FEW FERMION SYSTEMS

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1. The Problem: Layout

As a case study we look at a few electron Quantum Dot (QD). We concentrate on *heterostructure* QDs. In heterostructures two slabs of differently doped semiconductor stacked together:

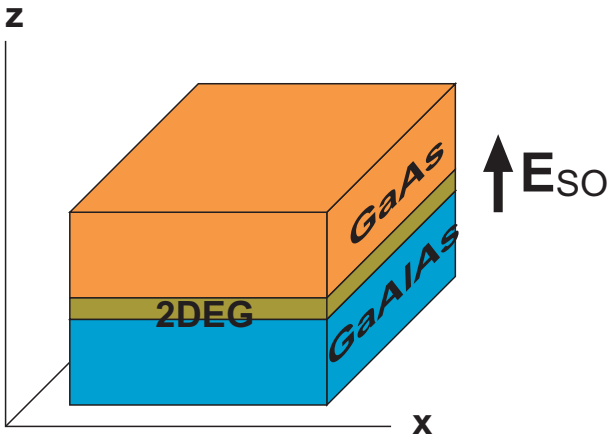

Fig. 1.1 A semiconductor heterostructure

- in the vicinity of the contact surface electrons can move freely parallel to the surface
- in the perpendicular direction (z-axis in the figure) the confining potential keeps the electrons on the lowest energy level restraining the perpendicular motion (excitation energies are of the order of 100s of meVs)

The electrons trapped in the contact layer

- effectively form a *Two Dimensional Electron Gas* (2DEG)
- feel an average non-zero electric field $\boldsymbol{E}_{\mathrm{SO}}$ parallel to the z-axis due to the asymmetric confining potential caused by the inversion asymmetry of the structure
- feel the electron-electron Coulomb interaction which is screened by the other electrons and the substrate material (dielectric constant being of the order ≈ 10)
- reside at the bottom of the conduction band which gives them an *effective mass* only a fraction of their free mass.

Quantum dots can be formed from heterostructures for example by etching like

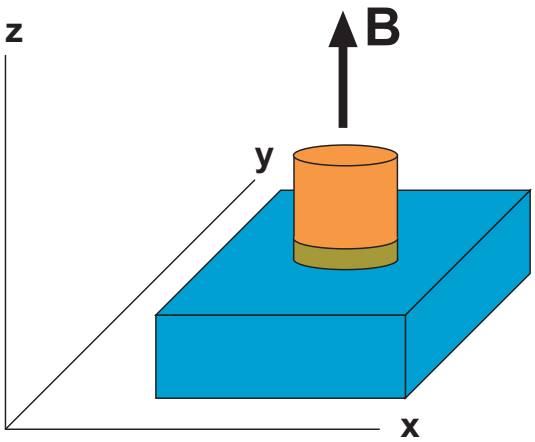

Fig. 1.2 A heterostructure QD.

or by electric gates on the outer surface of the slabs. Now the electrons in the contact layer

- are confined to a restricted area in the xy-plane. To a very good approximation the confining potential V_{conf} for cylindrically shaped structures is parabolic, i.e. $V_{\text{conf}} \propto r^2$, where $\boldsymbol{r}$ is the two dimensional radius vector lying in the xy-plane
- inherit the properties (effective mass, dielectric constant, ...) from the original heterostructure

QDs are often probed by an external magnetic field perpendicular to the field and by observing their absorption spectra.
We can now write down the Hamiltonian describing the electrons in a QD. It consists of the familiar single particle terms

- the kinetic energy
$$T = \frac{1}{2m}\boldsymbol{\Pi}^2,$$
where m is the effective mass of the electron, typically of the order of few hundredths or tenths of electron mass m_0, and $\boldsymbol{\Pi}$ is the momentum operator
- the parabolic potential $V_{\text{conf}}(\boldsymbol{r})$ confining the electrons in the xy-plane
$$V_{\text{conf}}(\boldsymbol{r}) = \frac{1}{2}m\omega_0^2 r^2,$$
where typically the strength of V_{conf} is such that the excitations energies $\hbar\omega_0$ are of the order of few meVs.

The persistent average electric field resident in the contact layer results a single particle interaction called the *Spin-Orbit* (SO) coupling which is of the form

$$H_{\mathrm{SO}} = \frac{\alpha}{\hbar}\left[\boldsymbol{\sigma} \times \boldsymbol{\Pi}\right]_z$$

The parameter α determines the strength of the coupling and is typically of the order of few meV nm. The components of the vector $\boldsymbol{\sigma}$ are the Pauli spin matrices, i.e

$$\begin{aligned} \boldsymbol{\sigma} &= \boldsymbol{\sigma}_x \boldsymbol{x} i + \boldsymbol{\sigma}_y \boldsymbol{j} + \boldsymbol{\sigma}_z \boldsymbol{k} \\ &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \boldsymbol{i} + \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \boldsymbol{j} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \boldsymbol{k}. \end{aligned}$$

This interaction is also known as the *Rashba* term.
To handle external electromagnetic fields $\boldsymbol{E}_{\mathrm{r}}$ and $\boldsymbol{B}$ we introduce the *vector potential* $\boldsymbol{A}$ such that

$$\begin{aligned} \boldsymbol{B} &= \nabla \times \boldsymbol{A} \\ \boldsymbol{E}_{\mathrm{r}} &= -\frac{\partial}{\partial t}\boldsymbol{A} \end{aligned}$$

The external static magnetic field

$$\boldsymbol{B} = B\hat{\boldsymbol{z}}$$

- modifies the momentum operator as

  $$\boldsymbol{\Pi} = \boldsymbol{p} - e\boldsymbol{A}$$

  where $\boldsymbol{p} = -\mathrm{i}\hbar\nabla$ is the ordinary momentum

- the vector potential can be taken, for example as

  $$\boldsymbol{A} = \boldsymbol{A}_B = \frac{B}{2}(-y, x, 0)$$

- couples to the spin of each electron by the Zeeman term

  $$H_{\mathrm{Z}} = g\mu_B B\sigma_z,$$

  where g is the Lande factor ranging typically from -0.4 to -40, μ_B the Bohr magneton and σ_z a Pauli spin matrix.

To probe the energy levels of the QD we subject it to an external radiation field with the electric component

$$\boldsymbol{E}_{\mathrm{r}}(t) = \boldsymbol{E}_{\mathrm{r}} \cos \Omega t$$

- in *dipole approximation* the amplitude $\boldsymbol{E}_{\mathrm{r}}$ is spatially constant (and, ofcourse also temporally)

- the frequency of the field is $\Omega/2\pi$
- the corresponding vector potential will then be

$$\boldsymbol{A}_{\mathrm{r}} = -\frac{\boldsymbol{E}_{\mathrm{r}}}{\Omega}\sin\Omega t$$

The total vector potential is now given by

$$\boldsymbol{A} = \boldsymbol{A}_B + \boldsymbol{A}_{\mathrm{r}} = \frac{B}{2}(-y, x, 0) - \frac{\boldsymbol{E}_{\mathrm{r}}}{\Omega}\sin\Omega t.$$

Thus far all terms in the Hamiltonian have been single particle terms, i.e. they operate on one particle at a time. In principle it is a simple straightforward task to find, for example the energy spectrum and eigenstates of this kind of Hamiltonian.
The problem gets remarkably more complicated when we add the mutual Coulomb interactions

$$V_{\mathrm{Coul}} = \frac{1}{2}\sum_{i\neq j}^{N_e}\frac{e^2}{4\pi\varepsilon\varepsilon_0|\boldsymbol{r}_i - \boldsymbol{r}_j|}.$$

Here N_e is the number of electrons labeled by the subscripts i and j.
The total Hamiltonian modelling a heterostructure QD now reads as

$$\begin{aligned} H &= \sum_{i=1}^{N_e}[T_i + V_{\mathrm{conf}}(\boldsymbol{r}_i) + H_{\mathrm{SO}\,i} + H_{Z\,i}] + V_{\mathrm{Coul}} \\ &= \sum_{i=1}^{N_e}\frac{1}{2m}\boldsymbol{\Pi}_i^2 + \sum_{i=1}^{N_e}\frac{1}{2}m\omega_0^2 r_i^2 \\ &\quad + \sum_{i=1}^{N_e}\frac{\alpha}{\hbar}\left[\boldsymbol{\sigma}\times\boldsymbol{\Pi}_i\right]_z + \sum_{i=1}^{N_e} g\mu_B B\sigma_{z\,i} \\ &\quad + \frac{1}{2}\sum_{i\neq j}^{N_e}\frac{e^2}{4\pi\varepsilon\varepsilon_0|\boldsymbol{r}_i - \boldsymbol{r}_j|} \end{aligned}$$

where the kinematic momentum $\boldsymbol{\Pi}_i$ is

$$\begin{aligned} \boldsymbol{\Pi}_i &= \boldsymbol{p}_i - e\boldsymbol{A}_i = \boldsymbol{p}_i - e\boldsymbol{A}_{B\,i} - e\boldsymbol{A}_{\mathrm{r}\,i} \\ &= -\mathrm{i}\hbar\nabla_i - \frac{eB}{2}(-y_i, x_i, 0) + \frac{e\boldsymbol{E}_{\mathrm{r}}}{\Omega}\sin\Omega t. \end{aligned}$$

The Task

Our aim is to find the absorption spectrum for our QD. It turns out that we can proceed in steps:

1. solve the static problem, i.e. find the energy eigenstates of the total Hamiltonian H when the radiation field $\boldsymbol{E}_{\mathrm{r}}(t)$ vanishes or, equivalently when $\boldsymbol{A}_{\mathrm{r}} = 0$

(a) solve the single particle problem, that is forget the mutual Coulomb interaction

i. from the single particle Hamiltonian drop out all the terms you cannot handle analytically and solve the remaining problem by paper and pencil

ii. handle numerically the dropped terms

(b) handle the interactions numerically

2. handle the the time dependence numerically.

2. Exact diagonalization

Consider N-particle *static* Hamiltonian

$$H = H_0 + H'.$$

Here H_0 is

- the single particle term, e.g.

$$H_0 = \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m} \nabla_i^2 + V(\boldsymbol{r}_i) \right],$$

- usually tractable, i.e. we can easily solve the problem

$$H_0 \Phi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N) = E \Phi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N),$$

and H' contains everything else, i.e.

