Fermionic Algebra and Fock Space

Earlier in class we saw how the harmonic-oscillator-like bosonic commutation relations

$$\left[\hat{a}_\alpha, \hat{a}_\beta\right] \;=\; 0, \quad \left[\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger\right] \;=\; 0, \quad \left[\hat{a}_\alpha, \hat{a}_\beta^\dagger\right] \;=\; \delta_{\alpha,\beta} \tag{1}$$

give rise to the bosonic Fock space in which the oscillator modes α correspond to the single-particle quantum states $|\alpha\rangle$. In this note, we shall see how the fermionic anti-commutation relations

$$\left\{\hat{a}_\alpha, \hat{a}_\beta\right\} \;=\; 0, \quad \left\{\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger\right\} \;=\; 0, \quad \left\{\hat{a}_\alpha, \hat{a}_\beta^\dagger\right\} \;=\; \delta_{\alpha,\beta} \tag{2}$$

give rise to the fermionic Fock space. Again, the modes α will correspond to the single-particle quantum states. For simplicity, I will assume discrete modes — for example, momenta (and spins) of a free particle in a big but finite box.

Hilbert Space of a Single Fermionic Mode

A single bosonic mode is equivalent to a harmonic oscillator; the relation $[\hat{a}, \hat{a}^\dagger] = 1$ gives rise to an infinite-dimensional Hilbert space spanning states $|n\rangle$ for $n = 0, 1, 2, 3, \ldots, \infty$. A single fermionic mode is different — its Hilbert space spans just two states, $|0\rangle$ and $|1\rangle$. In accordance with the Fermi statistics, multiple quanta in the same mode are not allowed.

To see how this works, note that there are three non-trivial anticommutation relations for a single pair of creation and annihilation operators, namely

$$\hat{a}\hat{a}^\dagger \;+\; \hat{a}^\dagger\hat{a} \;=\; 1 \tag{3}$$

and also

$$\{\hat{a}, \hat{a}\} \;=\; \{\hat{a}^\dagger, \hat{a}^\dagger\} \;=\; 0 \quad \Longleftrightarrow \quad \hat{a}\hat{a} \;=\; \hat{a}^\dagger\hat{a}^\dagger \;=\; 0. \tag{4}$$

For the bosons we had defined the number-of-quanta operator as $\hat{n} = \hat{a}^\dagger\hat{a}$, while the product of $\hat{a}$ and $\hat{a}^\dagger$ in the opposite order was $\hat{a}\hat{a}^\dagger = \hat{n} + 1$. For the fermions we also

define the number-of-quanta operator as $\hat{n} = \hat{a}^\dagger\hat{a}$, but now the product of $\hat{a}$ and $\hat{a}^\dagger$ in the opposite order is $\hat{a}\hat{a}^\dagger = 1 - \hat{n}$. Consequently, for the fermions

$$\hat{n}(1 - \hat{n}) \;=\; \hat{a}^\dagger\hat{a}\hat{a}\hat{a}^\dagger \;=\; 0 \quad \text{because} \;\; \hat{a}\hat{a} \;=\; 0, \tag{5}$$

which means that all the eigenvalues of $\hat{n}$ must obey $n(1 - n) = 0$. This immediately gives us the *Pauli principle:* the only allowed occupation numbers for the fermions are $n = 0$ and $n = 1$.

The algebra of the fermionic creation / annihilation operators closes in the two-dimensional Hilbert space spanning one $|n = 0\rangle$ state and one $|n = 1\rangle$ state. Specifically,

$$
\begin{aligned}
\hat{a}\,|0\rangle &\;=\; 0, &\text{(6.a)}\\
\hat{a}^\dagger\,|0\rangle &\;=\; |1\rangle, &\text{(6.b)}\\
\hat{a}\,|1\rangle &\;=\; |0\rangle, &\text{(6.c)}\\
\hat{a}^\dagger\,|1\rangle &\;=\; 0, &\text{(6.d)}
\end{aligned}
$$

or in matrix notations

$$\hat{a} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \hat{a}^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad \text{for} \quad |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{7}$$

These matrices obviously obey the anticommutation relations (3) and (4). Less obviously, there are no other solutions for the fermionic algebra. To prove that, we start by noting that $\hat{a}(1 - \hat{n}) = \hat{a}\hat{a}\hat{a}^\dagger = 0$ (because $\hat{a}\hat{a} = 0$) and $\hat{a}^\dagger\hat{n} = \hat{a}^\dagger\hat{a}^\dagger\hat{a} = 0$ (because $\hat{a}^\dagger\hat{a}^\dagger = 0$). Also, by definition of the eigenstates $|0\rangle$ and $|1\rangle$ of $\hat{n}$, $\;|1\rangle = \hat{n}\,|1\rangle$ and $|0\rangle = (1 - \hat{n})\,|0\rangle$. Consequently,

$$
\begin{aligned}
\hat{a}\,|0\rangle &\;=\; \hat{a}(1 - \hat{n})\,|0\rangle \;=\; 0, &\text{(6.a)}\\
\hat{a}^\dagger\,|1\rangle &\;=\; \hat{a}^\dagger\hat{n}\,|1\rangle \;=\; 0. &\text{(6.d)}
\end{aligned}
$$

Next, we check that $\hat{a}^\dagger \left|0\right\rangle$ and $\hat{a} \left|1\right\rangle$ are eigenstates of $\hat{n}$ with respective eigenvalues 1 and 0 as in eqs. (6,b–c):

$$
\begin{aligned}
(\hat{n} - 1)\big(\hat{a}^\dagger \left|0\right\rangle\big) &= -\hat{a}\hat{a}^\dagger\hat{a}^\dagger \left|0\right\rangle = 0 \quad \text{because } \hat{a}^\dagger\hat{a}^\dagger = 0, \\
(\hat{n} - 0)\big(\hat{a} \left|1\right\rangle\big) &= \hat{a}^\dagger\hat{a}\hat{a} \left|1\right\rangle = 0 \quad \text{because } \hat{a}\hat{a} = 0.
\end{aligned}
\tag{8}
$$

This means that $\hat{a}^\dagger \left|0\right\rangle \propto$ some $\left|1\right\rangle$ and $\hat{a} \left|1\right\rangle \propto$ some $\left|0\right\rangle$, but we need to make sure that applying $\hat{a}$ to $\hat{a}^\dagger \left|0\right\rangle$ we get back to the same state $\left|0\right\rangle$ we stated from, and likewise applying $\hat{a}^\dagger$ to $\hat{a} \left|1\right\rangle$ brings us back to the original $\left|1\right\rangle$:

$$
\begin{aligned}
\hat{a}\big(\left|1\right\rangle = \hat{a}^\dagger \left|0\right\rangle\big) &= \hat{a}\hat{a}^\dagger \left|0\right\rangle = (1 - \hat{n}) \left|0\right\rangle = \text{same } \left|0\right\rangle, \\
\hat{a}^\dagger\big(\left|0\right\rangle = \hat{a} \left|1\right\rangle\big) &= \hat{a}^\dagger\hat{a} \left|1\right\rangle = \hat{n} \left|1\right\rangle = \text{same } \left|1\right\rangle.
\end{aligned}
\tag{9}
$$

Finally, to make sure there are no numerical factors in eqs. (6,b–c) let's check the normalization: if $\left|1\right\rangle = \hat{a}^\dagger \left|0\right\rangle$ then $\left\langle 1|1\right\rangle = \left\langle 0\right| \hat{a}\hat{a}^\dagger \left|0\right\rangle = \left\langle 0\right| (1 - \hat{n}) \left|0\right\rangle = 1 \times \left\langle 0|0\right\rangle$ and likewise, if $\left|0\right\rangle = \hat{a} \left|1\right\rangle$ then $\left\langle 0|0\right\rangle = \left\langle 1\right| \hat{a}^\dagger\hat{a} \left|1\right\rangle = \left\langle 1\right| \hat{n} \left|1\right\rangle = 1 \times \left\langle 1|1\right\rangle$. In other words, both eqs. (6,b–c) as written are consistent with normalized states $\left\langle 0|0\right\rangle = \left\langle 1|1\right\rangle = 1$.

