II. SECOND QUANTIZATION

A. Occupation Number Representation

Dealing with symmetric or antisymmetric many-particle states is simplified considerably by using the occupation number representation (second quantization). Instead of working in the space of a fixed number of particles, one uses the vector space which is comprised of the vacuum state $|0\rangle$, which contains no particles, the complete set of sp states $\{|\alpha\rangle\}$, the complete set of (anti)symmetric two-particle states $\{|\alpha_1\alpha_2\rangle\}$, and so on until infinite particle number. This space is referred to as Fock space. Completeness of the states in this space, using ordered sp quantum numbers, is expressed by

$$\sum_{N=0}^{\infty} \sum_{\alpha_1\alpha_2...\alpha_N} |\alpha_1\alpha_2...\alpha_N\rangle \langle\alpha_1\alpha_2...\alpha_N| \; = \; 1. \tag{66}$$

First the case of fermions will be discussed. An important operator is the particle addition (creation) operator defined by

$$a_\alpha^\dagger \, |\alpha_1\alpha_2...\alpha_N\rangle \equiv |\alpha\alpha_1\alpha_2...\alpha_N\rangle \tag{67}$$

which adds to an N-particle antisymmetric state in which N particles occupy sp levels $\{\alpha_1, \alpha_2, ..., \alpha_N\}$ a particle with quantum numbers α resulting in an antisymmetric $N+1$-particle state. Note that if the level characterized by α is already occupied, the result is zero. Observe that the $N+1$-particle state containing α may not yet be ordered and the ordering of α among the α_i could therefore result in a minus sign.

The adjoint of $a_\alpha^\dagger$ is called a particle removal (destruction) operator and has the property that upon acting on an antisymmetric N-particle state, it produces an antisymmetric $N-1$-particle state provided the sp state α is occupied (otherwise the result is zero). These properties can be obtained by considering

$$\begin{aligned} a_\alpha \, |\alpha_1\alpha_2...\alpha_N\rangle \; &= \sum_{M=0}^{\infty} \sum_{\alpha'_1\alpha'_2...\alpha'_M} |\alpha'_1\alpha'_2...\alpha'_M\rangle \, \langle\alpha'_1\alpha'_2...\alpha'_M| \, a_\alpha \, |\alpha_1\alpha_2...\alpha_N\rangle \\ &= \sum_{M=0}^{\infty} \sum_{\alpha'_1\alpha'_2...\alpha'_M} |\alpha'_1\alpha'_2...\alpha'_M\rangle \, \langle\alpha_1\alpha_2...\alpha_N| \, a_\alpha^\dagger \, |\alpha'_1\alpha'_2...\alpha'_M\rangle^* \\ &= \sum_{M=0}^{\infty} \sum_{\alpha'_1\alpha'_2...\alpha'_M} |\alpha'_1\alpha'_2...\alpha'_M\rangle \, \langle\alpha_1\alpha_2...\alpha_N|\alpha\alpha'_1\alpha'_2...\alpha'_M\rangle^*. \end{aligned} \tag{68}$$

The last line is obtained by using the definition of the particle addition operator. States containing different particle number are naturally orthogonal to each other; this implies that $M = N-1$. As discussed above, the normalization of the antisymmetric states is real and one can omit the complex conjugation sign. In addition, it is clear that once α has been ordered among the α' states, one can simply apply the normalization result discussed above. Suppose α must be placed before α'_i. If $i = 1$, no sign change will result, therefore ordering leads to the phase $(-1)^{i-1}$. The normalization condition gives

$$\langle\alpha_1\alpha_2...\alpha_N|\alpha'_1\alpha'_2...\alpha\alpha'_i...\alpha'_M\rangle \; = \; \delta_{\alpha_1,\alpha'_1}\delta_{\alpha_2,\alpha'_2}...\delta_{\alpha_i,\alpha}\delta_{\alpha_{i+1},\alpha'_i}...\delta_{\alpha_N,\alpha'_{N-1}}. \tag{69}$$

As a result one obtains

$$a_\alpha \, |\alpha_1\alpha_2...\alpha_N\rangle = (-1)^{i-1} \, |\alpha_1\alpha_2...\alpha_{i-1}\alpha_{i+1}...\alpha_N\rangle \qquad if \;\; \alpha = \alpha_i \tag{70}$$

otherwise

$$a_\alpha \, |\alpha_1\alpha_2...\alpha_N\rangle = \; 0 \qquad if \;\; \alpha \neq \alpha_i. \tag{71}$$

