\dagger}_{\tilde{\lambda}} = \langle \lambda | \tilde{\lambda} \rangle c^{\dagger}_{\lambda}; \quad c_{\tilde{\lambda}} = \langle \tilde{\lambda} | \lambda \rangle c_{\lambda}$$

We note that $|\lambda\rangle$ are any type of normalized single-body states.

2 Single-Body Operators in Second Quantization

A single-body operator is an operator $\hat{O}_1$ that has the form:

$$\hat{O}_1 = \sum_{n=1}^{N} \hat{o}_n$$

Where $\hat{o}_n$ only acts on particle n.
Examples:

$$\hat{o}_n = \frac{\vec{p}_n^{\,2}}{2m}; \quad \hat{o}_n = V(\vec{r}_n)$$

Now take $\hat{O}_1$ as diagonal in a basis $|\lambda_i\rangle$ such that:

$$\hat{O}_1 = \sum_{n=1}^{N} o_n |\lambda_n\rangle\langle\lambda_n|; \quad \hat{n}_{\lambda_n} = a^{\dagger}_{\lambda_n} a_{\lambda_n}$$

Where $o_n = \langle \lambda_n | \hat{o}_n | \lambda_n \rangle$ are eigenvalues of $\hat{o_n}$ that correspond to the state $|\lambda_n\rangle$. In this case we may compute matrix elements of a many-body state $|n_{\lambda_1}, n_{\lambda_2}, \ldots\rangle$ as:

$$\langle n_{\lambda_1}, n_{\lambda_2}, \ldots | \hat{O}_1 | n_{\lambda_1}, n_{\lambda_2}, \ldots \rangle = \sum_{n=1}^{N} o_n n_{\lambda_n} \langle n_{\lambda_1}, n_{\lambda_2}, \ldots | n_{\lambda_1}, n_{\lambda_2}, \ldots \rangle = \sum_{n=1}^{N} o_n n_{\lambda_n}$$

We get the same result if:

$$\hat{O}_1 = \sum_{m=1}^{N} o_m n_{\lambda_m} = \sum_{m=1}^{N} o_m a^{\dagger}_{\lambda_m} a_{\lambda_m}$$

We can of course also rewrite this in an arbitrary basis to find:

$$\hat{O}_1 = \sum_{\mu\nu} \langle \mu | \hat{o} | \nu \rangle a_\mu^\dagger a_\nu$$

Here again we stress that $|\nu\rangle$ and $|\mu\rangle$ are any single particle states.

3 Two-Body Operators in Second Quantization

A similar thing can be done for two-body operators of the form:

$$\hat{O}_2 = \sum_{ij} \hat{o}_{ij}$$

Here $\hat{o}_{ij}$ acts on two particles i and j.
Example:

$$\hat{o}_{ij} = \frac{e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{r}_j|}$$

After some similar computations that are similar to the ones for the one body operator (see Altland and Simons for details) one may find that:

$$\hat{O}_2 = \frac{1}{2} \sum_{\lambda\lambda'\mu\mu'} \langle \mu\mu' | \hat{o}_{ij} | \lambda\lambda' \rangle a_\mu^\dagger a_{\mu'}^\dagger a_\lambda a_{\lambda'}$$

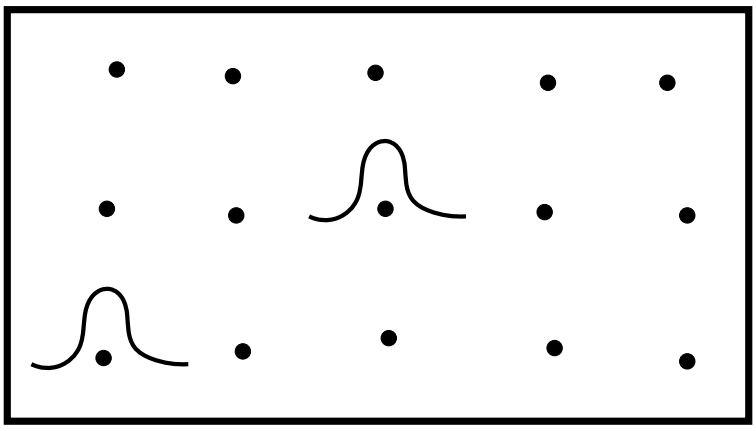
Again we stress that $|\mu\rangle$ etc. are single particle states, which could for instance be obtained by DFT.

