Theoretical Nuclear Physics Formularium

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1 First and second quantized operators

We started the course with direct product states, *i.e.*

$$|1:\alpha, 2:\beta, \ldots\rangle \,, \tag{1}$$

which are orthonormalized, such that for example

$$\langle 1:\alpha, 2:\beta, 3:\gamma, \ldots | 1:\mu, 2:\nu, 3:\rho, \ldots\rangle = \delta_{\alpha\mu}\delta_{\beta\nu}\delta_{\gamma\rho}\ldots \,. \tag{2}$$

Slater determinants are defined as

$$|\alpha_1 \cdots \alpha_N\rangle = \sqrt{N!}\mathcal{A}\,|1:\alpha_1, \ldots, N:\alpha_N\rangle \,, \tag{3}$$

with $\mathcal{A}$ the anti-symmetrizer operator.

A k-body operator K, in first quantization, is defined via its action

$$|1:\alpha, 2:\beta, \ldots\rangle \mapsto K\,|1:\alpha, 2:\beta, \ldots\rangle \,, \tag{4}$$

and we write

$$K = \frac{1}{k!}\sum_{i\neq j\neq \ldots \neq l}^{N} k(i, j, \ldots, l)\,, \tag{5}$$

where $k(i, j, \ldots, l)$ acts non trivially as

$$|i:\alpha, j:\beta, \ldots, l:\delta\rangle \mapsto k(i, j, \ldots, l)\,|i:\alpha, j:\beta, \ldots, l:\delta\rangle \tag{6}$$

In second quantization, the canonical commutation relations are

$$\{a_\mu, a_\nu^+\} = \delta_{\mu\nu}\,. \tag{7}$$

Operators are decomposed as (watch out: reversed order for annihilator indices)

$$K = \frac{1}{k!} \sum_{\alpha \cdots \beta \gamma \cdots \delta} k_{\alpha \cdots \beta \gamma \cdots \delta} a_\alpha^+ \cdots a_\beta^+ a_\delta \cdots a_\gamma \,, \tag{8}$$

where the matrix elements are

$$k_{\alpha \cdots \beta \gamma \cdots \delta} = \langle i : \alpha, \ldots, l : \beta | k(i, \ldots, l) | i : \gamma, \ldots, l : \delta \rangle \ . \tag{9}$$

For example, 1-body operators in first quantization are written as

$$F = \sum_{i=1}^{N} f(i) \,, \tag{10}$$

and in second quantization are written as

$$F = \sum_{\alpha\beta} f_{\alpha\beta} a_\alpha^+ a_\beta \,. \tag{11}$$

To go from 1^{st} to 2^{nd} quantization in this case, use that

$$f_{\alpha\beta} = \langle 1 : \alpha | f(1) | 1 : \beta \rangle \ . \tag{12}$$

A useful result from Practice 1 is

$$[F, a_{\alpha_i}^+] = \sum_{\alpha} f_{\alpha\alpha_i} a_\alpha^+ \,. \tag{13}$$

The local density operator is

$$\rho(\vec{r}) = \sum_{i=1}^{N} \rho_{\vec{r}}(i) \,, \tag{14}$$

where *e.g.* $\rho_{\vec{r}}(1)$ is defined in the basis $|1 : \vec{r}\sigma\tau\rangle$ via

$$\langle 1 : \vec{r}_1 \sigma_1 \tau_1 | \rho_{\vec{r}(1)} | 1 : \vec{r}_1' \sigma_1' \tau_1' \rangle = \delta(\vec{r} - \vec{r}_1) \delta(\vec{r}_1 - \vec{r}_1') \delta_{\sigma_1 \sigma_1'} \delta_{\tau_1 \tau_1'} \,. \tag{15}$$

The number operator is defined in 2^{nd} quantization as

$$N = \sum_{\alpha} a_\alpha^+ a_\alpha \tag{16}$$

and has the Slater determinants as eigenstates.

The kinetic energy operator of one particle has matrix elements (in an arbitrary basis)

$$t_{\alpha\beta} = \langle 1 : \alpha | t(1) | 1 : \beta \rangle = \frac{\hbar^2}{2m} \int \mathrm{d}\vec{r} \sum_{\sigma\tau} \vec{\nabla} \varphi_\alpha^*(\vec{r}\sigma\tau) \cdot \vec{\nabla} \varphi_\beta(\vec{r}\sigma\tau) \,. \tag{17}$$

The nuclear Hamiltonian in second quantized form is (omitting 3-body interactions)

$$H = T + V = \sum_{\alpha\beta} t_{\alpha\beta} a^+_\alpha a_\beta + \left(\frac{1}{2!}\right)^2 \sum_{\alpha\beta\gamma\delta} \overline{v}_{\alpha\beta\gamma\delta} a^+_\alpha a^+_\beta a_\delta a_\gamma + \dots \,, \tag{18}$$

with antisymmetrized matrix elements:

$$\overline{v}_{\alpha\beta\gamma\delta} \equiv v_{\alpha\beta\gamma\delta} - v_{\alpha\beta\delta\gamma} \,, \tag{19}$$

which, in the above summation, has the symmetries

$$\overline{v}_{\alpha\beta\gamma\delta} = -\overline{v}_{\alpha\beta\delta\gamma} = -\overline{v}_{\beta\alpha\gamma\delta} = +\overline{v}_{\beta\alpha\delta\gamma} \,. \tag{20}$$