One therefore also obtains

$$a_\alpha \, |0\rangle \; = \; 0. \tag{72}$$

The particle addition and removal operators obey the following, extremely important operator relations (sometimes called fundamental anticommutation relations) :

$$\{a_\alpha, a^\dagger_\beta\} = a_\alpha a^\dagger_\beta + a^\dagger_\beta a_\alpha = \delta_{\alpha,\beta}, \tag{73}$$

$$\{a_\alpha, a_\beta\} = 0, \tag{74}$$

and

$$\{a^\dagger_\alpha, a^\dagger_\beta\} = 0. \tag{75}$$

As an example how to derive these results, a typical analysis will be given. Consider an N-particle ket in which α is not occupied:

$$\begin{aligned} a_\alpha a^\dagger_\alpha \left|\alpha_1\alpha_2...\alpha_N\right\rangle &= a_\alpha \left|\alpha\alpha_1\alpha_2...\alpha_N\right\rangle \\ &= \left|\alpha_1\alpha_2...\alpha_N\right\rangle . \end{aligned} \tag{76}$$

In addition

$$a^\dagger_\alpha a_\alpha \left|\alpha_1\alpha_2...\alpha_N\right\rangle = 0. \tag{77}$$

These two results combined show that

$$\{a_\alpha, a^\dagger_\alpha\} \left|\alpha_1\alpha_2...\alpha_N\right\rangle = \left|\alpha_1\alpha_2...\alpha_N\right\rangle \tag{78}$$

When the N-particle ket does contain the sp state α one can assume without loss of generality that $\alpha_1 = \alpha$. One then obtains

$$a_\alpha a^\dagger_\alpha \left|\alpha\alpha_2...\alpha_N\right\rangle = 0 \tag{79}$$

and

$$\begin{aligned} a^\dagger_\alpha a_\alpha \left|\alpha\alpha_2...\alpha_N\right\rangle &= a^\dagger_\alpha \left|\alpha_2...\alpha_N\right\rangle \\ &= \left|\alpha\alpha_2...\alpha_N\right\rangle \end{aligned} \tag{80}$$

which shows that

$$\{a_\alpha, a^\dagger_\alpha\} \left|\alpha\alpha_2...\alpha_N\right\rangle = \left|\alpha\alpha_2...\alpha_N\right\rangle . \tag{81}$$

Since this procedure can be applied for any N and as shown for fixed N for any state, one concludes that

$$\{a_\alpha, a^\dagger_\alpha\} = 1. \tag{82}$$

A similar strategy can be used for the proof of the other operator identities.

Antisymmetric N-particle states can now be obtained by repeated application of particle addition operators to the vacuum state

$$\begin{aligned} \left|\alpha_1\alpha_2\alpha_3...\alpha_N\right\rangle &= a^\dagger_{\alpha_1} \left|\alpha_2\alpha_3...\alpha_N\right\rangle \\ &= a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \left|\alpha_3...\alpha_N\right\rangle \\ &= ... \\ &= a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} ... a^\dagger_{\alpha_N} \left|0\right\rangle \\ &= \prod_i a^\dagger_{\alpha_i} \left|0\right\rangle . \end{aligned} \tag{83}$$

Note that the third anticommutation relation automatically ensures that the Pauli principle is incorporated in the above construction. For example:

$$\begin{aligned} \left|\alpha_1\alpha_2\alpha_3...\alpha_N\right\rangle &= a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} ... a^\dagger_{\alpha_N} \left|0\right\rangle \\ &= -a^\dagger_{\alpha_2} a^\dagger_{\alpha_1} ... a^\dagger_{\alpha_N} \left|0\right\rangle \\ &= 0 \end{aligned} \tag{84}$$

when $\alpha_1 = \alpha_2$.