- the intractable single particle terms,
- the mutual interaction

$$\frac{1}{2} \sum_{i \neq j}^{N} U(\boldsymbol{r}_i - \boldsymbol{r}_j).$$

Since H_0 is Hermitian, its eigenstates Φ_n,

$$H_0 \Phi_n = E_n \Phi_n,$$

form a complete orthonormal basis. Thus, the solutions to the problem

$$H \Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N) = E \Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N)$$

can be written as superpositions

$$\Psi = \sum_{n=0} c_n \Phi_n.$$

The superposition coefficients

$$c = \begin{pmatrix} c_0 \\ c_1 \\ \vdots \end{pmatrix}$$

satisfy the eigenvalue equation

$$\mathcal{H} c = E c,$$

where the elements of the matrix $\mathcal{H}$ are given by

$$\begin{aligned} \mathcal{H}_{ij} &= \langle \Phi_i | H | \Phi_j \rangle \\ &= \int \Phi_i^*(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) H \Phi_j(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) \, \mathrm{d}\boldsymbol{r}_1 \cdots \mathrm{d}\boldsymbol{r}_N. \end{aligned}$$

In principle the matrix $\mathcal{H}$ is infinite dimensional. In certain cases, for example when

- the number of particles is small, $N \approx 10$
- it is possible, e.g. by applying clever boundary values, to map the actual many body problem approximately to a few body problem
- in the energy spectrum $\{E_n\}$ of H_0 there are big gaps as compared to perturbation H',

the matrix $\mathcal{H}$ can be truncated to finite size, say $r \times r$. The process

1. reducing the Hamiltonian to a finite $r \times r$-matrix $\mathcal{H}$,
2. diagonalizing $\mathcal{H}$, usually numerically,

is called *the exact diagonalization method*.
In practice we must have $r \approx 50\,000$. Occasionally matrices of order of millions can be diagonalized.

3. Occupation representation demystified

according to S. Raimes, *Many-Electron Theory.*

3.1 Non-interacting states

Consider the Hamiltonian

$$H_0 = \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m} \nabla_i^2 + V(\boldsymbol{r}_i) \right]$$

and the corresponding Schrödinger equation

$$H_0 \Phi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N) = E \Phi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N). \qquad (*)$$

Supposing that the functions $f_i(\boldsymbol{r})$ satisfy single particle equations

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\boldsymbol{r}) \right] f_i(\boldsymbol{r}) = \epsilon_i f_i(\boldsymbol{r}_i)$$

it is easy to see that

$$\Phi = f_1(\boldsymbol{r}_1) f_2(\boldsymbol{r}_2) \cdots f_N(\boldsymbol{r}_N) \qquad (**)$$

satisfy the many particle equation $(*)$ with the eigenvalue

$$E = \sum_{i=1}^{N} \epsilon_i.$$

However, the simple product $(**)$ is not correct, since

1. the spin degrees of freedom are not incorporated.
2. the statistics is wrong: wave functions describing fermions must be antisymmetric and the ones describing boson symmetric in the coordinates of the particles.

Spin coordinates

We introduce the spin coordinate ξ taking values ± 1 and the spin wave functions $\chi_\uparrow$ and $\chi_\downarrow$ as

$$\begin{aligned} \chi_\uparrow(\xi) &= \begin{cases} 1 & \text{if } \xi = 1 \\ 0 & \text{if } \xi = -1 \end{cases} \\ \chi_\downarrow(\xi) &= \begin{cases} 0 & \text{if } \xi = 1 \\ 1 & \text{if } \xi = -1. \end{cases} \end{aligned}$$

If there are no terms depending on the spin in the Hamiltonian H_0 we can rewrite the single particle solution like

$$\phi_i(\boldsymbol{x}) = f_i(\boldsymbol{r}) \chi_i(\xi),$$

where χ_i is either $\chi_\uparrow$ or $\chi_\downarrow$ and

$$\boldsymbol{x} = (\boldsymbol{r}, \xi).$$

Integration over $\boldsymbol{x}$ implies summation over ξ, e.g.

$$\int \phi_i^*(\boldsymbol{x})\phi_j(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \sum_{\xi=\pm 1} \int f_i^*(\boldsymbol{r}) f_j(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}\chi_i(\xi)\chi_j(\xi).$$

In particular, we have

$$\int |\phi_i(\boldsymbol{x})|^2 \mathrm{d}\boldsymbol{x} = \int |f_i(\boldsymbol{r})|^2 \mathrm{d}\boldsymbol{r} \sum_{\xi=\pm 1} \chi_i^2(\xi) = 1,$$

provided that the spatial wave functions are normalized.

Fermions
We start with the product $\phi_1(\boldsymbol{x}_1)\phi_2(\boldsymbol{x}_2)\cdots\phi_N(\boldsymbol{x}_N)$ and

1. permute the coordinates $\boldsymbol{x}_i$ in every possible way. There are $N!$ ways to do this. It is clear that we still have many particle wave functions satisfying the equation $(*)$.
2. change sign every time we exchange two coordinates.
3. sum up all these terms.

When we denote by

- P a permutation of the coordinates $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$,
- p the number of exchanges required for the permutaion P,

we end up with the antisymmetric normalized wave function

$$\Phi = \frac{1}{(N!)^{1/2}} \sum_P (-1)^p P\phi_1(\boldsymbol{x}_1)\phi_2(\boldsymbol{x}_2)\cdots\phi_N(\boldsymbol{x}_N).$$

By definition this can be rewritten as the determinant

$$\Phi = \frac{1}{(N!)^{1/2}} \begin{vmatrix} \phi_1(\boldsymbol{x}_1) & \phi_1(\boldsymbol{x}_2) & \cdots & \phi_1(\boldsymbol{x}_N) \\ \phi_2(\boldsymbol{x}_1) & \phi_2(\boldsymbol{x}_2) & \cdots & \phi_2(\boldsymbol{x}_N) \\ \vdots & \vdots & & \vdots \\ \phi_N(\boldsymbol{x}_1) & \phi_N(\boldsymbol{x}_2) & \cdots & \phi_N(\boldsymbol{x}_N) \end{vmatrix},$$

which is known as the *Slater determinant*.

3.2 Determinantal wave functions

As eigenstates of the single particle Hamiltonian the wave functions $\phi_i(\boldsymbol{x})$ form a complete, orthonormal set, i.e.

$$\sum_i \phi_i^*(\boldsymbol{x}')\phi_i(\boldsymbol{x}) = \delta(\boldsymbol{x} - \boldsymbol{x}').$$

and

$$\int \phi_i^*(\boldsymbol{x})\phi_j(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \delta_{ij}.$$

From these states we construct all possible non-interacting states of N fermions by

1. picking up N different integers $a_1, a_2, \ldots, a_N$ or, equivalently, N different wave functions
$$\phi_{a_1}, \phi_{a_2}, \ldots, \phi_{a_N}$$
from the infinite set
$$\phi_1, \phi_2, \ldots$$
in every possible way and

2. forming the determinants

$$\Phi_a(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) = \frac{1}{(N!)^{1/2}} \sum_P (-1)^p P\phi_{a_1}(\boldsymbol{x}_1)\cdots\phi_{a_N}(\boldsymbol{x}_N).$$

Let

$$\Phi_b(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) = \frac{1}{(N!)^{1/2}} \sum_P (-1)^p P\phi_{b_1}(\boldsymbol{x}_1)\cdots\phi_{b_N}(\boldsymbol{x}_N).$$

be another determinant.
For short we denote by $\mathrm{d}\tau'$ the volume element $\mathrm{d}\boldsymbol{x}_1\cdots\mathrm{d}\boldsymbol{x}_N$ and let the prime$'$ indicate the summation over spin coordinates.
Consider an N-particle operator $F(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N)$. We say that F is *symmetric* if $PF = F$.
We have
if F is a symmetric operator then

$$\int \Phi_b^* F \Phi_a \mathrm{d}\tau' = (N!)^{1/2} \int\int \Phi_b^* F\phi_{a_1}(\boldsymbol{x}_1)\cdots\phi_{a_N}(x_N)\mathrm{d}\tau'.$$

Proof We have

$$\begin{aligned}
&\int \Phi_b^* F \Phi_a \mathrm{d}\tau' \\
&\quad = \frac{1}{(N!)^{1/2}} \int \Phi_b^* F \\
&\qquad \sum_P (-1)^p P \phi_{a_1}(\boldsymbol{x}_1) \cdots \phi_{a_N}(\boldsymbol{x}_N)\, \mathrm{d}\tau'.
\end{aligned}$$

We note that

- since P has no effect on F we can move F to the right over P.
- introducing the operator P^{-1} undoing the effect of P the determinant Φ_b^* can also be moved over P multiplying it by P^{-1}.
- the number of exchanges, p, is exactly the same in P^{-1} as in P and every exchange of coordinates in the determinantal wave function merely changes its sign.
- we can exchange the sum and the integration.

We end up with

$$\begin{aligned}
&\int \Phi_b^* F \Phi_a \mathrm{d}\tau' \\
&\quad = \frac{1}{(N!)^{1/2}} \sum_P (-1)^p \\
&\qquad P \int (P^{-1}\Phi_b^*) F \phi_{a_1}(\boldsymbol{x}_1) \cdots \phi_{a_N}(\boldsymbol{x}_N)\, \mathrm{d}\tau' \\
&\quad = \frac{1}{(N!)^{1/2}} \sum_P P \int \Phi_b^* F \phi_{a_1}(\boldsymbol{x}_1) \cdots \phi_{a_N}(\boldsymbol{x}_N)\, \mathrm{d}\tau' \\
&\quad = (N!)^{1/2} \int \Phi_b^* F \phi_{a_1}(\boldsymbol{x}_1) \cdots \phi_{a_N}(\boldsymbol{x}_N)\, \mathrm{d}\tau'.
\end{aligned}$$

We can now show that determinantal wave functions are normalized. Due to the orthogonality of the single particle function we can write

$$\begin{aligned}
&\int \Phi_a^* \Phi_a \mathrm{d}\tau' \\
&\quad = (N!)^{1/2} \int \Phi_a^* \phi_{a_1}(\boldsymbol{x}_1) \cdots \phi_{a_N}(\boldsymbol{x}_N)\, \mathrm{d}\tau' \\
&\quad = \int \left[\sum_P (-1)^p P \phi_{a_1}^*(\boldsymbol{x}_1) \cdots \phi_{a_N}^*(\boldsymbol{x}_N) \right] \\
&\qquad \times \phi_{a_1}(\boldsymbol{x}_1) \cdots \phi_{a_N}(\boldsymbol{x}_N)\, \mathrm{d}\tau' \\
&\quad = \int |\phi_{a_1}(\boldsymbol{x}_1)|^2 \cdots |\phi_{a_N}(\boldsymbol{x}_N)|^2\, \mathrm{d}\tau'
\end{aligned}$$

$$= \int |\phi_{a_1}(\boldsymbol{x}_1)|^2 \mathrm{d}\boldsymbol{x}_1 \cdots \int |\phi_{a_N}(\boldsymbol{x}_N)|^2 \mathrm{d}\boldsymbol{x}_N = 1.$$