Multiple Fermionic Modes

Now consider multiple fermionic creation and annihilation operators $\hat{a}^\dagger_\alpha$ and $\hat{a}_\alpha$ that are hermitian conjugates of each other and satisfy the anti-commutation relations (2). For each mode α we define the occupation number operator

$$
\hat{n}_\alpha \;\overset{\text{def}}{=}\; \hat{a}^\dagger_\alpha \hat{a}_\alpha.
\tag{10}
$$

All these operators commute with each other; moreover, each $\hat{n}_\alpha$ commutes with creation and annihilation operators for all the other modes $\beta \neq \alpha$. Indeed, using the Leibniz rules for commutators and anti-commutators

$$
\begin{aligned}
[A, BC] &= [A, B]C + B[A, C] = \{A, B\}C - B\{A, C\}, \\
[AB, C] &= A[B, C] + [A, C]B = A\{B, C\} - \{A, C\}B, \\
\{A, BC\} &= [A, B]C + B\{A, C\} = \{A, B\}C - B[A, C], \\
\{AB, C\} &= A[B, C] + \{A, C\}B = A\{B, C\} - [A, C]B,
\end{aligned}
\tag{11}
$$

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we obtain

$$
\begin{aligned}
\big[\hat{n}_\alpha, \hat{a}_\beta\big] &= \big[\hat{a}_\alpha^\dagger \hat{a}_\alpha, \hat{a}_\beta\big] = \hat{a}_\alpha^\dagger \{\hat{a}_\alpha, \hat{a}_\beta\} - \{\hat{a}_\alpha^\dagger, \hat{a}_\beta\}\hat{a}_\alpha = \hat{a}_\alpha^\dagger \times 0 - \delta_{\alpha\beta} \times \hat{a}_\alpha \\
&= -\delta_{\alpha\beta} \times \hat{a}_\beta \to 0 \quad \text{for } \beta \neq \alpha, \tag{12} \\
\big[\hat{n}_\alpha, \hat{a}_\beta^\dagger\big] &= \big[\hat{a}_\alpha^\dagger \hat{a}_\alpha, \hat{a}_\beta^\dagger\big] = \hat{a}_\alpha^\dagger \{\hat{a}_\alpha, \hat{a}_\beta^\dagger\} - \{\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger\}\hat{a}_\alpha = \hat{a}_\alpha^\dagger \times \delta_{\alpha\beta} - 0 \times \hat{a}_\alpha \\
&= +\delta_{\alpha\beta} \times \hat{a}_\beta \to 0 \quad \text{for } \beta \neq \alpha, \tag{13} \\
\big[\hat{n}_\alpha, \hat{a}_\beta^\dagger \hat{a}_\gamma\big] &= \hat{a}_\beta^\dagger \big[\hat{n}_\alpha, \hat{a}_\gamma\big] + \big[\hat{n}_\alpha, \hat{a}_\beta^\dagger\big]\hat{a}_\gamma = -\hat{a}_\beta^\dagger \times \delta_{\alpha\gamma}\hat{a}_\gamma + \delta_{\alpha\beta}\hat{a}_\beta^\dagger \times \hat{a}_\gamma \\
&= \big(\delta_{\alpha\beta} - \delta_{\alpha\gamma}\big)\hat{a}_\beta^\dagger \hat{a}_\gamma \to 0 \quad \text{for } \beta = \gamma, \tag{14} \\
\big[\hat{n}_\alpha, \hat{n}_\beta\big] &= \big[\hat{n}_\alpha, \hat{a}_\beta^\dagger \hat{a}_\beta\big] = 0. \tag{15}
\end{aligned}
$$

The fact that all the $\hat{n}_\alpha$ commute with each other allows us to diagonalize all of them at once. This gives us the occupation-number basis of states $|\text{set of all } n_\alpha\rangle$ for the whole Hilbert space of the theory. Similar to the bosonic case, we may use the $\hat{a}_\alpha^\dagger$ and $\hat{a}_\alpha$ operators to raise or lower any particular n_α without changing the other occupation numbers n_β; this means that all the occupation numbers may take any allowed values independently from each other. However, the only allowed values of the fermionic occupation numbers are 0 and 1 — multiple quanta in the same mode are not allowed.

Note that for a finite set of M modes the fermionic Hilbert space has a finite dimension 2^M. This fact is important for understanding the ground state degeneracies of fermionic fields in some non-trivial backgrounds that have zero-energy fermionic modes: For M zero modes, the ground level of the whole QFT has 2^M degenerate states.

Fermionic Fock Space

Now suppose there is an infinite but discrete set of fermionic modes α corresponding to some 1–particle quantum states $|\alpha\rangle$ with wave functions $\phi_\alpha(\mathbf{x})$. (By abuse of notations, I am including the spin and the other non-spatial quantum numbers into

$\mathbf{x} = (x, y, z, \mathrm{spin}, \mathit{etc}.)$.) In this case, the fermionic Hilbert space

$$\mathcal{F} = \bigotimes_\alpha \mathcal{H}_{\mathrm{mode}\,\alpha} \;(\text{spanning } |n_\alpha = 0\rangle \text{ and } |n_\alpha = 1\rangle) \tag{16}$$

has infinite dimension and we may interpret is as the *Fock space* of arbitrary number of identical fermions. Indeed, let the operator

$$\hat{N} = \sum_\alpha \hat{n}_\alpha \tag{17}$$

count the net number of fermionic quanta in all the modes, $N = 0, 1, 2, 3 \ldots, \infty$. Let's reorganize $\mathcal{F}$ into the eigenblocks of $\hat{N}$:

$$\mathcal{F} = \bigoplus_{N=0}^\infty \mathcal{H}_N = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \mathcal{H}_3 \oplus \cdots. \tag{18}$$

The $\mathcal{H}_0$ block here spans a unique state with $N = 0$, namely the vacuum state $|\mathrm{vac}\rangle = |\text{all } n_\alpha = 0\rangle$. The $\mathcal{H}_1$ block spans states with a single $n_\alpha = 1$ while all the other $n_\beta = 0$. Similar to the bosonic case, we may identify such states $|n_\alpha = 1; \text{other } n = 0\rangle = \hat{a}_\alpha^\dagger |\mathrm{vac}\rangle$ with the single-particle states $|\alpha\rangle$ and hence the $\mathcal{H}_1$ block of $\mathcal{F}$ with the Hilbert space of a single particle.

The $\mathcal{H}_2$ block of $\mathcal{F}$ spans states

$$\left|n_\alpha = n_\beta = 1; \text{other } n = 0\right\rangle = \hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger |\mathrm{vac}\rangle \tag{19}$$

with $\alpha \neq \beta$ and only such states — the fermionic Fock space does not allow states $|n_\alpha = 2; \text{other } n = 0\rangle$ with doubly occupied modes. Moreover, since the creation operators $\hat{a}_\alpha^\dagger$ and $\hat{a}_\beta^\dagger$ anti-commute with each other, exchanging $\alpha \leftrightarrow \beta$ results in the same physical state but with an opposite sign. Consequently, the occupation numbers

define the fermionic state only up to an overall sign; to be more precise, we define

$$|\alpha, \beta\rangle \overset{\text{def}}{=} \hat{a}_\beta^\dagger \hat{a}_\alpha^\dagger |\text{vac}\rangle = -|\beta, \alpha\rangle. \tag{20}$$

Likewise, the $\mathcal{H}_3$ block spans states

$$|\alpha, \beta, \gamma\rangle = \hat{a}_\gamma^\dagger \hat{a}_\beta^\dagger \hat{a}_\alpha^\dagger |\text{vac}\rangle \tag{21}$$

for 3 *different* modes α, β, γ; the $\mathcal{H}_4$ block spans states

$$|\alpha, \beta, \gamma, \delta\rangle = \hat{a}_\delta^\dagger \hat{a}_\gamma^\dagger \hat{a}_\beta^\dagger \hat{a}_\alpha^\dagger |\text{vac}\rangle \tag{22}$$

for 4 *different* modes $\alpha, \beta, \gamma, \delta$, *etc.*, *etc.* In all cases, the order of the modes $\alpha, \beta, \gamma, \ldots$ does not matter physically but affects the overall sign of the state,

$$|\text{any permutation of } \alpha, \beta, \ldots, \omega\rangle = |\alpha, \beta, \ldots, \omega\rangle \times (-1)^{\text{parity of the permutation}}. \tag{23}$$

Thus, each $\mathcal{H}_N$ (for $N \geq 2$) is a Hilbert space of N identical Fermions.