In dealing with boson addition and removal operators it is convenient to to use the notation that characterizes the occupation of each sp state

$$|\alpha_1\alpha_2...\alpha_N\rangle = \left[\frac{N!}{n_\alpha! n_{\alpha'}!...}\right]^{1/2} S\ |\alpha_1\alpha_2...\alpha_N) = |n_\alpha n_\beta ...\rangle \tag{85}$$

which identifies how many particles occupy a sp level α etc. Addition and removal operators may be introduced as in the case of fermions. For sp states one has

$$|\alpha\rangle = a_\alpha^\dagger |0\rangle . \tag{86}$$

For two-particle states one has

$$|\alpha\beta\rangle = a_\alpha^\dagger a_\beta^\dagger |0\rangle \tag{87}$$

when $\alpha \neq \beta$. In the case $\alpha = \beta$ one must include an extra normalization factor

$$|\alpha\alpha\rangle = |n_\alpha = 2\rangle = \frac{1}{\sqrt{2}} a_\alpha^\dagger a_\alpha^\dagger |0\rangle . \tag{88}$$

In the general case one obtains

$$|n_\alpha n_\beta ... n_\omega\rangle = \frac{1}{[n_\alpha! n_\beta! ... n_\omega!]^{1/2}} \left(a_\alpha^\dagger\right)^{n_\alpha} \left(a_\beta^\dagger\right)^{n_\beta} ... \left(a_\omega^\dagger\right)^{n_\omega} |0\rangle \tag{89}$$

with a corresponding result for the bra states. The particle addition and removal operators obey the following fundamental commutation relations :

$$[a_\alpha, a_\beta^\dagger] = a_\alpha a_\beta^\dagger - a_\beta^\dagger a_\alpha = \delta_{\alpha,\beta}, \tag{90}$$

$$[a_\alpha, a_\beta] = 0, \tag{91}$$

and

$$[a_\alpha^\dagger, a_\beta^\dagger] = 0. \tag{92}$$

These results can be obtained in a similar way as for the fermion operators and are related to the requirement that symmetric states are obtained after the action of an addition or removal operator of a boson sp state. It should be noted that the commutation relations for one sp state are identical to those for harmonic oscillator quanta. It is therefore not surprising that the following relations hold

$$a_\alpha^\dagger |n_\alpha n_\beta ... n_\omega\rangle = \sqrt{n_\alpha + 1}\, |n_\alpha + 1\ n_\beta ... n_\omega\rangle , \tag{93}$$

$$a_\alpha |n_\alpha n_\beta ... n_\omega\rangle = \sqrt{n_\alpha}\, |n_\alpha - 1\ n_\beta ... n_\omega\rangle , \tag{94}$$

and similarly for operators involving other sp quantum numbers. The results of Eqs. (93) and (94) can be verified by using Eq. (89) and the commutation relations.

B. Operators in Fock Space

Relevant operators to consider in many-particle systems involve only the coordinates of one or two (and in unusual cases three) particles. It is therefore important to translate the action of such operators into the language of particle addition and removal operators. Consider first this translation for an operator which acts only on one particle. Such a one-body operator, F, acting in a sp space can be written as

$$F = \sum_\alpha \sum_\beta |\alpha\rangle \langle\alpha| F |\beta\rangle \langle\beta| . \tag{95}$$

In an N-particle space the corresponding extension of this operator is simply

$$\begin{aligned} F_N &= F(1) + F(2) + ... + F(N) \\ &= \sum_{i=1}^{N} F(i) \end{aligned} \tag{96}$$

where each operator $F(i)$ acts only on particle i. The action of $F(i)$ on a product state is given by

$$\begin{aligned} F(i)|\alpha_1\alpha_2\alpha_3...\alpha_N) &= |\alpha_1\rangle\,|\alpha_2\rangle\,...\,|\alpha_{i-1}\rangle \left\{\sum_{\beta_i} |\beta_i\rangle \,\langle\beta_i|\,F\,|\alpha_i\rangle\right\} |\alpha_{i+1}\rangle\,...\,|\alpha_N\rangle \\ &= \sum_{\beta_i} \langle\beta_i|\,F\,|\alpha_i\rangle\,|\alpha_1...\alpha_{i-1}\beta_i\alpha_{i+1}...\alpha_N). \end{aligned} \tag{97}$$