Suppose now, that in the determinants Φ_a and Φ_b we have

$$\begin{aligned} a_i &= b_i \text{ when } i \neq j \\ a_j &\neq b_j, \end{aligned}$$

i.e. the determinants differ in one single particle state. Then

$$\begin{aligned} &\int \Phi_a^* \Phi_b \mathrm{d}\tau' \\ &\quad = \int \left[\sum_P (-1)^p P \phi_{a_1}^*(\boldsymbol{x}_1) \cdots \phi_{a_N}^*(\boldsymbol{x}_N) \right] \\ &\qquad \times \phi_{b_1}(\boldsymbol{x}_1) \cdots \phi_{b_N}(\boldsymbol{x}_N) \, \mathrm{d}\tau' \\ &\quad = \int |\phi_{a_1}(\boldsymbol{x}_1)|^2 \mathrm{d}\boldsymbol{x}_1 \cdots \int \phi_{a_j}^*(\boldsymbol{x}_j) \phi_{b_j}(\boldsymbol{x}_j) \, \mathrm{d}\boldsymbol{x}_j \\ &\qquad \cdots \int |\phi_{a_N}(\boldsymbol{x}_N)|^2 \mathrm{d}\boldsymbol{x}_N = 0. \end{aligned}$$

It is easy to see that the same holds if they differ in more than one wave function.
Thus the determinants Φ_a form an orthonormal set. It can also be shown that in the space of antisymmetric functions they form a complete set. So, *every antisymmetric function Ψ of N variables can be written as a superposition*

$$\Psi = \sum_a B_a \Phi_a.$$

3.3 Matrix elements

Our original problem

$$H\Psi = E\Psi$$

can now be converted to the matrix form

$$\sum_a (H_{ba} - E) B_a = 0, \qquad (*)$$

where

$$H_{ba} = \langle \Phi_b | H | \Phi_a \rangle = \int \Phi_b^* (H_0 + H') \Phi_a \mathrm{d}\tau'. \qquad (**)$$

We recall that H' is a sum of intractable single particle terms and terms describing mutual interactions. It can be written in terms of *one body operators*, i.e. operators acting on one particle at a time, and of *two body operators*, i.e. operators acting on two particles at a time like

$$H' = \sum_{i=1}^{N} u(\boldsymbol{r}_i) + \frac{1}{2} \sum_{i \neq j}^{N} v(\boldsymbol{r}_i, \boldsymbol{r}_j).$$

Thus calculation of the elements H_{ba} involves treatment of one body and two body operators.
In general, our operators are either one body operators

$$\Omega^{(1)} = \sum_{i=1}^{N} \eta(\boldsymbol{x}_i)$$

or two body operators

$$\Omega^{(2)} = \frac{1}{2} \sum_{i \neq j}^{N} \vartheta(\boldsymbol{x}_i, \boldsymbol{x}_j).$$

We use the notation

$$\langle i|\eta|j\rangle = \int \phi_i^*(\boldsymbol{x})\eta(\boldsymbol{x})\phi_j(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x},$$

and

$$\begin{aligned}\langle ij|\vartheta|kl\rangle \quad = \quad & \int\int \Big[\phi_i^*(\boldsymbol{x}_1)\phi_j^*(\boldsymbol{x}_2)\vartheta(\boldsymbol{x}_1,\boldsymbol{x}_2) \\ & \times \phi_k(\boldsymbol{x}_1)\phi_l(\boldsymbol{x}_2)\Big]\,\mathrm{d}\boldsymbol{x}_1\mathrm{d}\boldsymbol{x}_2.\end{aligned}$$

When fermions are involved *the relative orders of the labels (i,j,k,l) and the dummy variables $(\boldsymbol{x}_1,\boldsymbol{x}_2)$ are crucial* in the latter definition.

Matrix elements of one body operators
We start with

$$\begin{aligned}&\langle\Phi_b|\Omega^{(1)}|\Phi_a\rangle \\ &\quad = \int \Phi_b^*\Omega^{(1)}\Phi_a\,\mathrm{d}\tau' \\ &\quad = (N!)^{1/2}\int \Phi_b^*\Omega^{(1)}\phi_{a_1}(\boldsymbol{x}_1)\cdots\phi_{a_N}(\boldsymbol{x}_N)\,\mathrm{d}\tau' \\ &\quad = (N!)^{1/2}\sum_{i=1}^{N}\int \Phi_b^*\eta(\boldsymbol{x}_i)\phi_{a_1}(\boldsymbol{x}_1)\cdots\phi_{a_N}(\boldsymbol{x}_N)\,\mathrm{d}\tau'.\end{aligned}$$

Case (i): $\Phi_a = \Phi_b$, i.e. $b_i = a_i\ \forall i$. Now, due to the orthonormality of the ϕ_{a_i}, we can write

$$\begin{aligned}&(N!)^{1/2}\int \Phi_b^*\eta(\boldsymbol{x}_i)\phi_{a_1}(\boldsymbol{x}_1)\cdots\phi_{a_N}(\boldsymbol{x}_N)\,\mathrm{d}\tau' \\ &\quad = \int\left[\sum_P (-1)^p P\phi_{a_1}^*(\boldsymbol{x}_1)\cdots\phi_{a_N}^*(\boldsymbol{x}_N)\right] \\ &\qquad \eta(\boldsymbol{x}_i)\phi_{a_1}(\boldsymbol{x}_1)\cdots\phi_{a_N}(\boldsymbol{x}_N)\,\mathrm{d}\tau' \\ &\quad = \int \phi_{a_i}^*(\boldsymbol{x}_i)\eta(\boldsymbol{x}_i)\phi_{a_i}(\boldsymbol{x}_i)\,\mathrm{d}\boldsymbol{x}_i.\end{aligned}$$

Consequently

$$\langle \Phi_a | \Omega^{(1)} | \Phi_a \rangle = \sum_{i=1}^{N} \langle a_i | \eta | a_i \rangle.$$

Case (ii): Φ_a and Φ_b differ in one function. Suppose, that

$$\begin{aligned} a_i &= b_i \text{ when } i \neq k \\ a_k &\neq b_k. \end{aligned}$$

We have

$$\begin{aligned} &(N!)^{1/2} \int \Phi_b^* \eta(\boldsymbol{x}_i) \phi_{a_1}(\boldsymbol{x}_1) \cdots \phi_{a_N}(\boldsymbol{x}_N) \, \mathrm{d}\tau' \\ &\quad = \int \left[\sum_P (-1)^p P \phi_{a_1}^*(\boldsymbol{x}_1) \cdots \phi_{b_k}^*(\boldsymbol{x}_k) \cdots \phi_{a_N}^*(\boldsymbol{x}_N) \right] \\ &\qquad \eta(\boldsymbol{x}_i) \phi_{a_1}(\boldsymbol{x}_1) \cdots \phi_{a_k}(\boldsymbol{x}_k) \cdots \phi_{a_N}(\boldsymbol{x}_N) \, \mathrm{d}\tau' \\ &\quad = \begin{cases} 0, & \text{if } i \neq k \\ \int \phi_{b_k}^*(\boldsymbol{x}_k) \eta(\boldsymbol{x}_k) \phi_{a_k}(\boldsymbol{x}_k) \, \mathrm{d}\boldsymbol{x}_k, & \text{if } i = k. \end{cases} \end{aligned}$$

So

$$\langle \Phi_b | \Omega^{(1)} | \Phi_a \rangle = \langle b_k | \eta | a_k \rangle.$$

Case (iii): Φ_a and Φ_b differ in two functions, say

$$\begin{aligned} a_i &= b_i \text{ when } i \neq k, l \\ a_k &\neq b_k, b_l \\ a_l &\neq b_k, b_l. \end{aligned}$$

Now

$$\begin{aligned} &(N!)^{1/2} \int \Phi_b^* \eta(\boldsymbol{x}_i) \phi_{a_1}(\boldsymbol{x}_1) \cdots \phi_{a_N}(\boldsymbol{x}_N) \, \mathrm{d}\tau' \\ &\quad = \int \Bigg[\sum_P (-1)^p P \phi_{a_1}^*(\boldsymbol{x}_1) \cdots \phi_{b_k}^*(\boldsymbol{x}_k) \cdots \\ &\qquad \phi_{b_l}^*(\boldsymbol{x}_l) \cdots \phi_{a_N}^*(\boldsymbol{x}_N) \Bigg] \\ &\qquad \eta(\boldsymbol{x}_i) \phi_{a_1}(\boldsymbol{x}_1) \cdots \phi_{a_k}(\boldsymbol{x}_k) \cdots \\ &\qquad \phi_{a_l}(\boldsymbol{x}_l) \cdots \phi_{a_N}(\boldsymbol{x}_N) \, \mathrm{d}\tau' \\ &= 0, \ \forall i \end{aligned}$$

so that

$$\langle \Phi_b | \Omega^{(1)} | \Phi_a \rangle = 0.$$

Clearly this holds also when the determinants differ in more than two functions.

We can summarize:
One body operators have non zero matrix elements only between two determinantal wave functions which are either the same or differ in a single one particle wave function.