A system of two identical fermions has an antisymmetric wave-function of two arguments, $\psi(\mathbf{x}_1, \mathbf{x}_2) = -\psi(\mathbf{x}_2, \mathbf{x}_1)$. A complete basis for such wavefunctions can be made from antisymmetrized tensor products of single-particle wave-functions

$$\phi_{\alpha\beta}(\mathbf{x}_1, \mathbf{x}_2) = \frac{\phi_\alpha(\mathbf{x}_1)\phi_\beta(\mathbf{x}_2) - \phi_\beta(\mathbf{x}_1)\phi_\alpha(\mathbf{x}_2)}{\sqrt{2}} = -\phi_{\alpha\beta}(\mathbf{x}_2, \mathbf{x}_1). \tag{24}$$

Note that such wave functions are not only antisymmetric in $\mathbf{x}_1 \leftrightarrow \mathbf{x}_2$ but also separately antisymmetric in $\alpha \leftrightarrow \beta$, $\phi_{\beta\alpha}(\mathbf{x}_1, \mathbf{x}_2) = -\phi_{\alpha\beta}(\mathbf{x}_1, \mathbf{x}_2)$, so we may identify them as wave functions of two-fermions states $|\alpha, \beta\rangle = \hat{a}_\beta^\dagger \hat{a}_\alpha^\dagger |\text{vac}\rangle = -|\beta, \alpha\rangle \in \mathcal{H}_2$.

Likewise, a wavefunction of N identical fermions is totally antisymmetric in its N arguments,

$$\psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) = \psi(\text{any permutation of } \mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) \times (-1)^{\text{parity of permutation}}. \tag{25}$$

A complete basis for such wavefunctions obtains from totally antisymmetrized products of N different single-particle wave-functions

$$\phi_{\alpha_1, \ldots, \alpha_N}(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \sum_{(\tilde{\alpha}_1, \ldots, \tilde{\alpha}_N)}^{\substack{\text{all permutations} \\ \text{of } (\alpha_1, \ldots, \alpha_N)}} \phi_{\tilde{\alpha}_1}(\mathbf{x}_1) \times \cdots \times \phi_{\tilde{\alpha}_N}(\mathbf{x}_N) \times (-1)^{\text{parity}}$$

$$= \frac{1}{\sqrt{N!}} \det \begin{vmatrix} \phi_{\alpha_1}(\mathbf{x}_1) & \phi_{\alpha_2}(\mathbf{x}_1) & \cdots & \phi_{\alpha_N}(\mathbf{x}_1) \\ \phi_{\alpha_1}(\mathbf{x}_2) & \phi_{\alpha_2}(\mathbf{x}_2) & \cdots & \phi_{\alpha_N}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{\alpha_1}(\mathbf{x}_N) & \phi_{\alpha_2}(\mathbf{x}_N) & \cdots & \phi_{\alpha_N}(\mathbf{x}_N) \end{vmatrix}. \tag{26}$$

The determinant here — called the *Slater determinant* — is properly antisymmetric in $(\mathbf{x}_1, \ldots, \mathbf{x}_N)$, and it's also antisymmetric with respect to the single-particle states $(\alpha_1, \ldots, \alpha_N)$, which allows us to identify it as the wave-function of the N-fermion state

$$|\alpha_1, \alpha_2, \ldots, \alpha_N\rangle = \hat{a}_{\alpha_N}^\dagger \cdots \hat{a}_{\alpha_2}^\dagger \hat{a}_{\alpha_1}^\dagger |\text{vac}\rangle \in \mathcal{N}_N. \tag{27}$$

To complete the wave-function picture of the Fermionic Fock space, let me spell out the action of the creation operators $\hat{a}_\alpha^\dagger$ and the annihilation operators $\hat{a}_\alpha$. For any N-fermions state $|N; \psi\rangle$ with a totally-antisymmetric wave function $\psi(\mathbf{x}_1, \ldots, \mathbf{x}_N)$, the state $|N+1; \psi'\rangle = \hat{a}_\alpha^\dagger |N; \psi\rangle$ has a totally antisymmetric function of $N+1$ variables

$$\psi'(\mathbf{x}_1, \ldots, \mathbf{x}_{N+1}) = \frac{1}{\sqrt{N+1}} \sum_{i=1}^{N+1} (-1)^{N+1-i} \phi_\alpha(\mathbf{x}_i) \times \psi(\mathbf{x}_1, \ldots, \cancel{\mathbf{x}}_i, \ldots, \mathbf{x}_{N+1}) \tag{28}$$

while the state $|N-1, \psi''\rangle = \hat{a}_\alpha |N, \psi\rangle$ has a totally antisymmetric function of $N-1$

variables

$$\psi''(\mathbf{x}_1, \ldots, \mathbf{x}_{N-1}) = \sqrt{N} \int d^3\mathbf{x}_N \, \phi_\alpha^*(\mathbf{x}_N) \times \psi(\mathbf{x}_1, \ldots, \mathbf{x}_{N-1}, \mathbf{x}_N). \qquad (29)$$

The proof of these formulae is left out as an optional exercise to the students.

Thanks to the relations (29) and (28), the Fock-space formulae for the additive one-body operators work similarly to the bosonic case: If in N-fermion Hilbert spaces

$$\hat{A}_{\text{tot}} = \sum_{i=1}^{N} \hat{A}_1(i^{\text{th}}) \qquad (30)$$

where each $\hat{A}_1(i^{\text{th}})$ acts only on the ith particle, then in the Fock space

$$\hat{A}_{\text{tot}} = \sum_{\alpha,\beta} \langle \alpha | \, \hat{A}_1 \, | \beta \rangle \times \hat{a}_\alpha^\dagger \hat{a}_\beta \, . \qquad (31)$$

For example, for the free non-relativistic electrons in a box with $\alpha = (\mathbf{p}, s)$ we have

$$\begin{aligned}
\hat{H}_{\text{tot}} &= \sum_{\mathbf{p},s} \frac{\mathbf{p}^2}{2m} \times \hat{a}_{\mathbf{p},s}^\dagger \hat{a}_{\mathbf{p},s} \, , \\
\hat{\mathbf{P}}_{\text{tot}} &= \sum_{\mathbf{p},s} \mathbf{p} \times \hat{a}_{\mathbf{p},s}^\dagger \hat{a}_{\mathbf{p},s} \, , \\
\hat{\mathbf{S}}_{\text{tot}} &= \sum_{\mathbf{p},s,s'} \langle \tfrac{1}{2}, s' | \, \hat{\mathbf{S}} \, | \tfrac{1}{2}, s \rangle \times \hat{a}_{\mathbf{p},s'}^\dagger \hat{a}_{\mathbf{p},s} \, .
\end{aligned} \qquad (32)$$

Likewise, the two-body additive operators that act in N-fermion spaces as

$$\hat{B}_{\text{tot}} = \tfrac{1}{2} \sum_{i \neq j} \hat{B}_2(i^{\text{th}}, j^{\text{th}}) \qquad (33)$$

in the Fock space become

$$\hat{B}_{\text{tot}} = \tfrac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} B_{\alpha,\beta,\gamma,\delta} \times \hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger \hat{a}_\delta \hat{a}_\gamma \quad \langle\!\langle \text{note the order!} \rangle\!\rangle$$
$$\text{where } B_{\alpha,\beta,\gamma,\delta} = (\langle \alpha | \otimes \langle \beta |) \, \hat{B}_2 \, (|\gamma\rangle \otimes |\delta\rangle) \, . \qquad (34)$$

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For example, a spin-blind potential $V_2(\mathbf{x}_1 - \mathbf{x}_2)$ becomes

$$
\begin{aligned}
\hat{V}_{\text{tot}} &= \tfrac{1}{2} \sum_{i \neq j} V_2(\mathbf{x}_i - \mathbf{x}_j) \\
&= \frac{1}{2L^3} \sum_{\mathbf{q}} W(\mathbf{q}) \sum_{\mathbf{p}_1, \mathbf{p}_2} \sum_{s_1, s_2} \hat{a}^\dagger_{\mathbf{p}_1+\mathbf{q}, s_1} \hat{a}^\dagger_{\mathbf{p}_2-\mathbf{q}, s_2} \hat{a}_{\mathbf{p}_2, s_2} \hat{a}_{\mathbf{p}_1, s_1} \qquad (35)
\end{aligned}
$$

$$
\text{where } W(\mathbf{q}) = \int d^3\mathbf{x}\, V_2(\mathbf{x}) e^{-i\mathbf{q}\mathbf{x}}.
$$

Note that while the formulae for this operator in the bosonic and the fermionic Fock spaces have similar forms, the actual operators are quite different because the two Fock spaces have different algebras of the creation and annihilation operators and different quantum states (symmetric vs. antisymmetric). Thus, the physical effect of similar $V_2(\mathbf{x}_1 - \mathbf{x}_2)$ potentials for the fermions and for the bosons may be quite different from each other.