Note that the matrix elements of F do not depend on which particle is considered. The matrix element $\langle\beta_i|\,F\,|\alpha_i\rangle$ in the above expression will therefore be the same for any particle. Calculation of this matrix element for another particle will in fact only involve a change in dummy variables. For the operator F_N one then obtains

$$\begin{aligned} F_N\,|\alpha_1\alpha_2\alpha_3...\alpha_N) &= F(1)\,|\alpha_1\rangle\,|\alpha_2\rangle\,...\,|\alpha_N\rangle \\ &+ |\alpha_1\rangle\,F(2)\,|\alpha_2\rangle\,...\,|\alpha_N\rangle + ... \\ &+ |\alpha_1\rangle\,|\alpha_2\rangle\,...F(N)\,|\alpha_N\rangle \\ &= \sum_{\beta_1} \langle\beta_1|\,F\,|\alpha_1\rangle\,|\beta_1\alpha_2...\alpha_N) \\ &+ \sum_{\beta_2} \langle\beta_2|\,F\,|\alpha_2\rangle\,|\alpha_1\beta_2...\alpha_N) + ... \\ &+ \sum_{\beta_N} \langle\beta_N|\,F\,|\alpha_N\rangle\,|\alpha_1\alpha_2...\beta_N) \\ &= \sum_{i=1}^{N}\sum_{\beta_i} \langle\beta_i|\,F\,|\alpha_i\rangle\,|\alpha_1\alpha_2...\alpha_{i-1}\beta_i\alpha_{i+1}...\alpha_N). \end{aligned} \tag{98}$$

To obtain the action of F_N on an antisymmetric or symmetric N-particle state, one notes that F_N is symmetric and therefore commutes with the antisymmetrizer A or the symmetrizeR S (remember the example of two particles in which H commutes with P_{12}). As a result

$$F_N\,|\alpha_1\alpha_2\alpha_3...\alpha_N\rangle = \sum_{i=1}^{N}\sum_{\beta_i} \langle\beta_i|\,F\,|\alpha_i\rangle\,|\alpha_1\alpha_2...\alpha_{i-1}\beta_i\alpha_{i+1}...\alpha_N\rangle\,. \tag{99}$$

One can now show that the Fock space operator (note the “ˆ” notation for a Fock-space operator)

$$\hat{F} = \sum_{\alpha\beta} \langle\alpha|\,F\,|\beta\rangle\; a^\dagger_\alpha a_\beta \tag{100}$$

gives the same result for any N when acting on Eq. (83) for fermions and Eq. (89) for bosons. In order to show this, consider the following commutator in the case of fermions

$$\begin{aligned} [\hat{F}, a^\dagger_{\alpha_i}] &= \sum_{\alpha\beta} \langle\alpha|\,F\,|\beta\rangle\,[a^\dagger_\alpha a_\beta, a^\dagger_{\alpha_i}] \\ &= \sum_{\alpha\beta} \langle\alpha|\,F\,|\beta\rangle\,(a^\dagger_\alpha a_\beta a^\dagger_{\alpha_i} - a^\dagger_{\alpha_i} a^\dagger_\alpha a_\beta) \\ &= \sum_{\alpha\beta} \langle\alpha|\,F\,|\beta\rangle\,a^\dagger_\alpha(a_\beta a^\dagger_{\alpha_i} + a^\dagger_{\alpha_i} a_\beta) \\ &= \sum_{\alpha\beta} \langle\alpha|\,F\,|\beta\rangle\,a^\dagger_\alpha \delta_{\beta,\alpha_i} \end{aligned}$$

$$
\begin{aligned}
&= \sum_{\alpha} \langle \alpha | F | \alpha_i \rangle a_{\alpha}^{\dagger} \\
&= \sum_{\beta_i} \langle \beta_i | F | \alpha_i \rangle a_{\beta_i}^{\dagger}.
\end{aligned} \tag{101}
$$

This result is also obtained for bosons. One can use this result in the following manipulation

$$
\begin{aligned}
\hat{F} | \alpha_1 \alpha_2 \alpha_3 ... \alpha_N \rangle &= \hat{F} a_{\alpha_1}^{\dagger} a_{\alpha_2}^{\dagger} ... a_{\alpha_N}^{\dagger} |0\rangle \\
&= [\hat{F}, a_{\alpha_1}^{\dagger}] a_{\alpha_2}^{\dagger} ... a_{\alpha_N}^{\dagger} |0\rangle + a_{\alpha_1}^{\dagger} \hat{F} a_{\alpha_2}^{\dagger} ... a_{\alpha_N}^{\dagger} |0\rangle \\
&= [\hat{F}, a_{\alpha_1}^{\dagger}] a_{\alpha_2}^{\dagger} ... a_{\alpha_N}^{\dagger} |0\rangle \\
&+ a_{\alpha_1}^{\dagger} [\hat{F}, a_{\alpha_2}^{\dagger}] ... a_{\alpha_N}^{\dagger} |0\rangle + ... \\
&+ a_{\alpha_1}^{\dagger} a_{\alpha_2}^{\dagger} ... [\hat{F}, a_{\alpha_N}^{\dagger}] |0\rangle \\
&= \sum_{i=1}^{N} \sum_{\beta_i} \langle \beta_i | F | \alpha_i \rangle a_{\alpha_1}^{\dagger} ... a_{\alpha_{i-1}}^{\dagger} a_{\beta_i}^{\dagger} a_{\alpha_{i+1}}^{\dagger} ... a_{\alpha_N}^{\dagger} |0\rangle \\
&= \sum_{i=1}^{N} \sum_{\beta_i} \langle \beta_i | F | \alpha_i \rangle | \alpha_1 ... \alpha_{i-1} \beta_i \alpha_{i+1} ... \alpha_N \rangle
\end{aligned} \tag{102}
$$

