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Solid State Theory I

Mini Review

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2nd quantization

The Hilbert space of a system composed of N (for the moment distinguishable) subsystems is given by the tensor product of individual Hilbert spaces

$$\mathcal{H}_N = \mathcal{H}_{S_1} \otimes \mathcal{H}_{S_2} \otimes \ldots \otimes \mathcal{H}_{S_N}. \tag{0.1}$$

A complete basis for this space is given by the tensor product

$$\{|\alpha_{i_1}\rangle \otimes |\alpha_{i_2}\rangle \otimes \ldots \otimes |\alpha_{i_N}\rangle\}, \tag{0.2}$$

where $\{|\alpha_{i_n}\rangle\}$ is a complete set of orthonormal vectors that span the Hilbert space of the system n.
The closure relation for $\mathcal{H}$ is given by

$$\begin{aligned}\sum_{i_1,i_2,\ldots,i_N} |\alpha_{i_1}\rangle \otimes |\alpha_{i_2}\rangle \otimes \ldots \otimes |\alpha_{i_N}\rangle\langle\alpha_{i_1}| \otimes \langle\alpha_{i_2}| \otimes \ldots \otimes \langle\alpha_{i_N}| = \\ \Big(\sum_{i_1} |\alpha_{i_1}\rangle\langle\alpha_{i_1}|\Big) \ldots \Big(\sum_{i_N} |\alpha_{i_N}\rangle\langle\alpha_{i_N}|\Big)\& = \\ \mathbf{1}_1 \otimes \ldots \otimes \mathbf{1}_N.\end{aligned} \tag{0.3}$$

As short-hand for the tensor product above, we will write

$$|\alpha_{i_1}, \alpha_{i_2}, \ldots, \alpha_{i_N}\rangle = |\alpha_{i_1}\rangle \otimes |\alpha_{i_2}\rangle \otimes \ldots \otimes |\alpha_{i_N}\rangle. \tag{0.4}$$

In the case of indistinguishable particles, it can be shown in relativistic quantum field theory that, in three dimensions, the joint wave-function of such a system can have one of two possible symmetries under the interchange of two particles:

- it is symmetric in the case of particles of integer spin (bosons), or
- it is anti-symmetric in the case of particles of half-integer spin (fermions).

This so-called spin-statistics theorem has to be accepted at our level as a fact of life and moreover, it does not hold in two dimensions (the particles with strange interchange properties that are found in certain two-dimensional electron gases are called anyons). If one takes this observation into account, one concludes that the (un-normalised) wave-function of such systems of indistinguishable particles has to have the form

$$\big|\alpha_1, \alpha_2, \ldots, \alpha_N\big\} = \frac{1}{\sqrt{N!}} \sum_P \xi^{\sigma(P)} \big|\alpha_{P(1)}, \alpha_{P(2)}, \ldots, \alpha_{P(N)}\big), \tag{0.5}$$

where P represents one of the $N!$ possible permutations of the numbers $\{1, 2, \ldots, N\}$ and $\xi = \pm 1$, having the plus sign for bosons and the minus sign for fermions. The function $\sigma(P)$ is the order of the permutation, i.e. the number, modulo 2, of transpositions of two numbers at a time that is necessary to perform in order to bring the N numbers in that permutation to their natural order $1 < 2 < ... < N$. It can be shown, e.g. by induction, that a given permutation can always be decomposed into a product of transpositions. Such a decomposition is not unique, but the number of transpositions necessary is either even or odd and thus the order of a permutation is a well-defined quantity. Using the orthonormal character of the basis of each individual particle, it is easy to convince oneself that a second state $\big|\alpha'_1, \alpha'_2, \ldots, \alpha'_N\big\}$ is orthogonal to $\big|\alpha_1, \alpha_2, \ldots, \alpha_N\big\}$ unless the set of the α's constitute a permutation of $\alpha_1, \ldots, \alpha_N$. Thus, one has

$$\big\{\alpha_1, \alpha_2, \ldots, \alpha_N\big|\alpha'_1, \alpha'_2, \ldots, \alpha'_N\big\} = \sum_P \prod_i^N \delta_{\alpha_i, \alpha'_{P(i)}} \parallel \big|\alpha_1, \alpha_2, \ldots, \alpha_N\big\} \parallel^2 , \tag{0.6}$$

where only one of the terms in the summation above is non-zero. Applying the definition given in (0.5), one obtains for the square of the norm of $\big|\alpha_1, \alpha_2, \ldots, \alpha_N\big\}$ the result