Fermionic Particles and Holes

Consider a system of fermions with a one-body Hamiltonian of the form

$$
\hat{H} = \sum_{\alpha} \mathcal{E}_\alpha \hat{a}^\dagger_\alpha \hat{a}_\alpha + E_0. \qquad (36)
$$

When **all** particle energies $\mathcal{E}_\alpha$ are positive, the ground state of the system is the vacuum state $|\text{vac}\rangle$ with all $n_\alpha = 0$. In terms of the creation and annihilation operators, $|\text{vac}\rangle$ can be identified as the unique state killed by all the annihilation operators, $\hat{a}_\alpha |\text{vac}\rangle = 0 \; \forall \alpha$. The excited states of the Hamiltonian (36) are N-particle states which obtain by applying creation operators to the vacuum, $|\alpha_1, \ldots, \alpha_N\rangle = \hat{a}^\dagger_{\alpha_N} \cdots \hat{a}^\dagger_{\alpha_1} |\text{vac}\rangle$; the energy of such a state is $E = E_0 + \mathcal{E}_{\alpha_a} + \cdots \mathcal{E}_{\alpha_N} > E_0$.

Now suppose for a moment that all the particle energies $\mathcal{E}_\alpha$ are negative instead of positive. In this case, adding particles decreases the energy, so the ground state of

the system is not the vacuum but rather the full-to-capacity state

$$|\text{full}\rangle \;=\; |\text{all } n_\alpha = 1\rangle \;=\; \prod_{\text{all }\alpha} \hat{a}_\alpha^\dagger \, |\text{vac}\rangle \tag{37}$$

with energy

$$E_{\text{full}} \;=\; E_0 \;+\; \sum_{\text{all }\alpha} \mathcal{E}_\alpha \,. \tag{38}$$

Never mind whether the sum here is convergent; if it is not, we may add an infinite constant to the E_0 to cancel the divergence. What's important to us here are the energy differences between this ground state and the excited states.

The excited states of the system are not completely full but have a few *holes*. That is, $n_{\alpha_1} = \cdots = n_{\alpha_N} = 0$ for some N modes $(\alpha_1, \ldots, \alpha_N)$, while all the *other* $n_\beta = 1$. The energy of such a state is

$$E \;=\; E_0 \;+\; \sum_{\beta \neq \alpha_a, \ldots, \alpha_N} \mathcal{E}_\beta \;=\; E_{\text{full}} \;-\; \sum_{i=1}^{N} \mathcal{E}_{\alpha_i} \;>\; E_{\text{full}} \,. \tag{39}$$

In other words, an un-filled hole in mode α carries a positive energy $-\mathcal{E}_\alpha$.

In terms of the operator algebra, the $|\text{full}\rangle$ state is the unique state killed by all the creation operators, $\hat{a}_\alpha^\dagger \, |\text{full}\rangle = 0 \;\forall \alpha$. The holes can be obtained by acting on the $|\text{full}\rangle$ state with the annihilation operators that remove one particle at a time. Thus,

$$|1 \text{ hole at } \alpha\rangle \;=\; \left| \hat{n}_\alpha = 0; \text{ other } n = 1 \right\rangle \;=\; \hat{a}_\alpha \, |\text{full}\rangle \tag{40}$$

and likewise

$$|N \text{ holes at } \alpha_1, \ldots, \alpha_N\rangle \;=\; \hat{a}_{\alpha_N} \cdots \hat{a}_{\alpha_1} \, |\text{full}\rangle \,. \tag{41}$$

Altogether, when the ground state is $|\text{full}\rangle$, the creation and the annihilation operators exchange their roles. Indeed, the $\hat{a}_\alpha$ make extra holes in the full or almost-full states while the $\hat{a}_\alpha^\dagger$ operators annihilates those holes (by filling them up). Also, the algebraic definition of the $|\text{full}\rangle$ and $|\text{vac}\rangle$ states are related by this exchange: $\hat{a}_\alpha \, |\text{vac}\rangle = 0 \;\forall \alpha$ vs. $\hat{a}_\alpha^\dagger \, |\text{full}\rangle = 0 \;\forall \alpha$.

To make this exchange manifest, let us define a new family of fermionic creation and annihilation operators,

$$\hat{b}_\alpha \;=\; \hat{a}_\alpha^\dagger, \quad \hat{b}_\alpha^\dagger \;=\; \hat{a}_\alpha. \tag{42}$$

Unlike the bosonic commutation relations (1), the fermionic anti-commutation relations (2) are symmetric between $\hat{a}$ and $\hat{a}^\dagger$, so the $\hat{b}_\alpha$ and $\hat{b}_\alpha^\dagger$ satisfy exactly the same anti-commutation relations as the $\hat{a}_\alpha$ and $\hat{a}_\alpha^\dagger$,

$$\begin{pmatrix} \{\hat{a}_\alpha, \hat{a}_\beta\} = 0 \\ \{\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger\} = 0 \\ \{\hat{a}_\alpha, \hat{a}_\beta^\dagger\} = \delta_{\alpha\beta} \end{pmatrix} \Longleftrightarrow \begin{pmatrix} \{\hat{b}_\alpha, \hat{b}_\beta\} = 0 \\ \{\hat{b}_\alpha^\dagger, \hat{b}_\beta^\dagger\} = 0 \\ \{\hat{b}_\alpha, \hat{b}_\beta^\dagger\} = \delta_{\alpha\beta} \end{pmatrix}. \tag{43}$$

Physically, the $\hat{b}_\alpha^\dagger$ operators *create holes* while the $\hat{b}_\alpha$ operators *annihilate holes*, and the holes obey exactly the same Fermi statistics as the original particles. In condensed-matter terminology, the holes are *quasi-particles*, but the only distinction between the quasi-particles and the true particles is that the later may exist outside the condensed matter. When viewed from the inside of condensed matter, this distinction becomes irrelevant.

Anyhow, from the hole point of view, the $|\text{full}\rangle$ state is the *hole vacuum* — the unique state with no holes at all, algebraically defined by $\hat{b}_\alpha |\text{full}\rangle = 0 \; \forall\alpha$. The excitations are N-hole states obtained by acting with hole-creation operators $\hat{b}_\alpha^\dagger$ on the hole-vacuum, $|\text{holes at } \alpha_1, \ldots, \alpha_N\rangle = \hat{b}_{\alpha_N}^\dagger \cdots \hat{b}_{\alpha_1}^\dagger |\text{full}\rangle$. And the Hamiltonian operator (36) of the system becomes

$$\begin{aligned} \hat{H} \;&=\; E_0 \;+\; \sum_\alpha \mathcal{E}_\alpha \left(\hat{a}_\alpha^\dagger \hat{a}_\alpha \;=\; \hat{b}_\alpha \hat{b}_\alpha^\dagger \;=\; 1 - \hat{b}_\alpha^\dagger \hat{b}_\alpha \right) \\ &=\; E_{\text{full}} \;+\; \sum_\alpha (-\mathcal{E}_\alpha) \hat{b}_\alpha^\dagger \hat{b}_\alpha \,, \end{aligned} \tag{44}$$

in accordance with individual holes having positive energies $-\mathcal{E}_\alpha > 0$.

