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$$\Omega = \sum_{n \text{ considered}} \left[\langle r^2 \rangle_n - \langle \vec{r}_n \rangle^2 \right]$$

$$= \Omega_I + \tilde{\Omega} \leftarrow \text{positive definite.}$$

$\downarrow$

gauge invariant

$\downarrow$

related to topology

2. Second quantization

A natural symmetry of all many-particle Hamiltonians is the invariance under the exchange of identical particles:

$$H(1,2,\dots i,\dots,j,\dots N) = H(1,2,\dots,j,\dots i,\dots,N).$$

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With other words, the cyclic group S_N of N elements is a symmetry group of H.

All permutations can be written as

$$P = \prod_{ij} P_{ij} \qquad P_{ij}^2 = \mathbb{1}$$

a product of pair-wise exchanges.
Due to the above we have that the eigenvalues of $P \in \{1, -1\}$.
S_N is not an abelian group and has therefore higher-dimensional irreducible representations. However, nature chose that the elementary particles are realized in two classes of 1D irreps:

$$P_{ij}\psi_{s/a}(\dots i, \dots j, \dots) = \psi_{s/a}(\dots j\ i) = \pm\psi_{s/a}(\dots i\ j).$$

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$\eta = +$: Bosons $\eta = -$: Fermions

We can the symmetrize states:

$$|i_1, \dots i_N\rangle = |i_1\rangle_1 \otimes |i_2\rangle_2 \otimes \dots \otimes |i_N\rangle_n$$

where i_1 is the quantum number of particle 1, etc. To symmetrize we write

$$S_\pm |i_1 \dots i_N\rangle = \frac{1}{N!} \sum_P (-1)^{\sigma_P} P |i_1 \dots i_N\rangle$$

While we could work like this, there are reasons not to do so:

i) cumbersome

ii) only fixed number of particles

iii) carries too much information

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We want to work with the occupation number basis

$$S_{\pm} |i_1, \dots, i_N\rangle = |n_1, n_2, \dots\rangle_{\pm}$$

where we don't label each particle with a quantum number, but we only keep track which single-particle state is occupied how many times and make sure that the symmetry under permutation is enforced. The total number of particles is given by

$$N = \sum_i n_i$$

and from the orthogonality and completeness of the single-particle states follows immediately that

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1.) $\langle n_1, n_2, \dots | n_1' n_2' \dots \rangle = \delta_{n_1 n_1'} \delta_{n_2 n_2'} \dots$

2.) $\sum_{n_1, n_2 \dots} | n_1 n_2 \dots \rangle \langle n_1 n_2 \dots | = \mathbb{1}$

We now introduce creation and annihilation operators

$$\hat{a}_i^+ | \dots, n_i, \dots \rangle = \sqrt{n_i + 1} \, | \dots, n_i + 1, \dots \rangle$$
$$\hat{a}_i | \dots, n_i + 1, \dots \rangle = \sqrt{n_i + 1} \, | \dots, n_i, \dots \rangle$$

It is left to the reader to prove that the second line follows from the first.

In order to keep the symmetrization of the Fock states, we need to enforce

$[\hat{a}_i, \hat{a}_j] = [\hat{a}_i^+, \hat{a}_j^+] = 0$; $[\hat{a}_i, \hat{a}_j^+] = \delta_{ij}$: Bosons

$\{\hat{a}_i, \hat{a}_j\} = \{\hat{a}_i^+, \hat{a}_j^+\} = 0$; $\{\hat{a}_i, \hat{a}_j^+\} = \delta_{ij}$: Fermions

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Note, that as a consequence of $\{\hat{a}_i^+, \hat{a}_i^+\} = 2\hat{a}_i^+\hat{a}_i^+ = 0$ the Pauli principle is automatically enforced.

The above (anti-) commutation relations define the algebra of second quantized operators. This algebra is invariant under canonical transformations. [Balian & Brezin Nuovo. Cim. B LXIV, 37 (1969)]. Here we constrain ourselves to normal transformations (i.e. not mixing $\hat{a}_i$ and $\hat{a}_i^+$).

If we write a unitary matrix U it is easy to check that

$$\hat{a}_\alpha^+ = \sum_i U_{\alpha i} \hat{a}_i^+$$

also fulfill the same algebra.

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2.1 Non-interacting Hamiltonians

A normal quadratic Hamiltonian can be written as

$$\mathcal{H} = \sum_{ij} a_i^+ H_{ij} a_j = \sum_k (\varepsilon_k - \mu) a_k^+ a_k$$

Put it back in i

Matrix element for doing so

remove particle from orbital j

$$a_j = \sum_k M_{jk} a_k$$

$$\sum_{ij} \sum_{kk'} a_k^+ \underbrace{M_{ki} H_{ij} M_{jk'}}_{\varepsilon_k \delta_{kk'}} a_{k'}$$

where H is a hermitian matrix with real eigenvalues ε_k. We added a Lagrange multiplier μ (the chemical potential) as $-\mu \hat{N} = -\mu \sum_k a_k^+ a_k$.