Matrix elements of two body operators
We start with

$$\begin{aligned}
&\langle\Phi_b|\Omega^{(2)}|\Phi_a\rangle \\
&\quad= \int \Phi_b^*\Omega^{(2)}\Phi_a \mathrm{d}\tau' \\
&\quad= (N!)^{1/2}\int \Phi_b^*\Omega^{(2)}\phi_{a_1}(\boldsymbol{x}_1)\cdots\phi_{a_N}(\boldsymbol{x}_N)\,\mathrm{d}\tau' \\
&\quad= \frac{1}{2}(N!)^{1/2}\sum_{i\neq j}^{N}\int \Phi_b^*\vartheta(\boldsymbol{x}_i,\boldsymbol{x}_j) \\
&\qquad\qquad \phi_{a_1}(\boldsymbol{x}_1)\cdots\phi_{a_N}(\boldsymbol{x}_N)\,\mathrm{d}\tau'.
\end{aligned}$$

Case (i): $\Phi_a = \Phi_b$. Then

$$\begin{aligned}
&(N!)^{1/2}\int \Phi_b^*\vartheta(\boldsymbol{x}_i,\boldsymbol{x}_j)\phi_{a_1}(\boldsymbol{x}_1)\cdots\phi_{a_N}(\boldsymbol{x}_N)\,\mathrm{d}\tau' \\
&\quad= \int\left[\sum_P(-1)^p P\phi_{a_1}^*(\boldsymbol{x}_1)\cdots\phi_{a_N}^*(\boldsymbol{x}_N)\right] \\
&\qquad \vartheta(\boldsymbol{x}_i,\boldsymbol{x}_j)\phi_{a_1}(\boldsymbol{x}_1)\cdots\phi_{a_N}(\boldsymbol{x}_N)\,\mathrm{d}\tau' \\
&\quad= \int\int\left[\phi_{a_i}^*(\boldsymbol{x}_i)\phi_{a_j}^*(\boldsymbol{x}_j)-\phi_{a_i}^*(\boldsymbol{x}_j)\phi_{a_j}^*(\boldsymbol{x}_i)\right] \\
&\qquad \vartheta(\boldsymbol{x}_i,\boldsymbol{x}_j)\phi_{a_i}(\boldsymbol{x}_i)\phi_{a_j}(\boldsymbol{x}_j)\,\mathrm{d}\boldsymbol{x}_i\mathrm{d}\boldsymbol{x}_j \\
&\quad= \langle a_i a_j|\vartheta|a_i a_j\rangle - \langle a_j a_i|\vartheta|a_i a_j\rangle,
\end{aligned}$$

where the second term comes from the permutation which interchanges $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$. Finally

$$\langle\Phi_a|\Omega^{(2)}|\Phi_a\rangle = \frac{1}{2}\sum_{i\neq j}^{N}\left[\langle a_i a_j|\vartheta|a_i a_j\rangle - \langle a_j a_i|\vartheta|a_i a_j\rangle\right].$$

Case (ii): Φ_a and Φ_b differ in one function, say

$$\begin{aligned}
a_i &= b_i \text{ when } i\neq k \\
a_k &\neq b_k.
\end{aligned}$$

Then

$$(N!)^{1/2}\int \Phi_b^*\vartheta(\boldsymbol{x}_i,\boldsymbol{x}_j)\phi_{a_1}(\boldsymbol{x}_1)\cdots\phi_{a_N}(\boldsymbol{x}_N)\,\mathrm{d}\tau'$$

$$
\begin{aligned}
&= \int \left[\sum_P (-1)^p P \phi^*_{a_1}(\boldsymbol{x}_1) \cdots \phi^*_{b_k}(\boldsymbol{x}_k) \cdots \phi^*_{a_N}(\boldsymbol{x}_N) \right] \\
&\qquad \vartheta(\boldsymbol{x}_i, \boldsymbol{x}_j) \phi_{a_1}(\boldsymbol{x}_1) \cdots \phi_{a_k}(\boldsymbol{x}_k) \cdots \phi_{a_N}(\boldsymbol{x}_N) \, \mathrm{d}\tau' \\
&= \begin{cases} \langle b_k a_j | \vartheta | a_k a_j \rangle - \langle a_j b_k | \vartheta | a_k a_j \rangle, & \text{when } i = k \\ \langle a_i b_k | \vartheta | a_i a_k \rangle - \langle b_k a_i | \vartheta | a_i a_k \rangle, & \text{when } j = k \\ 0, & \text{otherwise.} \end{cases}
\end{aligned}
$$

Now

$$
\begin{aligned}
\langle ij | \vartheta | kl \rangle &= \int\int \left[\phi^*_i(\boldsymbol{x}_1) \phi^*_j(\boldsymbol{x}_2) \vartheta(\boldsymbol{x}_1, \boldsymbol{x}_2) \right. \\
&\qquad \left. \times \phi_k(\boldsymbol{x}_1) \phi_l(\boldsymbol{x}_2) \right] \mathrm{d}\boldsymbol{x}_1 \mathrm{d}\boldsymbol{x}_2 \\
&= \int\int \left[\phi^*_i(\boldsymbol{x}_2) \phi^*_j(\boldsymbol{x}_1) \vartheta(\boldsymbol{x}_2, \boldsymbol{x}_1) \right. \\
&\qquad \left. \times \phi_k(\boldsymbol{x}_2) \phi_l(\boldsymbol{x}_1) \right] \mathrm{d}\boldsymbol{x}_1 \mathrm{d}\boldsymbol{x}_2 \\
&= \langle ji | \vartheta | lk \rangle
\end{aligned}
$$

supposing $\vartheta(\boldsymbol{x}_1, \boldsymbol{x}_2)$ to be symmetric.
Thus we end up with

$$
\begin{aligned}
&\langle \Phi_b | \Omega^{(2)} | \Phi_b \rangle \\
&\quad = \frac{1}{2} \sum_{j=1}^{N} \left[\langle b_k a_j | \vartheta | a_k a_j \rangle - \langle a_j b_k | \vartheta | a_k a_j \rangle \right] \\
&\qquad + \frac{1}{2} \sum_{i=1}^{N} \left[\langle a_i b_k | \vartheta | a_i a_k \rangle - \langle b_k a_i | \vartheta | a_i a_k \rangle \right] \\
&\quad = \sum_{i=1}^{N} \left[\langle a_i b_k | \vartheta | a_i a_k \rangle - \langle b_k a_i | \vartheta | a_i a_k \rangle \right].
\end{aligned}
$$

Case (iii): Φ_a and Φ_b differ in two functions,

$$
\begin{aligned}
a_i &= b_i \text{ when } i! = k, l \\
a_k &\neq b_k, b_l \\
a_l &\neq b_k, b_l
\end{aligned}
$$

say. Then

$$
(N!)^{1/2} \int \Phi^*_b \vartheta(\boldsymbol{x}_i, \boldsymbol{x}_j) \phi_{a_1}(\boldsymbol{x}_1) \cdots \phi_{a_N}(\boldsymbol{x}_N) \, \mathrm{d}\tau'
$$

$$
\begin{aligned}
&= \int \Bigg[\sum_P (-1)^p P \phi^*_{a_1}(\boldsymbol{x}_1) \cdots \phi^*_{b_k}(\boldsymbol{x}_k) \cdots \\
&\qquad \phi^*_{b_l}(\boldsymbol{x}_l) \cdots \phi_{a_N}(\boldsymbol{x}_N) \Bigg] \\
&\qquad \vartheta(\boldsymbol{x}_i, \boldsymbol{x}_j) \phi_{a_1}(\boldsymbol{x}_1) \cdots \phi_{a_k}(\boldsymbol{x}_k) \cdots \\
&\qquad \phi_{a_l}(\boldsymbol{x}_l) \cdots \phi_{a_N}(\boldsymbol{x}_N) \, \mathrm{d}\tau' \\
&= \begin{cases} \langle b_k b_l | \vartheta | a_k a_l \rangle - \langle b_l a_k | \vartheta | a_k a_l \rangle & \text{if } i = k, j = l \\ & \text{or } i = l, j = k \\ 0, & \text{otherwise.} \end{cases}
\end{aligned}
$$

Thus

$$
\begin{aligned}
&\langle \Phi_b | \Omega^{(2)} | \Phi_b \rangle \\
&\quad = \langle b_k b_l | \vartheta | a_k a_l \rangle - \langle b_l a_k | \vartheta | a_k a_l \rangle .
\end{aligned}
$$

Case (iv): Φ_a and Φ_b differ in more than two functions. Now

$$
\langle \Phi_b | \Omega^{(2)} | \Phi_b \rangle = 0,
$$

since every term in the exapnsion of the matrix element contains a factor $\phi^*_{b_k}(\boldsymbol{x}_k)\phi_{a_k}(\boldsymbol{x}_k)$ with $b_k \neq a_k$ which vanishes due to the orthogonality.
We summarize:
Two body operators have non zero matrix elements only between two determinantal wave function which are either the same or differ at most in two one particle functions.

3.4 Creation and destruction operators

The sign of the determinantal wave function

$$
\begin{aligned}
&\Phi_{a_1 a_2 \ldots a_N}(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N) \\
&\quad = \frac{1}{(N!)^{1/2}} \sum_P (-1)^p P \phi_{a_1}(\boldsymbol{x}_1) \phi_{a_2}(\boldsymbol{x}_2) \cdots \phi_{a_N}(\boldsymbol{x}_N)
\end{aligned}
$$

depends on the order of single particle states ϕ_{a_i}. To remove this arbitrariness we

- specify a linear order among the single particle states so, that you can write
$$
a_1 < a_2 \cdots < a_N .
$$
The order is arbitrary but *once fixed stick to it*. For example, you can use the order you tabulate your single particle states, or arrange your states in energetically ascending order.

- write the single particle wave functions in the determinants always in increasing order.

Destruction (or annihilation) operator
The destruction operator c_{a_k} is defined formally as

$$\begin{aligned} c_{a_k}\Phi^N_{a_1\ldots a_k\ldots a_N}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N) \\ &= \pm\Phi^{N-1}_{a_1\ldots a_{k-1}a_{k+1}\ldots a_N}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_{N-1}) \\ &= \pm\frac{1}{[(N-1)!]^{1/2}}\sum_P(-1)^p P\phi_{a_1}(\boldsymbol{x}_1)\cdots \\ &\qquad \phi_{a_{k-1}}(\boldsymbol{x}_{k-1})\phi_{a_{k+1}}(\boldsymbol{x}_k)\cdots\phi_{a_N}(\boldsymbol{x}_{N-1}), \end{aligned}$$

where the sign is

- *positive* if k is *odd*, i.e. ϕ_{a_k} is *preceded by even number of functions* in Φ^N.
- *negative* if k is *even*, i.e. ϕ_{a_k} is *preceded by odd number of functions* in Φ^N.