4 Typical and Useful Choices of One-Particle Basis

1. Position basis.
Example:

$$H = \sum_i \frac{\vec{p}_i^2}{2m} + V(\vec{r}) \rightarrow H = \int d^d r a^\dagger(\vec{r}) [-\frac{\nabla^2}{2m} + V(\vec{r})] a(\vec{r})$$

2. Wannier basis:



For a lattice of atoms one can find basis that is localized on atoms - so- called Wannier basis. This basis is often well-approximated by orbitals so you may think of it as something similar to atomic orbitals. Wannier states can be

used to write a second quantization model on a lattice for instance one may use it to find the so-called tight binding Hamiltonian by using our expressions for a one body operator

$$H_{TB} = \sum_{ij} t_{ij} c_i^\dagger c_j + H.C.$$

Here, i and j now label Wannier states for atomic sites i and j. The way to understand this Hamiltonian is that c_j destroys a particle at site j and $c_i^\dagger$ creates a particle at site i. In a sense the particle hops from site j to site i. The t_{ij} are sometimes called hopping elements and can be thought of something similar to a probability of hopping between sites (note this is not fully accurate because it has dimensions of energy).

A similar approach is possible with two-body operators. Of course this is complicated in general, but under certain conditions this can **approximately** lead to a Hamiltonian of the form:

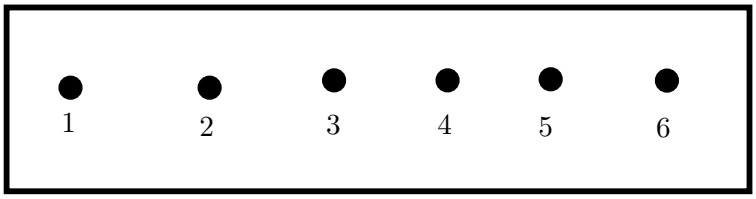
$$H_{Hubb} = H_{TB} + U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow}$$

The so-called Hubbard Hamiltonian. This Hamiltonian gives an energy penalty U to two electrons with opposite spin that sit at site i. This is similar to the Coulomb interaction that makes electrons repel one another. It should be noted that this term actually arises as second quantization form of the Coulomb interaction. However, there were additional approximations involved, which we will not detail here.

3. Momentum basis
4. Harmonic oscillator basis etc. One may choose any kind of useful basis

5 Turning Many-Body Hamiltonians into Numeric Code (Exact Diagonalization)

We will start with a simple example. More complicated examples are easy to guess from here. Consider a chain of 6 atoms:



Bosons:

We note that $a_3^\dagger$ was actually a short-hand notation for:

$$a_3^\dagger = \mathbb{1}_1 \otimes \mathbb{1}_2 \otimes a^\dagger \otimes \mathbb{1}_4 \otimes \mathbb{1}_5 \otimes \mathbb{1}_6$$

Where $\mathbb{1}_i$ is just an identity matrix of appropriate size and $a^\dagger$ is the usual harmonic oscillator raising operator:

$$a^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 & \dots & 0 & \dots \\ \sqrt{1} & 0 & 0 & 0 & \dots & 0 & \dots \\ 0 & \sqrt{2} & 0 & 0 & \dots & 0 & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots & \ddots & 0 & \dots \\ 0 & 0 & 0 & 0 & \sqrt{n} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix}$$

This can be truncated to some order but the identity operator needs to be made to match. Here, $\otimes$ is a tensor product. An example of how a tensor product works is given below:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \otimes \begin{pmatrix} e & f \\ g & h \end{pmatrix} = \left(\begin{array}{cc|cc} ae & af & be & bf \\ ag & ah & bg & bh \\ \hline ce & cf & de & df \\ cg & ch & dg & dh \end{array}\right)$$

The tensor product Mathematica is called KroneckerProduct.

Fermions:

For fermions we may take $c_3^\dagger$ as a short-hand also with:

$$c_3^\dagger = (-\sigma_1^z) \otimes (-\sigma_2^z) \otimes \sigma_3^+ \otimes \mathbb{1}_4 \otimes \mathbb{1}_5 \otimes \mathbb{1}_6$$

Here, σ_1^z is just the typical Pauli matrix and σ^+ is also just the conventional Pauli matrix. We see that Fermions carry a non-local operator string of Pauli matrices. Note that this what we describe above is essentially what is known as Jordan-Wigner transform:

$$c_j^\dagger = \prod_{k=1}^{j-1} (-\sigma_k^z)\sigma_j^+$$

$$c_j = \prod_{k=1}^{j-1} (-\sigma_k^z)\sigma_j^-$$

Homework

1. Prove that the Fermions rewritten in Jordan-Wigner form fulfill fermionic commutation relations (Hint: the string of σ_z operators is responsible for this)
2. Read a bit about the Wannier basis and become confident that there is a nice similarity to atomic orbitals
3. Build the following Hamiltonian for a 6 site lattice in Mathematica or equivalent and plot its eigenvalues (for t=1 U=2) sorted by size:

$$H = t \sum_i c_i^\dagger c_{i+1} + U \sum_i c_i^\dagger c_{i+1}^\dagger c_i c_{i+1}$$

Written by: Michael Rudolf Vogl
LaTeX Typeset by: Ibraheem Faisal Al-Yousef