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It is now easy to write down the partition function (*)

$$Z = \mathrm{Tr}\, e^{-\mathcal{H}/T} = \prod_k \sum_{n_k=0}^{n_{max}} e^{-\frac{(\varepsilon_k-\mu)n_k}{T}}$$

$$n_k^{max} = \begin{cases} 1 : F \\ \infty : B \end{cases}$$

$$= \prod_k \sum_{n_k=0}^{n_{max}} \left[e^{-\frac{(\varepsilon_k-\mu)}{T}}\right]^{n_k} =$$

$$= \prod_k \begin{cases} 1 + e^{-\frac{(\varepsilon_k-\mu)}{T}} & F \\ \dfrac{1}{1-e^{-(\varepsilon_k-\mu)/T}} & B \end{cases}$$

The free energy is immediately given by

$$F = -T \ln Z = \eta T \sum_k \ln\left[1 - \eta e^{-(\varepsilon_k-\mu)/T}\right].$$

Finally, we can calculate the equilibrium values for n_k by stating

$$\langle n_k \rangle = \frac{1}{Z} \mathrm{Tr}\left[\hat{a}_k^\dagger \hat{a}_k e^{-\mathcal{H}/T}\right] = \frac{\partial F}{\partial \varepsilon_k} = \quad (*)$$

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$$\boxed{\langle n_k \rangle = \frac{1}{e^{(\varepsilon_k-\mu)/T} - \eta}}$$

which are nothing but the Bose and Fermi functions.

2.2 Normal bilinear operators

Above we have seen a special bilinear operator: The Hamiltonian of non-interacting quantum particles. Because such bilinear operators are so ubiquitous, we want to analyze them a bit further. Let us define

$$\hat{A} = \sum_{ij} \hat{a}_i^+ A_{ij} \hat{a}_j \equiv \underline{\hat{a}}^+ \cdot A \cdot \underline{\hat{a}} .$$

We want to know the commutation relations of $\hat{A}$ with a linear operator

$$\hat{\underline{v}}^+ = \sum_i v_i \hat{a}_i^+ = \underline{v} \cdot \underline{\hat{a}}^+ .$$

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$$[\hat{A},\underline{\hat{v}}^+]_\eta = [\sum_{ij}\hat{a}_i^+ A_{ij}\hat{a}_j, \sum_n v_n \hat{a}_n^+]_\eta$$

$$= \sum_{ijn} A_{ij} v_n [\hat{a}_i^+\hat{a}_j, \hat{a}_n^+]_\eta$$

$[AB,C]_\eta = A[B,C]+\eta[A,C]B$

$$= \sum_{ijn} A_{ij} v_n \quad \hat{a}_i^+[\hat{a}_j,\hat{a}_n^+]_\eta + \eta[a_i^+, a_n^+]_\eta \hat{a}_j$$

$$= \sum_{ijn} A_{ij} v_n \quad \hat{a}_i^+ \delta_{jn} = \sum_{ij} A_{ij} v_j \hat{a}_i^+$$

$$= (A\cdot\underline{v})\cdot\underline{\hat{a}}^+$$

$\Rightarrow$ If $A\cdot\underline{v} = \sigma\underline{v} \Rightarrow \underline{\hat{v}}^+$ is an eigenoperator of $[\hat{A},\cdot]_\eta$. This can be used to write

$$e^{i\vartheta\hat{A}}\hat{v}^+ e^{-i\vartheta\hat{A}} = \hat{v}^+ + i\vartheta[\hat{A},\hat{v}^+] + \frac{(i\vartheta)^2}{2}[\hat{A},[\hat{A},\hat{v}^+]] + \ldots = e^{i\vartheta\sigma}\underline{\hat{v}}^+. \qquad (3)$$

This is useful as all unitary operators (such as symmetries) can be written as

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$$U_{\underline{\vartheta}} = e^{i \sum_\alpha \vartheta_\alpha \hat{A}_\alpha}$$

with a set of Hermitian generators and parameters ϑ_α. The corresponding many-particle operator $\hat{U}$ is defined as

$$\hat{U}_\vartheta = e^{i \sum_a \vartheta_a \hat{A}_a}$$

Using Eq. (3) it is straigthforward to show that

$$\hat{U}_\vartheta \, \hat{\underline{v}}^+ \, \hat{U}_\vartheta^{-1} = \left(U_\vartheta \, \underline{v} \right) \cdot \hat{\underline{a}}^+ .$$

Finally we state the identity .

$$[\hat{A}, \hat{B}] = \underline{\hat{a}}^+ \, [A, B] \cdot \underline{\hat{a}}$$

wich is easy to verify by the repeated use of $[AB, C] = A[B, C] + [A, C]B.$

A standard example for the manipulations above are the spin operators

$$\hat{S}^{\alpha} = \frac{1}{2} \sum_{s,s'=1}^{2} \hat{a}_s^{\dagger} \sigma^{\alpha}_{ss'} \hat{a}_{s'} \qquad \alpha = x, y, z$$

with

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Using $[\hat{A}, \hat{B}] = \hat{a}^{\dagger} [A, B] \hat{a}$ we find

$$[S^{\alpha}, S^{\beta}] = i \varepsilon_{\alpha\beta\gamma} S^{\gamma}$$