The effect of the destruction operator c_{a_k} is to convert an N particle determinantal wave function containing ϕ_{a_k} into an $N-1$ particle function not containing ϕ_{a_k}.
In the case Φ^N does not contain ϕ_{a_k} we define

$$c_{a_k}\Phi^N_{a_1\ldots a_N} = 0 \text{ if } a_k \notin \{a_1,\ldots,a_N\}.$$

Creation operator
The creation operator $c_l^\dagger$ is defined formally as

$$\begin{aligned} c_l^\dagger\Phi^N_{a_1\ldots a_j a_{j+1}\ldots a_N}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N) \\ &= \pm\Phi^{N+1}_{a_1}\ldots a_j l a_{j+1}\ldots a_N)(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_{N+1}) \\ &= \pm\frac{1}{[(N+1)!]^{1/2}}\sum_P(-1)^p P\phi_{a_1}(\boldsymbol{x}_1)\cdots\phi_{a_j}(\boldsymbol{x}_j) \\ &\qquad \phi_l(\boldsymbol{x}_{j+1})\phi_{a_{j+1}}(\boldsymbol{x}_{j+2})\cdots\phi_{a_N}(\boldsymbol{x}_{N+1}), \end{aligned}$$

where $a_j < l < a_{j+1}$ and the sign is

- *positive* if j is *even*, i.e. ϕ_l is *preceded by even number of functions* in Φ^{N+1}.
- *negative* if j is *odd*, i.e. ϕ_l is *preceded by odd number* of functions in Φ^{N+1}.

The effect of the creation operator $c_l^\dagger$ is to convert an N particle determinantal wave function not containing ϕ_l into an $N+1$ particle state containing ϕ_l.
In the case Φ^N contains ϕ_l we define

$$c_l^\dagger\Phi^N_{a_1\ldots a_N} = 0 \text{ if } l \in \{a_1,\ldots a_N\}.$$

Note that the sign associated with

- destruction operator is defined to be positive when the one particle function is destroyed in the first position, i.e.

$$c_{a_1}\Phi^N_{a_1a_2\ldots a_N} = \Phi^{N-1}_{a_2\ldots a_N},$$

and, otherwise, to correspond exchanges required to move the function to be removed in the first position, e.g.

$$\begin{aligned} c_{a_2}\Phi^N_{a_1a_2\ldots a_N} &= -c_{a_2}\Phi^N_{a_2a_1\ldots a_N} \\ &= -\Phi^{N-1}_{a_1a_3\ldots a_N}. \end{aligned}$$

- creation operator is defined to be positive when the one particle function is created in the first position, i.e.

$$c_l^\dagger\Phi^N_{a_1\ldots a_N} = \Phi^{N+1}_{la_1\ldots a_N},$$

and, otherwise, correspond to exchanges required to move the function inserted in the first position to its correct place, e.g.

$$\begin{aligned} c_l^\dagger\Phi^N_{a_1a_2\ldots a_N} &= \Phi^{N+1}_{la_1a_2\ldots a_N} \\ &= -\Phi^{N+1}_{a_1la_2\ldots a_N}, \end{aligned}$$

if $a_1 < l < a_2$.

3.5 Occupation numbers

Instead of specifying a determinantal wave function Φ by subscripts of the functions appearing in it we will get a more convenient notation by giving the *occupation number* n_i of each single particle state ϕ_i, i.e. we

- define n_i to be 1 or 0 according to whether the function ϕ_i is or is not contained in Φ.
- write N particle determinantal wave function like

$$\Phi^N(n_1, n_2, n_3, \ldots).$$

For example, we have

$$\Phi^N_{a_1a_2\ldots a_N} \equiv \Phi^N(0_1, 0_2, \ldots, 1_{a_1}, \ldots, 1_{a_2}, \ldots, 1_{a_N}, \ldots).$$

Sometimes we also use notation

$$|n_1, n_2, n_3, \ldots\rangle \equiv \Phi(n_1, n_2, n_3, \ldots),$$

or, more compactly, give only the indeces i of the states for which $n_i = 1$, e.g.

$$|0_1, 0_2, \ldots, 1_{a_1}, \ldots, 1_{a_2}, \ldots, 1_{a_N}, \ldots\rangle \equiv |a_1a_2\ldots a_N\rangle.$$

In the occupation representation the definition of the destruction operator c_k takes the form

$$\begin{aligned} c_k\Phi^N(\ldots 1_k \ldots) &= \theta_k\Phi^{N-1}(\ldots 0_k \ldots), \\ c_k\Phi^N(\ldots 0_k \ldots) &= 0. \end{aligned}$$

Here c_k leaves all other occupation numbers unchanged. The sign θ_k is given by

$$\theta_k = (-1)^{\sum_{j<k} n_j}$$

in accordance with our previous definition.
Similarly, the creation operator $c_k^\dagger$ is defined as

$$\begin{aligned} c_k^\dagger\Phi^N(\ldots 0_k \ldots) &= \theta_k\Phi^{N+1}(\ldots 1_k \ldots), \\ c_k^\dagger\Phi^N(\ldots 1_k \ldots) &= 0. \end{aligned}$$

All other occupation numbers are left untouched.
We can rewrite more compactly

$$\begin{aligned} c_k\Phi^N(\ldots n_k \ldots) &= \theta_k n_k\Phi^{N-1}(\ldots 0_k \ldots) \\ c_k^\dagger\Phi^N(\ldots n_k \ldots) &= \theta_k(1-n_k)\Phi^{N+1}(\ldots 1_k \ldots). \end{aligned}$$

3.6 Commutation relations

We have

$$c_l c_k\Phi^N(\ldots n_k \ldots n_l \ldots) = \theta_k n_k c_l\Phi^{N-1}(\ldots 0_k \ldots n_l \ldots)$$

and

$$c_k c_l\Phi^N(\ldots n_k \ldots n_l \ldots) = \theta_l n_l c_k\Phi^{N-1}(\ldots n_k \ldots 0_l \ldots),$$

where we have assumed that $k < l$. If either $n_k = 0$ or $n_l = 0$, both expressions are zero. So, suppose that $n_k = n_l = 1$. then

$$\begin{aligned} c_l c_k\Phi^N(\ldots 1_k \ldots 1_l \ldots) &= \theta_k c_l\Phi^{N-1}(\ldots 0_k \ldots 1_l \ldots) \\ &= \theta_k\theta_l'\Phi^{N-2}(\ldots 0_k \ldots 0_l \ldots), \end{aligned}$$

and

$$\begin{aligned} c_k c_l\Phi^N(\ldots 1_k \ldots 1_l \ldots) &= \theta_l c_k\Phi^{N-1}(\ldots 1_k \ldots 0_l \ldots) \\ &= \theta_l\theta_k'\Phi^{N-2}(\ldots 0_k \ldots 0_l \ldots). \end{aligned}$$

Above

- $\theta_l' = (-1)^p$, where p is the number of occupied states preceding ϕ_l in $\Phi^{N-1}(\ldots 0_k \ldots 1_l \ldots)$. Clearly $\theta_l' = -\theta_l$, since the number of the occupied states preceding ϕ_l has been reduced by one by the operator c_k.

- $\theta'_k = (-1)^q$, where q is the number of occupied states preceding ϕ_k in $\Phi^{N-1}(\ldots 1_k \ldots 0_l \ldots)$. Clearly $\theta'_k = \theta_k$, since no states preceding ϕ_k has been destroyed or created.

So, we have *the anticommutation rule*

$$c_l c_k \Phi^N = -c_k c_l \Phi^N \ \forall \Phi^N$$

and we can write

$$\{c_l, c_k\} \equiv c_l c_k + c_k c_l = 0.$$

Similarly we can show that creation operators obey the anticommutation rule

$$\{c_k^\dagger, c_l^\dagger\} = 0.$$

It is easy to see that these relations hold also for the cases $k > l$ and $k = l$. Consider now consecutive creation and destruction operations, c_k and $c_l^\dagger$ say. Supposing again $l > k$ we have

$$\begin{aligned} & c_l^\dagger c_k \Phi^N(\ldots n_k \ldots n_l \ldots) \\ & \quad = \theta_k n_k c_l^\dagger \Phi^{N-1}(\ldots 0_k \ldots n_l \ldots) \end{aligned}$$

and

$$\begin{aligned} & c_k c_l^\dagger \Phi^N(\ldots n_k \ldots n_l \ldots) \\ & \quad = \theta_l (1 - n_l) c_k \Phi^{N+1}(\ldots n_k \ldots 1_l \ldots). \end{aligned}$$

If either $n_k = 0$ or $n_l = 1$, both expressions vanish. We set $n_k = 1$ and $n_l = 0$. Then

$$\begin{aligned} c_l^\dagger c_k \Phi^N(\ldots 1_k \ldots 0_l \ldots) &= \theta_k c_l^\dagger \Phi^{N-1}(\ldots 0_k \ldots 0_l \ldots) \\ &= \theta_k \theta'_l \Phi^N(\ldots 0_k \ldots 1_l \ldots) \end{aligned}$$

and

$$\begin{aligned} c_k c_l^\dagger \Phi^N(\ldots 1_k \ldots 0_l \ldots) &= \theta_l c_k \Phi^{N+1}(\ldots 1_k \ldots 1_l \ldots) \\ &= \theta_l \theta'_k \Phi^N(\ldots 0_k \ldots 1_l \ldots). \end{aligned}$$

Again, it is evident that

- $\theta'_l = -\theta_l$ since we have destroyed one occupied state preceding ϕ_l in the final determinant Φ^N.
- $\theta'_k = \theta_k$, since no states preceeding ϕ_k in the intermediate determinant Φ^{N+1} has been destroyed or created.

So, we have

$$\{c_k, c_l^\dagger\} = 0 \text{ when } k < l.$$

It is clear, that the same holds also when $k > l$.