2 Operator relations and basis transformations

Position representation of $\vec{r}$, $\vec{p}$ operators

$$\hat{\vec{r}} = \vec{r}\times \,, \tag{21}$$

$$\hat{\vec{p}} = -i\hbar\vec{\nabla} \,, \tag{22}$$

$$\langle \vec{r}|\hat{\vec{r}}|\vec{r}'\rangle = \delta(\vec{r} - \vec{r}')\vec{r} \,, \tag{23}$$

$$\langle \vec{r}|\hat{\vec{p}}|\vec{r}'\rangle = -i\hbar\delta(\vec{r} - \vec{r}')\vec{\nabla} \,. \tag{24}$$

Completeness relation on $\mathcal{H}_1$:

$$\mathbb{1} = \sum_\alpha |\alpha\rangle \langle\alpha| \tag{25}$$

For a trivial Bogoliubov transformation,

$$\mathcal{B}_1 = \{|\mu\rangle\}, a^+_\mu \to \mathcal{B}'_1 = \{|\lambda\rangle\}, b^+_\mu \,, \tag{26}$$

we have the relations

$$|\mu\rangle = \sum_\lambda |\lambda\rangle \langle\lambda|\mu\rangle \equiv \sum_\lambda C_{\lambda\mu} |\lambda\rangle \,, \qquad \langle\mu| = \sum_\lambda \langle\mu|\lambda\rangle \langle\lambda| = \sum_\lambda C^*_{\lambda\mu} \langle\lambda| \,, \tag{27}$$

$$a^+_\mu = \sum_\lambda C_{\lambda\mu} b^+_\lambda \,, \qquad a_\mu = \sum_\lambda C^*_{\lambda\mu} b_\lambda \,. \tag{28}$$

The unitarity of the transformation can be expressed as

$$\sum_\lambda C^*_{\lambda\mu} C_{\lambda\mu'} = \delta_{\mu\mu'} \,, \tag{29}$$

from which the inverse transformation rules can be found, such as for example

$$b_\lambda^+ = \sum_\mu C^*_{\lambda_\mu} a^+_\mu \,. \tag{30}$$

For quasi-particles, a vacuum associated to a complete set of quasi-particle creation and annihilation operators $\{\beta_\alpha^+, \beta_\alpha\}$ satisfies $\beta_\alpha |\Phi\rangle = 0$. General Bogoliubov transformations from $\{\tilde\beta_\alpha, \tilde\beta_\alpha^+\}$ to $\{\beta_\lambda, \beta_\lambda^+\}$ read

$$\beta_\lambda = \sum_\alpha U^*_{\alpha\lambda}\tilde\beta_\alpha + V^*_{\alpha\lambda}\tilde\beta^+_\alpha \,, \tag{31}$$

$$\beta^+_\lambda = \sum_\alpha V_{\alpha\beta}\tilde\beta_\alpha + U_{\alpha\lambda}\tilde\beta^+_\alpha \,, \tag{32}$$

and the inverse

$$\tilde\beta_\alpha = \sum_\lambda U_{\alpha\lambda}\beta_\lambda + V^*_{\alpha\lambda}\beta^+_\lambda \,, \tag{33}$$

$$\tilde\beta^+_\alpha = \sum_\lambda V_{\alpha\beta}\beta_\lambda + U^*_{\alpha\lambda}\beta^+_\alpha \,. \tag{34}$$

This can be put in matrix form (see notes page 32). Note that Bogoliubov transformations change the vacuum and associated Hilbert spaces $\mathcal{H}_N$. A trivial transformation (*i.e.*, $V = 0$) does not change the associated vacua.

3 Wick theorem

Normal product: bring all annihilation operators to the right of all creation operators, and multiply by the signature of the permutation. Note: this depends on the set of operators and hence on the vacuum $|\Phi\rangle$. By definition, we have

$$\langle\Phi| : ABC...Z : |\Phi\rangle = 0 \,. \tag{35}$$

Contraction: the difference between an operator and its normal product, *i.e.*

$$\overbracket{AB} = AB - :AB: \,. \tag{36}$$

We have

$$\overbracket{AB} = \frac{\langle\Phi|AB|\Phi\rangle}{\langle\Phi|\Phi\rangle} \,. \tag{37}$$

Wick theorem: page 56 of the notes.
Generalized Wick theorem: page 63 of the notes.