Quantum Numbers of the Holes

Thus far, all I had assumed about the one-particle states $|\alpha\rangle$ corresponding to modes α is that they have definite energies $\mathcal{E}_\alpha$. But in most cases, they also have definite values of some other additive quantities, such as momentum $\mathbf{p}_\alpha$ (or lattice momentum, defined modulo ummklapp), spin (or rather S_α^z), electric charge, *etc.*, *etc.* For all such quantities, a hole has exactly opposite quantum numbers from the missing fermion. Indeed,

$$\hat{a}_\alpha^\dagger \hat{a}_\alpha \;=\; 1 \;-\; \hat{b}_\alpha^\dagger \hat{b}_\alpha \quad \Longrightarrow \quad \hat{A} \;=\; A_{\text{empty}} \;+\; \sum_\alpha A_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha \;=\; A_{\text{full}} \;+\; \sum_\alpha (-A_\alpha) \hat{b}_\alpha^\dagger \hat{b}_\alpha \,, \tag{45}$$

thus

$$\begin{aligned}
\hat{H} \;&=\; E_{\text{full}} \;+\; \sum_\alpha (-\mathcal{E}_\alpha) \hat{b}_\alpha^\dagger \hat{b}_\alpha \,, \\
\hat{\mathbf{P}}_{\text{net}} \;&=\; \mathbf{P}_{\text{full}} \;+\; \sum_\alpha (-\mathbf{p}_\alpha) \hat{b}_\alpha^\dagger \hat{b}_\alpha \,, \\
\hat{S}_{\text{net}}^z \;&=\; S_{\text{full}}^z \;+\; \sum_\alpha (-S_\alpha^z) \hat{b}_\alpha^\dagger \hat{b}_\alpha \,, \\
\hat{Q}_{\text{net}} \;&=\; Q_{\text{full}} \;+\; \sum_\alpha (-q = +e) \hat{b}_\alpha^\dagger \hat{b}_\alpha \,,
\end{aligned} \tag{46}$$

etc., *etc.* (On the last line I have assumed the original fermions were electrons whose electric charge is $q = -e$, so the holes have charge $+e$.) The physics behind all these formulae is very simple: creating a hole in a mode α of momentum $\mathbf{p}_\alpha$ means removing a fermion carrying that momentum, so the net momentum of the system changes by $-\mathbf{p}_\alpha$, which we interpret as the hole having momentum $-\mathbf{p}_\alpha$ — and likewise for the spin, energy, electric charge, and other quantum number of the holes.

Quite often we use the additive quantum numbers such as $\mathbf{p}$ and $s = S^z$ to label the one particles states, $|\alpha\rangle = |\mathbf{p}, s\rangle$. In such cases it is convenient to label the holes by their own quantum numbers rather than the QN of the missing fermions, so we define the hole creation and annihilation operators as

$$\hat{b}_{\mathbf{p},s} \;=\; \hat{a}_{-\mathbf{p},-s}^\dagger \,, \quad \hat{b}_{\mathbf{p},s}^\dagger \;=\; \hat{a}_{-\mathbf{p},-s} \,. \tag{47}$$

This definition leads to

$$\hat{\mathbf{P}}_{\text{net}} \;=\; \sum_{\mathbf{p},s}(+\mathbf{p})\hat{b}^{\dagger}_{\mathbf{p},s}\hat{b}_{\mathbf{p},s} \quad\text{and}\quad \hat{S}^{z}_{\text{net}} \;=\; \sum_{\mathbf{p},s}(+s)\hat{b}^{\dagger}_{\mathbf{p},s}\hat{b}_{\mathbf{p},s} \tag{48}$$

— assuming $\mathbf{P}_{\text{full}} = 0$ and $S^{z}_{\text{full}} = 0$, — but it does not change the sign of the holes' electric charge, thus

$$\hat{Q}_{\text{net}} \;=\; Q_{\text{full}} \;+\; \sum_{\mathbf{p},s}(-q = +e)\hat{b}^{\dagger}_{\mathbf{p},s}\hat{b}_{\mathbf{p},s}\,. \tag{49}$$

FERMI SEA

Now consider a more general fermionic system where the energies $\mathcal{E}_{\alpha}$ take both signs: negative for some modes α but positive for others. For example, the free-energy operator of the free fermion gas with a positive chemical potential $\mu = (p_f^2/2m)$

$$\hat{H} \;=\; \sum_{\mathbf{p},s}\left(\mathcal{E}_{\mathbf{p},s} \;=\; \frac{\mathbf{p}^2}{2m} - \mu\right)\hat{a}^{\dagger}_{\mathbf{p},s}\hat{a}_{\mathbf{p},s}\,, \tag{50}$$

has negative $\mathcal{E}_{\mathbf{p},s}$ for momenta inside the Fermi sphere ($|\mathbf{p}| < p_f$) but positive $\mathcal{E}_{\mathbf{p},s}$ for momenta outside that sphere ($|\mathbf{p}| > p_f$) For this system the ground state is the *Fermi sea* where

$$n_{\mathbf{p},s} \;=\; \Theta(|\mathbf{p}| < p_F) \;=\; \begin{cases} 1 & \text{for } |\mathbf{p}| < p_f, \\ 0 & \text{for } |\mathbf{p}| > p_f. \end{cases} \tag{51}$$

In terms of the creation and annihilation operators, the Fermi sea is the state

$$|\text{FS}\rangle \;=\; \prod_{\mathbf{p},s}^{|\mathbf{p}|<p_f\text{ only}} \hat{a}^{\dagger}_{\mathbf{p},s}\,|\text{vac}\rangle \tag{52}$$

which satisfies

$$\hat{a}_{\mathbf{p},s}\,|\text{FS}\rangle \;=\; 0 \text{ for } |\mathbf{p}| > p_f \quad\text{but}\quad \hat{a}^{\dagger}_{\mathbf{p},s}\,|\text{FS}\rangle \;=\; 0 \text{ for } |\mathbf{p}| < p_f\,. \tag{53}$$

We may treat this state as a quasi-particle vacuum if we redefine all the operators

killing the $|\text{FS}\rangle$ as annihilation operators. Thus, we define

$$\hat{b}_{\mathbf{p},s} = \hat{a}^\dagger_{-\mathbf{p},-s}, \quad \hat{b}^\dagger_{\mathbf{p},s} = \hat{a}_{-\mathbf{p},-s} \quad \textbf{for } |\mathbf{p}| < p_F \textbf{ only} \tag{54}$$

but keep the original $\hat{a}_{\mathbf{p},s}$ and $\hat{a}^\dagger_{\mathbf{p},s}$ operators for momenta outside the Fermi surface. Despite the partial exchange, the complete set or creation and annihilation operators satisfies the fermionic anticommutation relations:

$$\begin{aligned}
\textbf{all } \{\hat{a},\hat{a}\} &= \{\hat{b},\hat{b}\} = \{\hat{a},\hat{b}\} = 0, \\
\textbf{all } \{\hat{a}^\dagger,\hat{a}^\dagger\} &= \{\hat{b}^\dagger,\hat{b}^\dagger\} = \{\hat{a}^\dagger,\hat{b}^\dagger\} = 0, \\
\textbf{all } \{\hat{a},\hat{b}^\dagger\} &= \{\hat{b}^\dagger,\hat{a}\} = 0,
\end{aligned} \tag{55}$$

— provided we *restrict the $\hat{b}_{\mathbf{p},s}$ and the $\hat{b}^\dagger_{\mathbf{p},s}$ to $|\mathbf{p}| < p_f$ only and the $\hat{a}_{\mathbf{p},s}$ and the $\hat{a}^\dagger_{\mathbf{p},s}$ to $|\mathbf{p}| > p_f$ only* — while

$$\{\hat{a}_{\mathbf{p},s},\hat{a}^\dagger_{\mathbf{p}',s'}\} = \delta_{\mathbf{p},\mathbf{p}'}\delta_{s,s'} \quad \text{and} \quad \{\hat{b}_{\mathbf{p},s},\hat{b}^\dagger_{\mathbf{p}',s'}\} = \delta_{\mathbf{p},\mathbf{p}'}\delta_{s,s'}. \tag{56}$$