Set now $l = k$. If $n_k = 1$, we have

$$\begin{aligned} c_k^\dagger c_k \Phi^N(\ldots 1_k \ldots) &= \theta_k c_k^\dagger \Phi^{N-1}(\ldots 0_k \ldots) \\ &= \theta_k^2 \Phi^N(\ldots 1_k \ldots) \\ &= \Phi^N(\ldots 1_k \ldots) \end{aligned}$$

and

$$c_k c_k^\dagger \Phi^N(\ldots 1_k \ldots) = 0.$$

If, on the other hand, $n_k = 0$, we have

$$c_k^\dagger c_k \Phi^N(\ldots 0_k \ldots) = 0$$

and

$$\begin{aligned} c_k c_k^\dagger \Phi^N(\ldots 0_k \ldots) &= \theta_k c_k \Phi^{N+1}(\ldots 1_k \ldots) \\ &= \theta_k^2 \Phi^N(\ldots 0_k \ldots) \\ &= \Phi^N(\ldots 0_k \ldots). \end{aligned}$$

We see that we can write

$$\{c_k^\dagger, c_k\} = 1$$

or, together with the previous results,

$$\{c_l^\dagger, c_k\} = \delta_{kl}.$$

From the previous calculations we also deduce that

$$c_k^\dagger c_k \Phi^N(\ldots n_k \ldots) = n_k \Phi^N(\ldots n_k \ldots),$$

or in the operator form

$$c_k^\dagger c_k = n_k.$$

That's why $c_k^\dagger c_k$ is called the *number operator* for the one particle state ϕ_k. To summarize:

$$\begin{aligned} \{c_l, c_k\} &= 0 \\ \{c_l^\dagger, c_k^\dagger\} &= 0 \\ \{c_k^\dagger, c_l\} &= \delta_{kl} \\ c_k^\dagger c_k &= n_k. \end{aligned}$$

3.7 The vacuum

We define the *vacuum* (or *emty*) *state* Φ_{vac} to be the fictious 'zeroth order' determinant containing no single particle functions, i.e. we set

$$\Phi_{\text{vac}} \equiv \Phi(0_1, 0_2, 0_3, \ldots).$$

Applying successively creation operators on $\Phi_{\rm vac}$ we can construct all possible determinantal wave functions. For example

$$\begin{aligned} c_1^\dagger \Phi_{\rm vac} &= c_1^\dagger \Phi(0_1, 0_2, 0_3, \ldots) \\ &= \Phi^1(1_1, 0_2, 0_3, \ldots) \\ &= \phi_1(\boldsymbol{x}_1) \end{aligned}$$

and

$$\begin{aligned} c_3^\dagger c_1^\dagger c_2^\dagger \Phi_{\rm vac} &= c_3^\dagger c_1^\dagger c_2^\dagger \Phi(0_1, 0_2, 0_3, \ldots) \\ &= c_3^\dagger c_1^\dagger \Phi^1(0_1, 1_2, 0_3, \ldots) \\ &= c_3^\dagger \Phi^2(1_1, 1_2, 0_3, \ldots) \\ &= (-1)^2 \Phi^3(1_1, 1_2, 1_3, 0_4, \ldots) \\ &= \frac{1}{(3!)^{1/2}} \begin{vmatrix} \phi_1(\boldsymbol{x}_1) & \phi_1(\boldsymbol{x}_2) & \phi_1(\boldsymbol{x}_3) \\ \phi_2(\boldsymbol{x}_1) & \phi_2(\boldsymbol{x}_2) & \phi_2(\boldsymbol{x}_3) \\ \phi_3(\boldsymbol{x}_1) & \phi_3(\boldsymbol{x}_2) & \phi_3(\boldsymbol{x}_3) \end{vmatrix}. \end{aligned}$$

3.8 One and two body operators

We want to write the one and two body operators,

$$\begin{aligned} \Omega^{(1)} &= \sum_{i=1}^{N} \eta(\boldsymbol{x}_i) \\ \Omega^{(2)} &= \frac{1}{2} \sum_{i \neq j}^{N} \vartheta(\boldsymbol{x}_i, \boldsymbol{x}_j). \end{aligned} \qquad (*)$$

respectively, in terms of creation and destruction operators.
We claim that

$$\boxed{\begin{aligned} \Omega^{(1)} &= \sum_{i,j} \langle i|\eta|j\rangle c_i^\dagger c_j \\ \Omega^{(2)} &= \frac{1}{2} \sum_{i,j,k,l} \langle ij|\vartheta|kl\rangle c_i^\dagger c_j^\dagger c_l c_k. \end{aligned}} \qquad (**)$$

Here

- the single particle matrix elements are, as before,

$$\langle i|\eta|j\rangle = \int \phi_i^*(\boldsymbol{x}) \eta(\boldsymbol{x}) \phi_j(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}.$$

- the two particle matrix elements are, again as before,

$$\begin{aligned} &\langle ij|\vartheta|kl\rangle \\ &\quad = \int\int \phi_i^*(\boldsymbol{x}_1) \phi_j^*(\boldsymbol{x}_2) \vartheta(\boldsymbol{x}_1, \boldsymbol{x}_2) \\ &\qquad \phi_k(\boldsymbol{x}_1) \phi_l(\boldsymbol{x}_2) \, \mathrm{d}\boldsymbol{x}_1 \mathrm{d}\boldsymbol{x}_2. \end{aligned}$$

- the summation over indeces, i.e. over single particle states, goes over *all* values.
- *the relative order of operators with respect to the labeling indeces is important*. In particular, note the product $c_l c_k$.

To prove the equivalence of the two representations $(*)$ and $(**)$ we will proceed in the most straightforward way by showing that their matrix elements are identical.

One body operator in a one particle system
For one particle systems we have

$$\begin{aligned}\Phi_a &= \Phi^1(\ldots 1_k \ldots) = \phi_k(\boldsymbol{x}_1)\\ \Phi_b &= \Phi^1(\ldots 1_l \ldots) = \phi_l(\boldsymbol{x}_1).\end{aligned}$$

We see that the matrix elements of $\Omega^{(1)}$ in the representation $(*)$ in this case are given by

$$\langle\Phi_a|\Omega^{(1)}|\Phi_b\rangle = \langle\Phi_a|\eta(\boldsymbol{x}_1)|\Phi_b\rangle = \langle k|\eta|l\rangle.$$

In the representation $(**)$ we have

$$\begin{aligned}\langle\Phi_a|\Omega^{(1)}|\Phi_b\rangle &= \left\langle \Phi_a \left| \sum_{i,j} \langle i|\eta|j\rangle c_i^\dagger c_j \right| \Phi_b \right\rangle\\ &= \sum_{i,j} \langle i|\eta|j\rangle \ \langle\Phi_a|c_i^\dagger c_j|\Phi_b\rangle\\ &= \sum_{i,j} \langle i|\eta|j\rangle \ \int \Phi_a^* c_i^\dagger c_j \Phi_b \mathrm{d}\tau'.\end{aligned}$$

Now $c_j\Phi_b = 0$ unless $j = l$, in which case $c_l\Phi_b = \Phi_{\mathrm{vac}}$, and $c_i^\dagger\Phi_{\mathrm{vac}} = \Phi_a$ only if $i = k$. Thus

$$\langle\Phi_a|\Omega^{(1)}|\Phi_b\rangle = \langle k|\eta|l\rangle$$

holds also in the representation $(**)$.

Two body operator in a two particle system
For two particle systems we have

$$\begin{aligned}\Phi_a &= \Phi^2(\ldots 1_m \ldots 1_n \ldots)\\ &= \frac{1}{\sqrt{2}}\left[\phi_m(\boldsymbol{x}_1)\phi_n(\boldsymbol{x}_2) - \phi_n(\boldsymbol{x}_1)\phi_m(\boldsymbol{x}_2)\right]\\ \Phi_b &= \Phi^2(\ldots 1_p \ldots 1_q \ldots)\\ &= \frac{1}{\sqrt{2}}\left[\phi_p(\boldsymbol{x}_1)\phi_q(\boldsymbol{x}_2) - \phi_q(\boldsymbol{x}_1)\phi_p(\boldsymbol{x}_2)\right].\end{aligned}$$

In the representation $(*)$ we have

$$\begin{aligned}
&\langle\Phi_a|\Omega^{(2)}|\Phi_b\rangle \\
&\quad= \frac{1}{2}\sum_{i\neq j}^{2}\int \Phi_a^*\vartheta(\boldsymbol{x}_i,\boldsymbol{x}_j)\Phi_b \mathrm{d}\tau' \\
&\quad= \int \Phi_a^*\vartheta(\boldsymbol{x}_1,\boldsymbol{x}_2)\Phi_b \mathrm{d}\tau' \\
&\quad= \frac{1}{2}\int\Bigg[[\phi_m^*(\boldsymbol{x}_1)\phi_n^*(\boldsymbol{x}_2)-\phi_n^*(\boldsymbol{x}_1)\phi_m^*(\boldsymbol{x}_2)] \\
&\qquad\qquad \vartheta(\boldsymbol{x}_1,\boldsymbol{x}_2) \\
&\qquad [\phi_p(\boldsymbol{x}_1)\phi_q(\boldsymbol{x}_2)-\phi_q(\boldsymbol{x}_1)\phi_p(\boldsymbol{x}_2)]\Bigg]\mathrm{d}\boldsymbol{x}_1\mathrm{d}\boldsymbol{x}_2 \\
&\quad= \frac{1}{2}\left[\langle mn|\vartheta|pq\rangle-\langle mn|\vartheta|qp\rangle\right. \\
&\qquad \left.-\langle nm|\vartheta|pq\rangle+\langle nm|\vartheta|qp\rangle\right] \\
&\quad= \langle mn|\vartheta|pq\rangle-\langle mn|\vartheta|qp\rangle.
\end{aligned}$$

In the representation $(**)$ we write

$$\begin{aligned}
\langle\Phi_a|\Omega^{(2)}|\Phi_b\rangle &= \left\langle \Phi_a\left|\frac{1}{2}\sum_{i,j,k,l}\langle ij|\vartheta|kl\rangle c_i^\dagger c_j^\dagger c_l c_k\right|\Phi_b\right\rangle \\
&= \frac{1}{2}\sum_{i,j,k,l}\langle ij|\vartheta|kl\rangle\int\Phi_a^* c_i^\dagger c_j^\dagger c_l c_k\Phi_b\mathrm{d}\tau'.
\end{aligned}$$

Due to the orthogonality of the determinantal wave functions the integral vanishes unless

$$c_i^\dagger c_j^\dagger c_l c_k\Phi_b = \pm\Phi_a,$$

or unless $l,k=p,q$ and $i,j=m,n$.
Consider the case $k=p,l=q,j=n,i=m$. We now have

$$\begin{aligned}
c_m^\dagger c_n^\dagger c_q c_p\Phi_b &= c_m^\dagger c_n^\dagger c_q c_p\Phi^2(\ldots 1_p\ldots 1_q\ldots) \\
&= c_m^\dagger c_n^\dagger c_q\Phi^1(\ldots 1_q\ldots) \\
&= c_m^\dagger c_n^\dagger\Phi_{\mathrm{vac}} \\
&= c_m^\dagger\Phi^1(\ldots 1_n\ldots) \\
&= \Phi^2(\ldots 1_m\ldots 1_n\ldots)=\Phi_b,
\end{aligned}$$

and the value of the integral is $+1$.
Using the anticommutation relations we have immediately

$$k=q,l=p,j=n,i=m, \qquad \int = -1$$

$$k = p, l = q, j = m, i = n, \qquad \int = -1$$
$$k = q, l = p, j = m, i = n, \qquad \int = +1$$

and end up with

$$\begin{aligned}
&\langle \Phi_a | \Omega^{(2)} | \Phi_b \rangle \\
&\quad = \frac{1}{2}[\langle mn|\vartheta|pq\rangle - \langle mn|\vartheta|qp\rangle \\
&\qquad -\langle nm|\vartheta|pq\rangle + \langle nm|\vartheta|qp\rangle] \\
&\quad = \langle mn|\vartheta|pq\rangle - \langle mn|\vartheta|qp\rangle
\end{aligned}$$

showing the equivalence of the two representation.