which proves the equivalence for fermions since this result can be obtained for any N. For bosons one proceeds in the same way to obtain the equivalence. As an example of a second quantized operator consider

$$
\hat{N} = \sum_{\alpha} a_{\alpha}^{\dagger} a_{\alpha}. \tag{103}
$$

Using the results of Eqs. (101) and (102) one easily obtains that

$$
\hat{N} | \alpha_1 ... \alpha_N \rangle = N | \alpha_1 ... \alpha_N \rangle \tag{104}
$$

for any N and any set α_i. This operator is therefore called the number operator since it simply counts the number of particles in the state on which it acts. When the state has a fixed number of particles it is an eigenstate of $\hat{N}$.

An example of an operator involving the coordinates of two particles, is the two-body interaction V. In order to establish the corresponding Fock-space operator, consider first the two-body operator V acting on states in the two-particle space

$$
V = \sum_{\alpha\beta} \sum_{\gamma\delta} |\alpha\beta)(\alpha\beta|V|\gamma\delta)(\gamma\delta|. \tag{105}
$$

In an N-particle space the corresponding extension of this operator is given by

$$
V_N = \left\{ \begin{array}{lllll}
V(1,2)+ & V(1,3)+ & V(1,4)+ & \ldots + & V(1,N)+ \\
 & V(2,3)+ & V(2,4)+ & \ldots + & V(2,N)+ \\
 & & V(3,4)+ & \ldots + & V(3,N)+ \\
 & & & \ddots & \vdots \\
 & & & & V(N-1,N)
\end{array} \right. = \sum_{i<j=1}^{N} V(i,j) = \frac{1}{2} \sum_{i \neq j}^{N} V(i,j), \tag{106}
$$

where each operator $V(i,j)$ acts only on particles i and j. The action of $V(i,j)$ on a product state of N particles is given by

$$
V(i,j)|\alpha_1 ... \alpha_i ... \alpha_j ... \alpha_N) = \sum_{\beta_i \beta_j} (\beta_i \beta_j |V| \alpha_i \alpha_j) |\alpha_1 ... \alpha_{i-1} \beta_i \alpha_{i+1} ... \alpha_{j-1} \beta_j \alpha_{j+1} ... \alpha_N). \tag{107}
$$

Note that the matrix elements of V do not depend on which pair of particles is considered. The matrix elements $(\beta_i \beta_j |V| \alpha_i \alpha_j)$ in the above expression will therefore be the same for any pair of particles as long as the same quantum numbers are involved. For the operator V_N one then obtains

$$V_N|\alpha_1\alpha_2\alpha_3...\alpha_N) = \sum_{i<j=1}^{N}\sum_{\beta_i\beta_j}(\beta_i\beta_j|V|\alpha_i\alpha_j)|\alpha_1...\beta_i...\beta_j...\alpha_N). \tag{108}$$

To obtain the action of V_N on an antisymmetric or symmetric N-particle state, one notes that V_N is symmetric and therefore commutes with the antisymmetrizer A or symmetrizer S. As a result

$$V_N\left|\alpha_1\alpha_2\alpha_3...\alpha_N\right\rangle = \sum_{i<j=1}^{N}\sum_{\beta_i\beta_j}(\beta_i\beta_j|V|\alpha_i\alpha_j)\left|\alpha_1...\beta_i...\beta_j...\alpha_N\right\rangle . \tag{109}$$