The Fermi sea $|\text{FS}\rangle$ is the quasi-particle vacuum state of these fermionic operators — it is killed by all the annihilation operators $\hat{a}_{\mathbf{p},s}$ and $\hat{b}_{\mathbf{p},s}$ *in the set.* The two types of creation operators $\hat{a}^\dagger_{\mathbf{p},s}$ and $\hat{b}^\dagger_{\mathbf{p},s}$ create two distinct types of quasi-particles — respectively, the extra fermions above the Fermi surface and the holes below the surface. Both types of quasi-particles have positive energies. Indeed, in terms of our new fermionic operators, the Hamiltonian becomes

$$\hat{H} = E_{\text{FS}} + \sum_{\mathbf{p},s}^{|\mathbf{p}|>p_f \text{ only}} \left(\frac{\mathbf{p}^2}{2m} - \mu > 0\right) \times \hat{a}^\dagger_{\mathbf{p},s}\hat{a}_{\mathbf{p},s} + \sum_{\mathbf{p},s}^{|\mathbf{p}|<p_f \text{ only}} \left(\mu - \frac{\mathbf{p}^2}{2m} > 0\right) \times \hat{b}^\dagger_{\mathbf{p},s}\hat{b}_{\mathbf{p},s}. \tag{57}$$

Graphically,
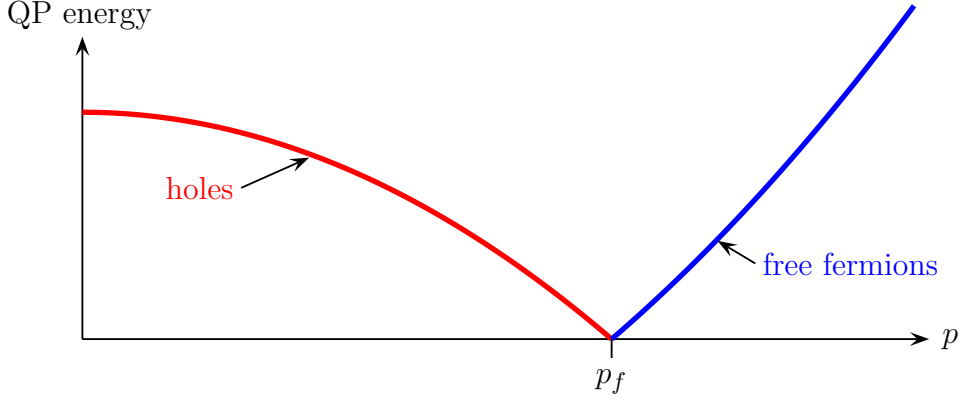
Besides energies, all the quasi-particles have definite momenta, spins S^z, and charges,

$$
\begin{aligned}
\hat{\mathbf{P}}_{\text{tot}} &= \sum_{\mathbf{p},s}^{|\mathbf{p}|>p_f \text{ only}} \mathbf{p} \times \hat{a}^\dagger_{\mathbf{p},s}\hat{a}_{\mathbf{p},s} + \sum_{\mathbf{p},s}^{|\mathbf{p}|<p_f \text{ only}} \mathbf{p} \times \hat{b}^\dagger_{\mathbf{p},s}\hat{b}_{\mathbf{p},s}, \\
\hat{S}^z_{\text{tot}} &= \sum_{\mathbf{p},s}^{|\mathbf{p}|>p_f \text{ only}} s \times \hat{a}^\dagger_{\mathbf{p},s}\hat{a}_{\mathbf{p},s} + \sum_{\mathbf{p},s}^{|\mathbf{p}|<p_f \text{ only}} s \times \hat{b}^\dagger_{\mathbf{p},s}\hat{b}_{\mathbf{p},s}, \\
\hat{Q}_{\text{tot}} &= \sum_{\mathbf{p},s}^{|\mathbf{p}|>p_f \text{ only}} (-e) \times \hat{a}^\dagger_{\mathbf{p},s}\hat{a}_{\mathbf{p},s} + \sum_{\mathbf{p},s}^{|\mathbf{p}|<p_f \text{ only}} (+e) \times \hat{b}^\dagger_{\mathbf{p},s}\hat{b}_{\mathbf{p},s} + Q_{\text{FS}}.
\end{aligned}
\tag{58}
$$

INTERACTING FERMIONS

Besides the free-fermion gas, the particle-hole formalism is very useful for many interacting-fermion systems such as atoms, nuclei, or condensed matter — especially the semiconductors. In the interacting systems, the ground state is quite complicated, but the simple excitations can be described in terms of a few extra particles and/or holes created and annihilated by the fermionic operators — $\hat{a}^\dagger_\alpha$ and $\hat{a}_\alpha$ for the extra particles, and $\hat{b}^\dagger_\alpha$ and $\hat{b}_\alpha$ for the holes. Thus

$$
\hat{H} = E_{\text{ground}} + \sum_\alpha^{\substack{\text{extra}\\\text{particles}}} (\mathcal{E}_\alpha - \mu > 0)\hat{a}^\dagger_\alpha\hat{a}_\alpha + \sum_\alpha^{\text{holes}} (\mu - \mathcal{E}_\alpha > 0)\hat{b}^\dagger_\alpha\hat{b}_\alpha + \hat{H}_{\text{interactions}}.
\tag{59}
$$

while the creation / annihilation operators obey the standard fermionic anti-commutation

15

relations

$$\{\hat{a}_\alpha, \hat{a}_\beta^\dagger\} = \{\hat{b}_\alpha, \hat{b}_\beta^\dagger\} = \delta_{\alpha,\beta}\,,$$
$$\text{all other } \{*, *\} = 0.$$

(60)

Due to interactions between the fermions already existing in the ground state, the $\hat{a}_\alpha^\dagger$ and $\hat{a}_\alpha$ operators not only create / annihilate an extra fermion but also adjust the state of the existing fermions to accommodate for the extra particle, and likewise for the $\hat{b}_\alpha^\dagger$ and $\hat{b}_\alpha$ operators creating / annihilating a hole. Consequently, the relation between these operators operators and the operators creating / annihilating the standalone fermions from the vacuum is quite complicated. But fortunately, we rarely need such relations. All we usually need are the anti-commutation relations (60), the fact that the ground state is annihilated by all the $\hat{a}_\alpha$ and $\hat{b}_\alpha$ operators, the quantum numbers of the extra particles and the holes, and their energies $\mathcal{E}_\alpha$.

Of particular importance are is the spectrum of fermion energies $\mathcal{E}_\alpha$. In atomic and nuclear physics it determines the shell structure of the atom/nucleus, while in condensed matter it distinguishes between metals, semi-metals, semiconductors, and insulators:
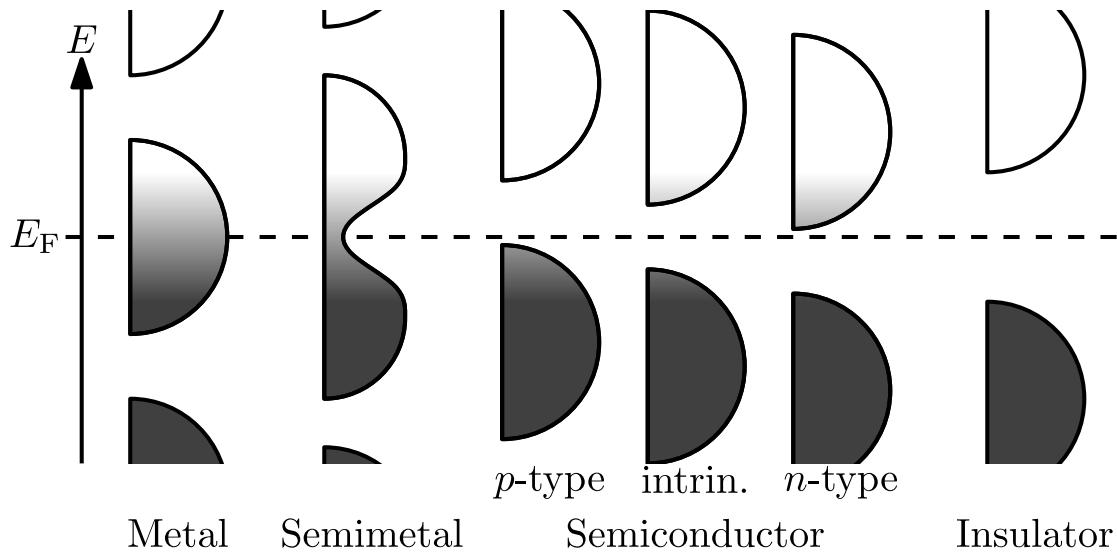
Relativistic Electrons and Positrons.