$$
\begin{aligned}
&\big\{\alpha_1, \alpha_2, \ldots, \alpha_N\big|\alpha_1, \alpha_2, \ldots, \alpha_N\big\} \\
&= \frac{1}{N!}\sum_{P,P'} \xi^{\sigma(P)+\sigma(P')} \big(\alpha_{P'(1)}, \alpha_{P'(2)}, \ldots, \alpha_{P'(N)}\big|\alpha_{P(1)}, \alpha_{P(2)}, \ldots, \alpha_{P(N)}\big) \qquad (0.7)\\
&= \frac{1}{N!}\sum_{P,P'} \xi^{\sigma(P)+\sigma(P')} \big(\alpha_1, \alpha_2, \ldots, \alpha_N\big|\alpha_{P'.P^{-1}(1)}, \alpha_{P.P'^{-1}(2)}, \ldots, \alpha_{P.P'^{-1}(N)}\big)\\
&= \sum_{\tilde{P}} \xi^{\sigma(\tilde{P})} \Big(\alpha_1, \alpha_2, \ldots, \alpha_N\big|\alpha_{\tilde{P}(1)}, \alpha_{\tilde{P}(2)}, \ldots, \alpha_{\tilde{P}(N)}\Big)\\
&= \sum_{\tilde{P}} \xi^{\sigma(\tilde{P})} \langle\alpha_1|\alpha_{\tilde{P}(1)}\rangle\langle\alpha_2|\alpha_{\tilde{P}(2)}\rangle \ldots \langle\alpha_N|\alpha_{\tilde{P}(N)}\rangle\\
&= \begin{cases} \det\left[\langle\alpha_i|\alpha_j\rangle\right], & \text{for fermions} \\ \operatorname{per}\left[\langle\alpha_i|\alpha_j\rangle\right], & \text{for bosons} \end{cases}, \qquad (0.8)
\end{aligned}
$$

where we have reordered the terms in the summation over P' on going from the first to the second line of this equation, and have reordered the summation over P such that it is performed over the permutation $\tilde{P} = P \cdot P'^{-1}$, with $\sigma(\tilde{P}) = \sigma(P) + \sigma(P')$, on going from the second to the third line. The summation over P' can then be performed and gives a simple factor $N!$. Since the vectors are supposed to be orthonormal, the determinant in (0.7) is equal to one if all α_i's are different and zero otherwise. The calculation of the permanent is a bit more involved but is nevertheless trivial.
Suppose there are k different αs, $\alpha_1, \ldots, \alpha_k$, such that $n_{\alpha_1} + \ldots + n_{\alpha_k} = N$. Since the wave-function for bosons is symmetric, one can reorder the αs that are equal in a contiguous fashion, *i.e.* we can write the wave-function as $|\alpha_1, \ldots, \alpha_1, \alpha_2, \ldots, \alpha_2, \ldots, \alpha_k, \ldots, \alpha_k\}$, where α_1 appears n_{α_1} times, etc. From this construction, it is now easy to see that the permanent that we wish to compute is that of a block-diagonal matrix in which each block is solely constituted of 1s. Since the permanent of a matrix that is composed of 1s is equal to the factorial of its dimension and the dimensions of each block matrix are $n_{\alpha_1}, \ldots, n_{\alpha_k}$, one sees that $\operatorname{per}[\langle\alpha_i|\alpha_j\rangle] = \prod_{i=1}^{k} n_{\alpha_i}!$.

One now defines the creation operator through the relation

$$\big|\mu, \alpha_1, \ldots, \alpha_N\big\} = c_\mu^\dagger\big|\alpha_1, \ldots, \alpha_N\big\}, \qquad (0.9)$$

i.e., this operator adds a particle in state μ to the many-particle state. If one wishes to add two particles to the system, to states μ and ν ($\mu \neq \nu$), say, one may apply first $c_\mu^\dagger$ and then $c_\nu^\dagger$, obtaining $|\mu, \nu, \alpha_1, \ldots, \alpha_N\}$ or the other way around, obtaining instead $|\nu, \mu, \alpha_1, \ldots, \alpha_N\}$. However, since $|\nu, \mu, \alpha_1, \ldots, \alpha_N\} = \xi|\mu, \nu, \alpha_1, \ldots, \alpha_N\}$, one concludes that

$$c_\mu^\dagger c_\nu^\dagger - \xi c_\nu^\dagger c_\mu^\dagger = 0, \qquad (0.10)$$

i.e. the creation operators commute in the case of bosons, but they anti-commute in the case of fermions. The same rule has to apply to the adjoint operators c_μ and c_ν, as results from considering the adjoint of the above equation.
It follows from (0.9) that

$$\big\{\alpha_1, \alpha_2, \ldots, \alpha_N \big| c_\mu \big| \mu, \alpha_1, \alpha_2, \ldots, \alpha_N \big\} = \| \ \big|\mu, \alpha_1, \alpha_2, \ldots, \alpha_N \big\} \ \|^2 . \tag{0.11}$$

Since the above scalar product is non-zero (in the case of fermions, one assumes that μ is different from all the αs), this implies that $c_\mu \alpha_1, \ldots, \alpha_N = C(\mu, \alpha_1, \ldots, \alpha_N) \big|\alpha_1, \ldots, \alpha_N\big\}$, with

$$C(\mu, \alpha_1, \ldots, \alpha_N) = \frac{\| \ \big|\mu, \alpha_1, \alpha_2, \ldots, \alpha_N\big\} \ \|^2}{\| \ \big|\alpha_1, \alpha_2, \ldots, \alpha_N\big\} \ \|^2} = n_\mu(\mu, \alpha_1, \alpha_2, \ldots, \alpha_N), \tag{0.12}$$

where $n_\nu(\mu, \alpha_1, \alpha_2, \ldots, \alpha_N)$ is the number of times the index μ appears in the series $\mu, \alpha_1, \alpha_2, \ldots, \alpha_N$.