One can now show that the Fock space operator (note again the ˆ for a Fock-space operator)

$$\hat{V} = \frac{1}{2}\sum_{\alpha\beta\gamma\delta}(\alpha\beta|V|\gamma\delta)a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \tag{110}$$

gives the same result for any N when acting on Eq. (83) for fermions and Eq. (89) for bosons. In order to show this in the case of fermions, consider the following commutator

$$\begin{aligned}
[\hat{V}, a^\dagger_{\alpha_i}] &= \frac{1}{2}\sum_{\alpha\beta\gamma\delta}(\alpha\beta|V|\gamma\delta)a^\dagger_\alpha a^\dagger_\beta[a_\delta a_\gamma, a^\dagger_{\alpha_i}] \\
&= \ldots\ldots a^\dagger_\alpha a^\dagger_\beta(a_\delta a_\gamma a^\dagger_{\alpha_i} - a^\dagger_{\alpha_i}a_\delta a_\gamma) \\
&= \ldots\ldots a^\dagger_\alpha a^\dagger_\beta(a_\delta(\delta_{\gamma,\alpha_i} - a^\dagger_{\alpha_i}a_\gamma) - a^\dagger_{\alpha_i}a_\delta a_\gamma) \\
&= \ldots\ldots a^\dagger_\alpha a^\dagger_\beta(a_\delta\delta_{\gamma,\alpha_i} - \delta_{\delta,\alpha_i}a_\gamma) \\
&= \frac{1}{2}\sum_{\alpha\beta\delta}(\alpha\beta|V|\alpha_i\delta)a^\dagger_\alpha a^\dagger_\beta a_\delta - \frac{1}{2}\sum_{\alpha\beta\gamma}(\alpha\beta|V|\gamma\alpha_i)a^\dagger_\alpha a^\dagger_\beta a_\gamma \\
&= \sum_{\alpha\beta\delta}(\alpha\beta|V|\alpha_i\delta)a^\dagger_\alpha a^\dagger_\beta a_\delta \\
&= \sum_{\beta_i\beta_{i'}\alpha_{i'}}(\beta_i\beta_{i'}|V|\alpha_i\alpha_{i'})a^\dagger_{\beta_i}a^\dagger_{\beta_{i'}}a_{\alpha_{i'}}.
\end{aligned} \tag{111}$$

In this sequence use has been made of the symmetry $V(i,j) = V(j,i)$ which implies

$$(\alpha\beta|V|\gamma\delta) = (\beta\alpha|V|\delta\gamma). \tag{112}$$

One can use this result in the following manipulation

$$\begin{aligned}
\hat{V}\left|\alpha_1\alpha_2\alpha_3...\alpha_N\right\rangle &= \hat{V}a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}...a^\dagger_{\alpha_N}\left|0\right\rangle \\
&= \sum_{i=1}^{N}a^\dagger_{\alpha_1}...[\hat{V}, a^\dagger_{\alpha_i}]...a^\dagger_{\alpha_N}\left|0\right\rangle \\
&= \sum_{i=1}^{N}\sum_{\beta_i\beta_{i'}\alpha_{i'}}(\beta_i\beta_{i'}|V|\alpha_i\alpha_{i'})a^\dagger_{\alpha_1}...a^\dagger_{\beta_i}a^\dagger_{\beta_{i'}}a_{\alpha_{i'}}a^\dagger_{\alpha_{i+1}}...a^\dagger_{\alpha_N}\left|0\right\rangle \\
&= \sum_{i=1}^{N}\sum_{j>i}^{N}\sum_{\beta_i\beta_j}(\beta_i\beta_j|V|\alpha_i\alpha_j)a^\dagger_{\alpha_1}...a^\dagger_{\beta_i}...a^\dagger_{\beta_j}...a^\dagger_{\alpha_N}\left|0\right\rangle
\end{aligned} \tag{113}$$

which proves the equivalence. Note that in the last equality use has been made of

$$\sum_{\beta_{i'}\alpha_{i'}}f(\beta_{i'},\alpha_{i'})[a^\dagger_{\beta_{i'}}a_{\alpha_{i'}}, a^\dagger_{\alpha_j}] = \sum_{\beta_{i'}}f(\beta_{i'},\alpha_j)a^\dagger_{\beta_{i'}} \tag{114}$$

for each $j > i$. Eq. (113) is equivalent to Eq. (108) and this result holds for any N. Eq. (110) therefore represents the extension of the two-particle operator V_N in Fock space. For bosons one can proceed in a similar fashion yielding the same result for the two-body interaction in Fock space (Eq. (110)). An alternative form for $\hat{V}$ in the case of fermions is given by

$$\hat{V} = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \, V \, | \gamma\delta \rangle \, a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \tag{115}$$

where

$$\begin{aligned} \langle \alpha\beta | \, V \, | \gamma\delta \rangle &\equiv (\alpha\beta|V|\gamma\delta) - (\alpha\beta|V|\delta\gamma) \\ &= \langle \alpha\beta | \, \hat{V} \, | \gamma\delta \rangle \, . \end{aligned} \tag{116}$$