4 Slater determinants and particle/hole excitations

Working in the basis $\mathcal{B}_1 = \{b_\alpha, b_\alpha^+\}$, a Slater determinant of $\mathcal{H}_N$ is defined like[1]

$$|\Phi\rangle = \prod_{i=1}^{N} b_i^+ |0\rangle \ . \tag{38}$$

The conventions used are such that

$a, b, c, \dots$	unoccupied/particle states
$i, j, k, \dots$	occupied/hole states

Taking the Slater determinant as Fermi vacuum and these conventions, we have

annihilators:	b_i^+	b_a
creators:	b_i	b_a^+

Particle/hole excitations: (watch out for the reversed order in the second part)

$$\left|\Phi_{ij\dots}^{ab\dots}\right\rangle = b_a^+ b_b^+ \cdots b_j b_i |\Phi\rangle \ . \tag{39}$$

In an arbitrary basis $\{a_\lambda, a_\lambda^+\}$, the elementary contractions are[2]

$$\contraction{}{a_\alpha^+}{}{a_\beta^+} a_\alpha^+ a_\beta^+ = 0 \tag{40}$$

$$\contraction{}{a_\alpha^+}{}{a_\beta} a_\alpha^+ a_\beta = \rho_{\beta\alpha} \tag{41}$$

$$\contraction{}{a_\alpha}{}{a_\beta^+} a_\alpha a_\beta^+ = \delta_{\alpha\beta} - \rho_{\alpha\beta} \tag{42}$$

$$\contraction{}{a_\alpha}{}{a_\beta} a_\alpha a_\beta = 0 \tag{43}$$

In basis $\mathcal{B}_1$, this is simplified as ρ becomes block-diagonal, *i.e.*:

$$\rho_{\beta\alpha} = \delta_{\beta i}\delta_{\alpha i} \ . \tag{44}$$

Therefore, we have:

$$\contraction{}{a_\alpha^+}{}{a_\beta} a_\alpha^+ a_\beta = \delta_{\alpha i}\delta_{\alpha\beta} \tag{45}$$

$$\contraction{}{a_\alpha}{}{a_\beta^+} a_\alpha a_\beta^+ = \delta_{\alpha a}\delta_{\alpha\beta} \tag{46}$$

[1] We are following the conventions of the lecture notes. Note that one should swap $a \leftrightarrow b$ when reading Practice 3.

[2] Watch out for the reversed order of indices in the definition of ρ.

5 Mean-field and Hartree-Fock

Using Wick theorem, the Hamiltonian in an arbitrary basis $\{a_\lambda, a_\lambda^+\}$ reads

$$H = \sum_{\alpha\beta} t_{\alpha\beta}\rho_{\alpha\beta} + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \overline{v}_{\alpha\beta\gamma\delta}\rho_{\gamma\alpha}\rho_{\delta\beta} + \sum_{\alpha\beta} h_{\alpha\beta} : a_\alpha^+ a_\beta : + \frac{1}{4}\sum_{\alpha\beta\gamma\delta} \overline{v}_{\alpha\beta\gamma\delta} : a_\alpha^+ a_\beta^+ a_\delta a_\gamma : , \tag{47}$$

where (see also equations (17) and (19))

$$h_{\alpha\beta} = t_{\alpha\beta} + \sum_{\gamma\delta} \overline{v}_{\alpha\gamma\beta\delta}\rho_{\delta\gamma} \,. \tag{48}$$

The HF partitioning is $H = H_0 + H_1$, with

$$H_0 = H_0^{0b} + H_0^{1b} \tag{49}$$

$$= \sum_{\alpha\beta} t_{\alpha\beta} + \tfrac{1}{2}\sum_{\alpha\beta\gamma\delta} \overline{v}_{\alpha\beta\gamma\delta}\rho_{\gamma\alpha}\rho_{\delta\beta} + \sum_{\alpha} e_\alpha : b_\alpha^+ b_\alpha : \tag{50}$$

$$H_1 = H_1^{1b} + H_1^{2b} \tag{51}$$

$$= \sum_{\alpha\beta} \breve{h}_{\alpha\beta} : b_\alpha^+ b_\beta : + \tfrac{1}{4}\sum_{\alpha\beta\gamma\delta} \overline{v}_{\alpha\beta\gamma\delta} : b_\alpha^+ b_\beta^+ b_\delta b_\gamma : , \tag{52}$$

where H^{nb} denotes the n-body part of the operator. Here, we defined

$$\breve{h}_{\alpha\beta} = h_{\alpha\beta} - e_\alpha \delta_{\alpha\beta} \,. \tag{53}$$

The Fermi vacuum from equation (38) and particle/hole excitations from (39) are orthonormalized eigenstates of H_0 in $\mathcal{H}_N$, with eigenvalues

$$\epsilon + (e_a + e_b + \cdots) - (e_i + e_j + \cdots) \,, \quad \epsilon = H_0^{0b} \,. \tag{54}$$

Koopman's theorem: Within HF, we have

$$\langle \Phi^a | H | \Phi^a \rangle - \langle \Phi | H | \Phi \rangle = e_a \,, \tag{55}$$

$$\langle \Phi_i | H | \Phi_i \rangle - \langle \Phi | H | \Phi \rangle = -e_i \,. \tag{56}$$

Brillouin's theorem: Within HF, H_1 does not couple $|\Phi\rangle$ to 1-particle/1-hole excitations:

$$\langle \Phi_i^a | H_1 | \Phi \rangle = 0 \,. \tag{57}$$