In the general case of a series of labels $\alpha_1, \ldots, \alpha_N$, in which the first is not necessarily equal to μ, the rule that generalizes this result and takes into account the symmetry of the wave-function is

$$c_\mu \big|\mu, \alpha_1, \alpha_2, \ldots, \alpha_N\big\} = \sum_{i=1}^{N} \xi^{i-1} \delta_{\mu,\alpha_i} \big|\alpha_1, \ldots, \alpha_{i-1}, \alpha_{i+1}, \ldots, \alpha_N\big\}. \tag{0.13}$$

Note in particular that the state with no particles, the vacuum, is annihilated by each one of the operators c_μ, *i.e.* $c_\mu|0\rangle = 0$. Using (0.13), we now have

$$\big[c_\mu c_\nu^\dagger - \xi c_\nu^\dagger c_\mu\big] \big|\mu, \alpha_1, \alpha_2, \ldots, \alpha_N\big\} = \delta_{\mu,\nu} \big|\mu, \alpha_1, \alpha_2, \ldots, \alpha_N\big\}. \tag{0.14}$$

Since the state $\big|\mu, \alpha_1, \alpha_2, \ldots, \alpha_N\big\}$ is arbitrary, we conclude that

$$\big[c_\mu c_\nu^\dagger\big]_{-\xi} = \delta_{\mu,\nu}, \tag{0.15}$$

i.e. these operators also obey commutation ($\xi = 1$) or anti-commutation ($\xi = -1$) relations among themselves, but with a commutator or anti-commutator that is non-zero, unlike above.
Note that the state that arises from the normalisation of $\big|\mu, \alpha_1, \alpha_2, \ldots, \alpha_N\big\} = c_{\alpha_1}^\dagger \ldots c_{\alpha_N}^\dagger |0\rangle$ can be written, up to a reordering of the operators, as

$$\big|n_{\alpha_1}, n_{\alpha_2}, \ldots, n_{\alpha_k}\big\rangle = \frac{(c_{\alpha_1}^\dagger)^{n_{\alpha_1}}}{\sqrt{n_{\alpha_1}!}} \ldots \frac{(c_{\alpha_k}^\dagger)^{n_{\alpha_k}}}{\sqrt{n_{\alpha_k}!}} \big|0\big\rangle, \tag{0.16}$$

where solely the occupation number of each mode is displayed. This form is valid both for bosons and fermions (but in the latter case, $n_\alpha = 0, 1$). It is relatively simple to show from the closure relation (0.3), after symmetrisation or anti-symmetrisation, that this set of states obeys the closure relation

$$\sum_{\{n_\alpha\}} \big|n_{\alpha_1}, n_{\alpha_2}, \ldots, n_{\alpha_k}\big\rangle \big\langle n_{\alpha_1}, n_{\alpha_2}, \ldots, n_{\alpha_k}\big| = \mathcal{P}_\xi, \tag{0.17}$$

where the sum is over all possible particle numbers on all possible modes and

$$\mathcal{P}_\xi = \sum_N \frac{1}{N!} \sum_{\alpha_1,\ldots,\alpha_N} \sum_P \xi^{\sigma(P)} \big|\alpha_1, \alpha_2, \ldots, \alpha_N\big)\big(\mu, \alpha_{P_1}, \alpha_{P_2}, \ldots, \alpha_{P_N}\big| \tag{0.18}$$

is the symmetrisation or anti-symmetrisation operator of the wave-functions.

One last note on a change of basis in second quantisation. It is known from elementary quantum mechanics that if $\{|\alpha_i\rangle\}$ is a complete basis of the one-particle Hilbert space and $\{|\beta_j\rangle\}$ is another complete basis, the two are related by an unitary transformation, *i.e.* $|\beta_j\rangle = \sum_i |\alpha_i\rangle U^\dagger_{ij}$, where $U_{ji} = \langle\beta_j|\alpha_i\rangle$. Since $|\alpha_i\rangle = c^\dagger_{\alpha_i}|0\rangle$ and $\beta_j\rangle = c^\dagger_{\beta_j}|0\rangle$, we conclude that $c^\dagger_{\beta_j} = \sum_i c^\dagger_{\alpha_i} U^\dagger_{ij}$. The adjoint of this equation is the desired transformation law

$$c_{\beta_j} = \sum_i U_{ji} c_{\alpha_i}. \tag{0.19}$$