Note that in the expression for $\hat{V}$ the order of the quantum numbers γ and δ in the matrix element is different from the ordering of the corresponding particle removal operators. Depending on the nature of the interaction V it can be useful to choose the unsymmetrized version of $\hat{V}$ (Eq. (110)) or the symmetrized version (Eq. (115)). As a result of the translation of a one-body and a two-body operator into Fock space formulation, it is possible to write the hamiltonian of a many-particle system in second quantized form

$$\begin{aligned} \hat{H} &= \hat{T} + \hat{V} \\ &= \sum_{\alpha\beta} \langle \alpha | \, T \, | \beta \rangle \, a_\alpha^\dagger a_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} (\alpha\beta|V|\gamma\delta) a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \end{aligned} \tag{117}$$

for both fermions and bosons. For fermions it also useful to consider

$$\hat{H} = \sum_{\alpha\beta} \langle \alpha | \, T \, | \beta \rangle \, a_\alpha^\dagger a_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \, V \, | \gamma\delta \rangle \, a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \, . \tag{118}$$

For a given choice of sp basis and two-body interaction V, it is possible to calculate the relevant one- and two-body matrix elements which appear in $\hat{H}$ (although this can be very tedious and computer time consuming sometimes). The calculation of matrix elements of $\hat{H}$ between many-particle states is therefore reduced to manipulating particle addition and removal operators using their anticommutation relations. In the case an explicit three-body interaction (symmetric in the coordinates of the particles) needs to be considered one can use the first quantized version in the N-particle space

$$W_N = \sum_{i<j<k=1}^{N} W(i,j,k) \tag{119}$$

and the Fock space operator

$$\hat{W} = \frac{1}{6} \sum_{\alpha\beta\gamma} \sum_{\alpha'\beta'\gamma'} \langle \alpha\beta\gamma | \, W \, | \alpha'\beta'\gamma' \rangle \, a_\alpha^\dagger a_\beta^\dagger a_\gamma^\dagger a_{\gamma'} a_{\beta'} a_{\alpha'} \, . \tag{120}$$

C. Some practical results

To explain the name second quantization it is useful to mention the confusing convention to denote the addition and removal operators for particles with quantum numbers $\mathbf{r}, m_s$ by

$$a_{\mathbf{r},m_s}^\dagger = \psi_{m_s}^\dagger(\mathbf{r}) \tag{121}$$

and

$$a_{\mathbf{r},m_s} = \psi_{m_s}(\mathbf{r}), \tag{122}$$

respectively. Using this basis the kinetic energy matrix element becomes

$$
\begin{aligned}
\langle \mathbf{r} m_s |\, T \,|\mathbf{r}' m_s' \rangle &= \langle \mathbf{r} m_s |\, \frac{\mathbf{p}^2}{2m} \,|\mathbf{r}' m_s' \rangle \\
&= \frac{-i\hbar}{2m} \nabla \cdot \langle \mathbf{r} m_s |\, \mathbf{p} \,|\mathbf{r}' m_s' \rangle \\
&= \frac{-\hbar^2}{2m} \nabla^2 \langle \mathbf{r} m_s | \mathbf{r}' m_s' \rangle \\
&= \frac{-\hbar^2}{2m} \nabla^2 \delta(\mathbf{r} - \mathbf{r}') \delta_{m_s, m_s'} .
\end{aligned}
\tag{123}
$$

For a conventional spin-independent two-particle interaction one has in addition

$$
(\mathbf{r}_1 m_{s_1}\ \mathbf{r}_2 m_{s_2} | V(\mathbf{r}, \mathbf{r}') | \mathbf{r}_3 m_{s_3}\ \mathbf{r}_4 m_{s_4}) = \delta(\mathbf{r}_1 - \mathbf{r}_3) \delta(\mathbf{r}_2 - \mathbf{r}_4) \delta_{m_{s_1}, m_{s_3}} \delta_{m_{s_2}, m_{s_4}} V(|\mathbf{r}_3 - \mathbf{r}_4|). \tag{124}
$$