Now consider a free Dirac spinor field $\hat{\Psi}_\alpha(x)$, for example the electron field. (Note change of notations: from now on, $\alpha, \beta, \ldots$ are Dirac indices running from 1 to 4 rather than the modes of fermionic creation and annihilation operators.) As I explained last lecture (see also my notes on Dirac spinors, Dirac equation, and Dirac fields), the Hamiltonian operator for a free Dirac spinor field is

$$\hat{H} \;=\; \int d^3\mathbf{x}\,\hat{\Psi}_\alpha^\dagger \mathcal{D}_{\alpha\beta}\hat{\Psi}_\beta \tag{61}$$

where

$$\mathcal{D}_{\alpha\beta} \;=\; \left(-i\gamma^0\vec{\gamma}\cdot\nabla \,+\, \gamma^0 m\right)_{\alpha\beta} \tag{62}$$

is the differential operator which acts as one-particle Hamiltonian in the coordinate basis. Apart from the specific form of this differential operator, the Hamiltonian (61) has a similar form to the Hamiltonian of a non-relativistic field theory, so *at first blush* we may thing of $\hat{\Psi}_\alpha(\mathbf{x})$ as a 4–component annihilation field while $\hat{\Psi}_\alpha^\dagger(\mathbf{x})$ is a 4–component creation field.

To expand such fields into the annihilation operators $\hat{a}(\mathbf{p},\ldots)$ and the creation operators $\hat{a}^\dagger(\mathbf{p},\ldots)$, we simply transform to the eigenbasis of the differential operator (62). First, we go to the momentum basis, where $\mathcal{D}$ reduces to a 4×4 matrix in Dirac indices,

$$\mathcal{D}_{\alpha\beta}(p) \;=\; \left(\gamma^0\vec{\gamma}\cdot\mathbf{p} \,+\, \gamma^0 m\right)_{\alpha\beta}. \tag{63}$$

The eigenvalues of this matrix are $(+E_\mathbf{p}, +E_\mathbf{p}, -E_\mathbf{p}, -E_\mathbf{p})$ where $E_\mathbf{p} = +\sqrt{\mathbf{p}^2 + m^2}$, so let me label the corresponding eigenvectors $U_\alpha(\mathbf{p}, \pm, s)$ by the momentum $\mathbf{p}$, the $\pm$ sign of energy, and some other index $s = \pm\frac{1}{2}$ (for example, the spin state) to distinguish between the degenerate eigenstates. Let's normalize the eigenvectors to

$$U^\dagger(\mathbf{p}, \pm, s)U(\mathbf{p}, \pm', s') \;=\; 2E_\mathbf{p} \times \delta_{\pm,\pm'}\delta_{s,s'}; \tag{64}$$

this will help with the relativistic normalization of the creation / annihilation operators.

Next, we define (in the Schrödinger picture)

$$
\begin{aligned}
\hat{a}(\mathbf{p}, \pm, s) &= \int d^3\mathbf{x}\, e^{-i\mathbf{px}} U^\dagger(p, \pm, s)\hat{\Psi}(\mathbf{x}), \\
\hat{a}^\dagger(\mathbf{p}, \pm, s) &= \int d^3\mathbf{x}\, e^{+i\mathbf{px}} \hat{\Psi}(\mathbf{x})^\dagger U(p, \pm, s),
\end{aligned}
\tag{65}
$$

so the reverse transform gives the expansion of the fields into the $\hat{a}$ and $\hat{a}^\dagger$ operators,

$$
\begin{aligned}
\hat{\Psi}_\alpha(\mathbf{x}) &= \int \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{1}{2E_\mathbf{p}} \sum_\pm \sum_s e^{+i\mathbf{px}} U_\alpha(\mathbf{p}, \pm, s) \times \hat{a}(\mathbf{p}, \pm, s), \\
\hat{\Psi}_\alpha^\dagger(\mathbf{x}) &= \int \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{1}{2E_\mathbf{p}} \sum_\pm \sum_s e^{-i\mathbf{px}} U_\alpha^*(\mathbf{p}, \pm, s) \times \hat{a}^\dagger(\mathbf{p}, \pm, s).
\end{aligned}
\tag{66}
$$

Note: the $1/2E_\mathbf{p}$ factor in this expansion stems from the $2E_\mathbf{p}$ factor in the normalization (64) of the U_α eigenvectors.

The anticommutation relations for the $\hat{a}$ and $\hat{a}^\dagger$ operators follow from the anticommutation relations for the fermionic fields. In the Schrödinger picture (or at equal times in other pictures), we have

$$
\begin{aligned}
\left\{\hat{\Psi}_\alpha(\mathbf{x}), \hat{\Psi}_\beta(\mathbf{y})\right\} &= 0, \\
\left\{\hat{\Psi}_\alpha^\dagger(\mathbf{x}), \hat{\Psi}_\beta^\dagger(\mathbf{y})\right\} &= 0, \\
\left\{\hat{\Psi}_\alpha(\mathbf{x}), \hat{\Psi}_\beta^\dagger(\mathbf{y})\right\} &= \delta_{\alpha\beta}\delta^{(3)}(\mathbf{x} - \mathbf{y}),
\end{aligned}
\tag{67}
$$

hence

$$
\begin{aligned}
\{\hat{a}(\mathbf{p}, \pm, s), \hat{a}(\mathbf{p}', \pm', s')\} &= 0, \\
\{\hat{a}^\dagger(\mathbf{p}, \pm, s), \hat{a}^\dagger(\mathbf{p}', \pm', s')\} &= 0, \\
\{\hat{a}(\mathbf{p}, \pm, s), \hat{a}^\dagger(\mathbf{p}', \pm', s')\} &= 2E_\mathbf{p} \times (2\pi)^3 \delta^{(3)}(\mathbf{p} - \mathbf{p}') \times \delta_{\pm,\pm'}\delta_{s,s'}
\end{aligned}
\tag{68}
$$

where the $2E_\mathbf{p}$ factor again stems from the $U_\alpha(\mathbf{p}, \pm, s)$ normalization (64).

Finally, the Dirac fields' Hamiltonian (61) becomes

$$\hat{H} = \int \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{1}{2E_\mathbf{p}} \sum_\pm \sum_s (\pm E_\mathbf{p}) \, \hat{a}^\dagger(\mathbf{p}, \pm, s)\hat{a}(\mathbf{p}, \pm, s). \tag{69}$$

No both positive and negative energy modes in this Hamiltonian. Consequently, the ground state is the Fermi-sea-like *Dirac sea* $|DS\rangle$ where all the negative-energy modes are filled while the positive-energy modes are empty,
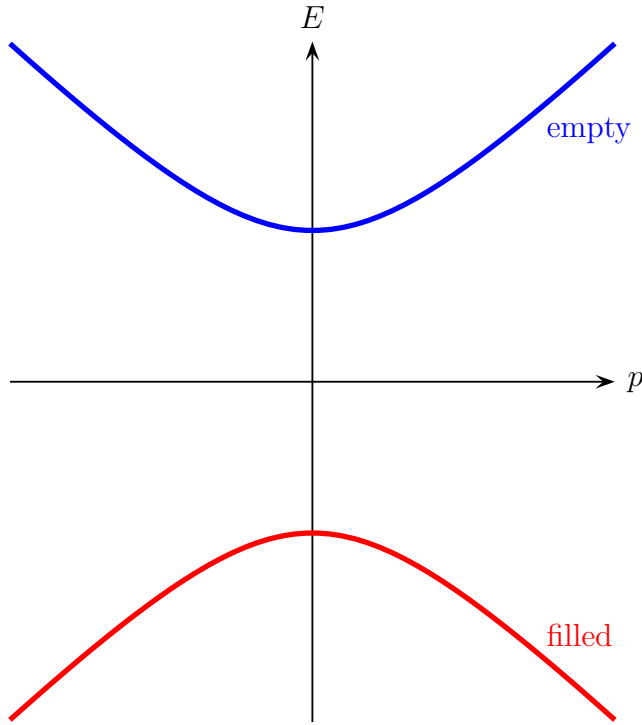
The Dirac sea state is annihilated by the $\hat{a}(\mathbf{p}, +, s)$ and the $\hat{a}^\dagger(\mathbf{p}, -, s)$ operators, so both types of the operators should be treated as the annihilation operators. The $\hat{a}(\mathbf{p}, +, s)$ operators annihilate the physical electrons e^- (which always have positive energies) while the $\hat{a}^\dagger(\mathbf{p}, -, s)$ operators annihilate the holes in the Dirac sea — which physically act as the electron anti-particles, the *positrons e^+*.