Matrix elements of one body operators
Let Φ_a and Φ_b be N-particle determinantal functions. In the representation $(**)$ we have

$$\begin{aligned}
\langle \Phi_b | \Omega^{(1)} | \Phi_b \rangle &= \int \Phi_b^* \left[\sum_{i,j} \langle i|\eta|j\rangle c_i^\dagger c_j \right] \Phi_a \mathrm{d}\tau' \\
&= \sum_{i,j} \langle i|\eta|j\rangle \int \Phi_b^* c_i^\dagger c_j \Phi_a \mathrm{d}\tau'.
\end{aligned}$$

Case (i): Diagonal elements, i.e. $\Phi_a = \Phi_b$. Now, due to the orthogonality,

$$\int \Phi_a^* c_i^\dagger c_j \Phi_a \mathrm{d}\tau'$$

vanishes unless

$$c_i^\dagger c_j \Phi_a = \pm \Phi_a.$$

The only possibility is that $i = j$, in which case

$$\int \Phi_a^* c_i^\dagger c_i \Phi_a d\tau' = n_i.$$

Thus, for diagonal elements we can write

$$\begin{aligned}
\langle \Phi_a | \Omega^{(1)} | \Phi_a \rangle &= \sum_i \langle i|\eta|i\rangle \int \Phi_a^* c_i^\dagger c_i \Phi_a \mathrm{d}\tau' \\
&= \sum_i \langle i|\eta|i\rangle n_i.
\end{aligned}$$

Since

$$\Phi_a = \Phi^N(\ldots, 1_{a_1}, \ldots, 1_{a_N}, \ldots),$$

i.e. only the states $a_1, a_2, \ldots, a_N$ are occupied, we have

$$n_i = \begin{cases} 1, & \text{for } i = a_1, a_2, \ldots, a_N \\ 0, & \text{otherwise.} \end{cases}$$

Consequently

$$\langle \Phi_a | \Omega^{(1)} | \Phi_a \rangle = \sum_{i=1}^{N} \langle a_i | \eta | a_i \rangle$$

in agreement with our earlier results for the representation $(*)$.
Case (ii): Φ_a and Φ_b differ in one function. Let us suppose that

$$\begin{aligned} \Phi_a &= \Phi^N(\ldots 0_k, 1_l \ldots) \\ \Phi_b &= \Phi^N(\ldots 1_k, 0_l \ldots) \end{aligned}$$

all the other occupations being the same in Φ_a and Φ_b. Note that we have assumed *the differing states to take consecutive positions* in the occupation representation, and

- in our earlier treatment of the corresponding case in the representation $(*)$ we assumed that the differing functions, ϕ_{a_k} and ϕ_{b_k}, occupy the same rows (or columns) in the determinants.
- in occupation representation above this would mean that the differing states take consecutive positions or, equivalently, that there are no occupied states between them.

Our assumption of the consecutive positions of l and k will not lead to any loss of generality, since

- we can always permute the state l (or k) to its proper position in Φ^N resulting only a *possible change of sign*.
- in the determinantal wave functions exactly the same permutation with the same change of sign will be required to carry the single particle function into its corresponding row (or column).

Now the integral

$$\int \Phi_b^* c_i^\dagger c_j \Phi_a \mathrm{d}\tau'$$

vanishes unless $j = l$ and $i = k$, when it has the value 1. Thus

$$\langle \Phi_b | \Omega^{(1)} | \Phi_a \rangle = \langle k | \eta | l \rangle$$

in agreement with our earlier result.
Case (iii): Φ_a and Φ_b differ in more than one function. Because $c_i^\dagger c_j$ can replace only one function in Φ_a with another one, it is clear that

$$c_i^\dagger c_j \Phi_a \neq \pm \Phi_b \ \forall i, j.$$

Correspondingly

$$\langle \Phi_b | \Omega^{(1)} | \Phi_a \rangle = 0,$$

again in agreement with the result for the representation $(*)$.
Thus, we have shown that for one body operators the representations $(*)$ and $(**)$ are equivalent.

Matrix elements of two body operators
Let Φ_a and Φ_b be N-particle determinantal functions. In the representation $(**)$ we have

$$\langle \Phi_b | \Omega^{(2)} | \Phi_a \rangle = \frac{1}{2} \sum_{i,j,k,l} \langle ij|\vartheta|kl\rangle \int \Phi_b^* c_i^\dagger c_j^\dagger c_l c_k \Phi_a \mathrm{d}\tau'.$$

Case (i): Diagonal elements,, i.e. $\Phi_a = \Phi_b$. Due to the orthogonality of the determinantal wave functions the integral

$$\int \Phi_a^* c_i^\dagger c_j^\dagger c_l c_k \Phi_a \mathrm{d}\tau'$$

vanishes unless

$$c_i^\dagger c_j^\dagger c_l c_k \Phi_a = \pm \Phi_a.$$

This can happen only when

1. Φ_a contains ϕ_k and ϕ_l, with $k \neq l$.
2. $i = k, j = l$ or $i = l, j = k$.

We have the two cases:

- if $j = k$ we must have $i = l$ and the anticommutation rules tell us that

$$c_i^\dagger c_j^\dagger c_l c_k = -c_i^\dagger c_l c_j^\dagger c_k = -c_i^\dagger c_i c_j^\dagger c_j = -n_i n_j.$$

- if $j = l$ we must have $i = k$ and from the anticommutation rules we have

$$c_i^\dagger c_j^\dagger c_l c_k = -c_i^\dagger c_j^\dagger c_k c_l = c_i^\dagger c_k c_j^\dagger c_l = c_i^\dagger c_i c_j^\dagger c_j = n_i n_j.$$

We can now write

$$\langle \Phi_a | \Omega^{(2)} | \Phi_a \rangle = \frac{1}{2} \sum_{i,j} n_i n_j [\langle ij|\vartheta|ij\rangle - \langle ij|\vartheta|ji\rangle].$$

Like before we have

$$n_i = \begin{cases} 1, & \text{for } i = a_1, a_2, \ldots, a_N \\ 0, & \text{otherwise} \end{cases}$$

so that

$$\langle \Phi_a | \Omega^{(2)} | \Phi_a \rangle = \frac{1}{2} \sum_{i,j} [\langle a_i a_j|\vartheta|a_i a_j\rangle - \langle a_i a_j|\vartheta|a_j a_i\rangle]$$

just like for representation $(*)$.
Case (ii): Φ_a and Φ_b differ in one function. Like in the treatment of $\Omega^{(1)}$ we suppose that

$$\begin{aligned}\Phi_a &= \Phi^N(\ldots 1_p 0_q \ldots)\\ \Phi_b &= \Phi^N(\ldots 0_p 1_q \ldots)\end{aligned}$$

all other occupations being the same. Our earlier discussion concerning the generality when choosing the differing functions occupying consecutive locations is valid here, too.
The integral

$$\int \Phi_b^* c_i^\dagger c_j^\dagger c_l c_k \Phi_a \mathrm{d}\tau'$$

vanishes unless

$$c_i^\dagger c_j^\dagger c_l c_k \Phi_a = \pm \Phi_b,$$

i.e. the operator $c_i^\dagger c_j^\dagger c_l c_k$ must destroy ϕ_p and create ϕ_q and nothing else. There are four possibilities:

1. $k = p, j = q, i = l$, so that
$$c_i^\dagger c_j^\dagger c_l c_k \Phi_a = c_i^\dagger c_q^\dagger c_i c_p \Phi_a = -c_i^\dagger c_i c_q^\dagger c_p \Phi_a = -n_i \Phi_b.$$
2. $k = p, i = q, j = l$, so that
$$c_i^\dagger c_j^\dagger c_l c_k \Phi_a = c_q^\dagger c_j^\dagger c_j c_p \Phi_a = c_j^\dagger c_j c_q^\dagger c_p \Phi_a = n_j \Phi_b.$$
3. $l = p, j = q, i = k$, so that
$$c_i^\dagger c_j^\dagger c_l c_k \Phi_a = c_i^\dagger c_q^\dagger c_p c_i \Phi_a = c_i^\dagger c_i c_q^\dagger c_p \Phi_a = n_i \Phi_b.$$
4. $l = p, i = q, j = k$, so that
$$c_i^\dagger c_j^\dagger c_l c_k \Phi_a = c_q^\dagger c_j^\dagger c_p c_j \Phi_a = -c_j^\dagger c_j c_q^\dagger c_p \Phi_a = -n_j \Phi_b.$$

We can now write

$$\begin{aligned}&\langle \Phi_b | \Omega^{(2)} | \Phi_a \rangle\\ &\quad = \frac{1}{2} \sum_{i,j,k,l} \langle ij|\vartheta|kl\rangle \int \Phi_b^* c_i^\dagger c_j^\dagger c_l c_k \Phi_a \mathrm{d}\tau'\\ &\quad = \frac{1}{2} \sum_j \langle qj|\vartheta|pj\rangle n_j - \frac{1}{2} \sum_i \langle iq|\vartheta|pi\rangle n_i\\ &\qquad + \frac{1}{2} \sum_i \langle iq|\vartheta|ip\rangle n_i - \frac{1}{2} \sum_j \langle qj|\vartheta|jp\rangle n_j\\ &\quad = \sum_i [\langle iq|\vartheta|ip\rangle - \langle qi|\vartheta|ip\rangle] n_i.\end{aligned}$$

We note that the number n_i is actually the one for ϕ_i in Φ_b. The occupation numbers n_i are, however, the same in Φ_a and Φ_b except when $i = p$ or $i = q$. In both cases the expression

$$\langle iq|\vartheta|ip\rangle - \langle qi|\vartheta|ip\rangle$$

vanishes, so that we can use

$$n_i = \begin{cases} 1, & \text{for } i = a_1, a_2, \ldots, a_N \\ 0, & \text{otherwise.} \end{cases}$$