Using these results the hamiltonian can be rewritten as

$$
\hat{H} = \sum_{m_s} \int d^3 r\ \psi^\dagger_{m_s}(\mathbf{r}) \{ \frac{-\hbar^2}{2m} \nabla^2 \} \psi_{m_s}(\mathbf{r}) + \frac{1}{2} \sum_{m_{s_1} m_{s_2}} \int d^3 r_1 \int d^3 r_2\ \psi^\dagger_{m_{s_1}}(\mathbf{r}_1) \psi^\dagger_{m_{s_2}}(\mathbf{r}_2) V(|\mathbf{r}_1 - \mathbf{r}_2|) \psi_{m_{s_2}}(\mathbf{r}_2) \psi_{m_{s_1}}(\mathbf{r}_1). \tag{125}
$$

This expression can of course easily lead to the wrong interpretation when one mistakenly thinks of ψ as a wave function. In order to avoid this pitfall the following notation will be used

$$
\hat{H} = \sum_{m_s} \int d^3 r\ a^\dagger_{\mathbf{r} m_s} \{ \frac{-\hbar^2}{2m} \nabla^2 \} a_{\mathbf{r} m_s} + \frac{1}{2} \sum_{m_{s_1} m_{s_2}} \int d^3 r_1 \int d^3 r_2\ a^\dagger_{\mathbf{r}_1 m_{s_1}} a^\dagger_{\mathbf{r}_2 m_{s_2}} V(|\mathbf{r}_1 - \mathbf{r}_2|) a_{\mathbf{r}_2 m_{s_2}} a_{\mathbf{r}_1 m_{s_1}} . \tag{126}
$$

A change of sp basis in sp space can be rewritten in the following way

$$
\begin{aligned}
a^\dagger_\alpha \,|0\rangle &= |\alpha\rangle \\
&= \sum_\lambda |\lambda\rangle \,\langle \lambda | \alpha \rangle \\
&= \sum_\lambda a^\dagger_\lambda \,|0\rangle \,\langle \lambda | \alpha \rangle .
\end{aligned}
\tag{127}
$$

This procedure can be repeated for $a^\dagger_\alpha$ acting on any state in Fock space and one therefore obtains the operator equation

$$
a^\dagger_\alpha = \sum_\lambda \langle \lambda | \alpha \rangle a^\dagger_\lambda \tag{128}
$$

and similarly

$$
a_\alpha = \sum_\lambda \langle \alpha | \lambda \rangle a_\lambda . \tag{129}
$$

Useful commutators for Fock-space operators have been used at various stages. Some of them are collected below. They include

$$
[\hat{F}, a^\dagger_\gamma] = \sum_\alpha \langle \alpha |\, F \,| \gamma \rangle \, a^\dagger_\alpha \tag{130}
$$

and therefore

$$
[\hat{F}, a_\gamma] = - \sum_\alpha \langle \gamma |\, F \,| \alpha \rangle \, a_\alpha . \tag{131}
$$

If F is diagonal in the chosen sp basis then

$$\begin{aligned}\hat{F} &= \sum_{\alpha} \langle\alpha|\, F \,|\alpha\rangle\, a_{\alpha}^{\dagger} a_{\alpha} \\ &= \sum_{\alpha} F_{\alpha} a_{\alpha}^{\dagger} a_{\alpha}.\end{aligned} \tag{132}$$

In that case

$$[\hat{F}, a_{\gamma}^{\dagger}] = F_{\gamma} a_{\gamma}^{\dagger} \tag{133}$$

and

$$[\hat{F}, a_{\gamma}] = -F_{\gamma} a_{\gamma}. \tag{134}$$

For a two-particle operator $\hat{G}$ one has

$$[\hat{G}, a_{\mu}^{\dagger}] = \sum_{\alpha\beta\delta} \langle\alpha\beta|\, G \,|\mu\delta\rangle\, a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} \tag{135}$$

and

$$[\hat{G}, a_{\mu}] = -\sum_{\beta\gamma\delta} \langle\mu\beta|\, G \,|\gamma\delta\rangle\, a_{\beta}^{\dagger} a_{\delta} a_{\gamma}. \tag{136}$$