Following the usual particle-hole formalism, we re-define the creation / annihila-

tion operators according to

$$
\begin{aligned}
\hat{a}_{\mathbf{p},s} &= \hat{a}(\mathbf{p},+,s) && \text{(annihilates an electron)}, \\
\hat{a}^\dagger_{\mathbf{p},s} &= \hat{a}^\dagger(\mathbf{p},+,s) && \text{(creates an electron)}, \\
\hat{b}_{\mathbf{p},s} &= \hat{a}^\dagger(-\mathbf{p},-,-s) && \text{(annihilates n positron)}, \\
\hat{b}^\dagger_{\mathbf{p},s} &= \hat{a}(-\mathbf{p},-,-s) && \text{(creates n positron)},
\end{aligned}
\tag{70}
$$

so that:

- All these operators obey the fermionic anticommutation relations;

- The Dirac sea state acts as the physical vacuum, so it is killed by all the annihilation operators, both $\hat{a}(\mathbf{p},s)\,|\text{DS}\rangle = 0$ and $\hat{b}(\mathbf{p},s)\,|\text{DS}\rangle = 0$;

- All the physical particles — both the electrons and the positrons — have positive energies $+E_{\mathbf{p}}$, thus

$$
\hat{H} = \int \frac{d^3\mathbf{p}}{(2\pi)^3}\frac{1}{2E_{\mathbf{p}}}\sum_s\left(+E_{\mathbf{p}}\hat{a}^\dagger_{\mathbf{p},s}\hat{a}_{\mathbf{p},s} + E_{\mathbf{p}}\hat{b}^\dagger_{\mathbf{p},s}\hat{b}_{\mathbf{p},s}\right) + \text{const.}
\tag{71}
$$

Finally, let's re-express the quantum fields in terms of the operators creating / annihilating the physical electrons and positrons. Let's define

$$
u_\alpha(\mathbf{p},s) = U_\alpha(\mathbf{p},+,s), \quad v_\alpha(\mathbf{p},s) = U_\alpha(-\mathbf{p},-,-s);
\tag{72}
$$

then the expansions (66) become

$$
\begin{aligned}
\hat{\Psi}_\alpha(\mathbf{x}) &= \int \frac{d^3\mathbf{p}}{(2\pi)^3}\frac{1}{2E_{\mathbf{p}}}\sum_s\left(e^{+i\mathbf{px}}u_\alpha(\mathbf{p},s)\times\hat{a}_{\mathbf{p},s} + e^{+i\mathbf{px}}v_\alpha(-\mathbf{p},-s)\times\hat{b}^\dagger_{-\mathbf{p},-s}\right) \\
&= \int \frac{d^3\mathbf{p}}{(2\pi)^3}\frac{1}{2E_{\mathbf{p}}}\sum_s\left(e^{+i\mathbf{px}}u_\alpha(\mathbf{p},s)\times\hat{a}_{\mathbf{p},s} + e^{-i\mathbf{px}}v_\alpha(\mathbf{p},s)\times\hat{b}^\dagger_{\mathbf{p},s}\right), \\
\hat{\Psi}^\dagger_\alpha(\mathbf{x}) &= \int \frac{d^3\mathbf{p}}{(2\pi)^3}\frac{1}{2E_{\mathbf{p}}}\sum_s\left(e^{-i\mathbf{px}}u^*_\alpha(\mathbf{p},s)\times\hat{a}^\dagger_{\mathbf{p},s} + e^{-i\mathbf{px}}v^*_\alpha(-\mathbf{p},-s)\times\hat{b}_{-\mathbf{p},-s}\right) \\
&= \int \frac{d^3\mathbf{p}}{(2\pi)^3}\frac{1}{2E_{\mathbf{p}}}\sum_s\left(e^{-i\mathbf{px}}u_\alpha(\mathbf{p},s)\times\hat{a}^\dagger_{\mathbf{p},s} + e^{+i\mathbf{px}}v_\alpha(\mathbf{p},s)\times\hat{b}_{\mathbf{p},s}\right).
\end{aligned}
\tag{73}
$$

Note: the $\hat{\Psi}$ field comprises the operators annihilating the electrons or creating the positrons, so its net effect on the electric charge is always $\Delta Q = +e$, while the $\hat{\Psi}^\dagger$

field comprises the operators creating the electrons or annihilating the positrons, so its net effect on the electric charge is always $\Delta Q = -e$.

The expansions (73) work in the Schrödinger picture of the quantum theory. In the Heisenberg picture we incorporate the time dependence according to the usual formulae for the free fields:

$$
\begin{aligned}
\left[\hat{a}_{\mathbf{p},s}, \hat{H}\right] &= +E_{\mathbf{p}} \times \hat{a}_{\mathbf{p},s} &\implies& \quad \hat{a}_{\mathbf{p},s}(t) = e^{-iE_p t} \times \hat{a}_{\mathbf{p},s}(0), \\
\left[\hat{a}^{\dagger}_{\mathbf{p},s}, \hat{H}\right] &= -E_{\mathbf{p}} \times \hat{a}^{\dagger}_{\mathbf{p},s} &\implies& \quad \hat{a}^{\dagger}_{\mathbf{p},s}(t) = e^{+iE_p t} \times \hat{a}^{\dagger}_{\mathbf{p},s}(0), \\
\left[\hat{b}_{\mathbf{p},s}, \hat{H}\right] &= +E_{\mathbf{p}} \times \hat{b}_{\mathbf{p},s} &\implies& \quad \hat{b}_{\mathbf{p},s}(t) = e^{-iE_p t} \times \hat{b}_{\mathbf{p},s}(0), \\
\left[\hat{b}^{\dagger}_{\mathbf{p},s}, \hat{H}\right] &= -E_{\mathbf{p}} \times \hat{b}^{\dagger}_{\mathbf{p},s} &\implies& \quad \hat{b}^{\dagger}_{\mathbf{p},s}(t) = e^{+iE_p t} \times \hat{b}^{\dagger}_{\mathbf{p},s}(0),
\end{aligned}
\tag{74}
$$

hence

$$
\begin{aligned}
\hat{\Psi}_\alpha(x) &= \int \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{1}{2E_{\mathbf{p}}} \sum_s \left(e^{-ipx} u_\alpha(\mathbf{p}, s) \times \hat{a}_{\mathbf{p},s} + e^{+ipx} v_\alpha(\mathbf{p}, s) \times \hat{b}^{\dagger}_{\mathbf{p},s} \right)^{p^0 = +E_{\mathbf{p}}}, \\
\hat{\Psi}^{\dagger}_\alpha(x) &= \int \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{1}{2E_{\mathbf{p}}} \sum_s \left(e^{+ipx} u^*_\alpha(\mathbf{p}, s) \times \hat{a}^{\dagger}_{\mathbf{p},s} + e^{-ipx} v^*_\alpha(\mathbf{p}, s) \times \hat{b}_{\mathbf{p},s} \right)^{p^0 = +E_{\mathbf{p}}}.
\end{aligned}
\tag{75}
$$