Writing a_k for p, b_k for q and a_i for i we end up with

$$\langle \Phi_b|\Omega^{(2)}|\Phi_a\rangle = \sum_{i=1}^{N}[\langle a_i b_k|\vartheta|a_i a_k\rangle - \langle b_k a_i|\vartheta|a_i a_k\rangle],$$

which is identical with our previous result in the representation $(*)$.
Case (iii): Φ_a and Φ_b differ in two functions. We suppose, that

$$\begin{aligned} \Phi_a &= \Phi^N(\ldots 1_p 0_r 1_q 0_s \ldots) \\ \Phi_b &= \Phi^N(\ldots 0_p 1_r 0_q 1_s \ldots), \end{aligned}$$

all other occupations being the same. Again, repeating our earlier arguments, we see that we will lose no generality when we assume the differing functions to occupy consecutive positions. It is also clear, that it does not matter whether $p < r$ or $r < p$ or whether $q < s$ or $s < q$.
Again the integral

$$\int \Phi_b^* c_i^\dagger c_j^\dagger c_l c_k \Phi_a \mathrm{d}\tau'$$

vanishes unless

$$c_i^\dagger c_j^\dagger c_l c_k \Phi_a = \pm\Phi_b.$$

This can happen only when the operator $c_l c_k$ destroys ϕ_p and ϕ_q and the operator $c_i^\dagger c_j^\dagger$ creates ϕ_r and ϕ_s in Φ_a.
We have four possibilities:

1. $i = r, j = s, l = p, k = q$, so that

$$c_i^\dagger c_j^\dagger c_k c_l \Phi_a = c_r^\dagger c_s^\dagger c_p c_q \Phi_a = -c_r^\dagger c_p c_s^\dagger c_q \Phi_a = -\Phi_b.$$

2. $i = r, j = s, l = q, k = p$, so that

$$c_i^\dagger c_j^\dagger c_k c_l \Phi_a = c_r^\dagger c_s^\dagger c_q c_p \Phi_a = c_r^\dagger c_p c_s^\dagger c_q \Phi_a = \Phi_b.$$

3. $i = s, j = r, l = p, k = q$, so that

$$c_i^\dagger c_j^\dagger c_k c_l \Phi_a = c_s^\dagger c_r^\dagger c_p c_q \Phi_a = c_r^\dagger c_p c_s^\dagger c_q \Phi_a = \Phi_b.$$

4. $i = s, j = r, l = q, k = p$, so that

$$c_i^\dagger c_j^\dagger c_k c_l \Phi_a = c_s^\dagger c_r^\dagger c_q c_p \Phi_a = -c_r^\dagger c_p c_s^\dagger c_q \Phi_a = -\Phi_b.$$

The matrix element will now be

$$\begin{aligned}
&\langle \Phi_b | \Omega^{(2)} | \Phi_a \rangle \\
&\quad = \frac{1}{2} \sum_{i,j,k,l} \langle ij|\vartheta|kl\rangle \int \Phi_b^* c_i^\dagger c_j^\dagger c_l c_k \Phi_a \mathrm{d}\tau' \\
&\quad = -\frac{1}{2} \langle rs|\vartheta|qp\rangle + \frac{1}{2} \langle rs|\vartheta|pq\rangle \\
&\qquad + \frac{1}{2} \langle sr|\vartheta|qp\rangle - \frac{1}{2} \langle sr|\vartheta|pq\rangle \\
&\quad = \langle rs|\vartheta|pq\rangle - \langle sr|\vartheta|pq\rangle.
\end{aligned}$$

Replacing p with a_k, q with a_l, r with b_k and s with b_l we end up with

$$\langle \Phi_b | \Omega^{(2)} | \Phi_a \rangle = \langle b_k b_l|\vartheta|a_k a_l\rangle - \langle b_l b_k|\vartheta|a_k a_l\rangle,$$

which again is exactly the result we obtained in the representation $(*)$.
Case (iv): Φ_a and Φ_b differ in more than two functions. Because the operator $c_i^\dagger c_j^\dagger c_l c_k$ can replace at most two functions in Φ_a, it is clear that

$$c_i^\dagger c_j^\dagger c_l c_k \Phi_a \neq \pm \Phi_b \ \forall i, j, k, l.$$

Correspondingly

$$\langle \Phi_b | \Omega^{(2)} | \Phi_a \rangle = 0,$$

again in agreement with our previous result.
Thus we have shown that the two representations $(*)$ and $(**)$ for $\Omega^{(2)}$ are equivalent.

3.9 Hermitean conjugacy of c and $c^\dagger$

Suppose that

$$\Phi_a = \Phi^{N+1}(\ldots 1_i \ldots)$$

and

$$\Phi_b = \Phi^N(\ldots 0_i \ldots)$$

all other occupation numbers being the same. Furthermore, suppose that

$$\Phi_b = c_i \Phi_a,$$

i.e. the number of occupied states preceding ϕ_i is even. Then

$$\int \Phi_b^* c_i \Phi_a \mathrm{d}\tau' = 1.$$

Denote by c_i^{H} the Hermitean conjugate of c_i. By definition

$$\int \Phi_b^* c_i \Phi_a \mathrm{d}\tau' = \left(\int \Phi_a^* c_i^{\mathrm{H}} \Phi_b \mathrm{d}\tau' \right)^* = 1.$$

Since the determinants Φ_a are arbitrary, except that they must contain ϕ_i, it is evident that

$$\Phi_a = c_i^{\mathrm{H}} \Phi_b,$$

so, that c_i^{H} creates the state ϕ_i, i.e.

$$c_i^{\mathrm{H}} = c_i^\dagger.$$

3.10 Field operators

Sometimes the many body theory is expressed in terms of *field operators* $\boldsymbol{\Psi}(\boldsymbol{x})$ and $\boldsymbol{\Psi}^\dagger(\boldsymbol{x})$ defined as

$$\begin{aligned} \boldsymbol{\Psi}(\boldsymbol{x}) &= \sum_i \phi_i(\boldsymbol{x}) c_i \\ \boldsymbol{\Psi}^\dagger(\boldsymbol{x}) &= \sum_i \phi_i^*(\boldsymbol{x}) c_i^\dagger. \end{aligned}$$

Now

$$\begin{aligned} &\{\boldsymbol{\Psi}(\boldsymbol{x}), \boldsymbol{\Psi}(\boldsymbol{x}')\} \\ &\quad = \sum_{i,j} \phi_i(\boldsymbol{x}) \phi_j(\boldsymbol{x}') c_i c_j + \sum_{i,j} \phi_j(\boldsymbol{x}') \phi_i(\boldsymbol{x}) c_j c_i \\ &\quad = \sum_{i,j} \phi_i(\boldsymbol{x}) \phi_j(\boldsymbol{x}') \{c_i, c_j\} = 0, \end{aligned}$$

and similarly for $\{\boldsymbol{\Psi}^\dagger(\boldsymbol{x}), \boldsymbol{\Psi}^\dagger(\boldsymbol{x}')\}$. Further

$$\begin{aligned} &\{\boldsymbol{\Psi}(\boldsymbol{x}), \boldsymbol{\Psi}^\dagger(\boldsymbol{x}')\} \\ &\quad = \sum_{i,j} \phi_i(\boldsymbol{x}) \phi_j^*(\boldsymbol{x}') c_i c_j^\dagger + \sum_{i,j} \phi_j^*(\boldsymbol{x}') \phi_i(\boldsymbol{x}) c_j^\dagger c_i \\ &\quad = \sum_{i,j} \phi_i(\boldsymbol{x}) \phi_j^*(\boldsymbol{x}') \{c_i, c_j^\dagger\} \\ &\quad = \sum_i \phi_i(\boldsymbol{x}) \phi_i^*(\boldsymbol{x}') = \delta(\boldsymbol{x} - \boldsymbol{x}') \end{aligned}$$

due to the completenes of the basis $\{\phi_i\}$.
We see that the field operators obey the anticommutation rules

$$\begin{aligned} \{\boldsymbol{\Psi}(\boldsymbol{x}), \boldsymbol{\Psi}(\boldsymbol{x}')\} &= 0 \\ \{\boldsymbol{\Psi}^\dagger(\boldsymbol{x}), \boldsymbol{\Psi}^\dagger(\boldsymbol{x}')\} &= 0 \\ \{\boldsymbol{\Psi}(\boldsymbol{x}), \boldsymbol{\Psi}^\dagger(\boldsymbol{x}')\} &= \delta(\boldsymbol{x} - \boldsymbol{x}'). \end{aligned}$$

Consider now the expression

$$\int \boldsymbol{\Psi}^\dagger(\boldsymbol{x})\eta(\boldsymbol{x})\boldsymbol{\Psi}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}.$$

We have

$$\begin{aligned}
&\int \boldsymbol{\Psi}^\dagger(\boldsymbol{x})\eta(\boldsymbol{x})\boldsymbol{\Psi}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \\
&\quad = \int \sum_i \phi_i^*(\boldsymbol{x})c_i^\dagger \eta(\boldsymbol{x}) \sum_j \phi_j(\boldsymbol{x})c_j \mathrm{d}\boldsymbol{x} \\
&\quad = \sum_{i,j} c_i^\dagger c_j \int \phi_i^*(\boldsymbol{x})\eta(\boldsymbol{x})\phi_j(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \\
&\quad = \sum_{i,j} \langle i|\eta|j\rangle c_i^\dagger c_j.
\end{aligned}$$

Similarly

$$\begin{aligned}
&\frac{1}{2}\int \boldsymbol{\Psi}^\dagger(\boldsymbol{x}_1)\boldsymbol{\Psi}^\dagger(\boldsymbol{x}_2)\vartheta(\boldsymbol{x}_1,\boldsymbol{x}_2)\boldsymbol{\Psi}(\boldsymbol{x}_2)\boldsymbol{\Psi}(\boldsymbol{x}_1)\,\mathrm{d}\boldsymbol{x}_1\mathrm{d}\boldsymbol{x}_2 \\
&\quad = \frac{1}{2}\int \sum_i \phi_i^*(\boldsymbol{x}_1)c_i^\dagger \sum_j \phi_j^*(\boldsymbol{x}_2)c_j^\dagger \vartheta(\boldsymbol{x}_1,\boldsymbol{x}_2) \\
&\qquad \sum_l \phi_l(\boldsymbol{x}_2)c_l \sum_k \phi_k(\boldsymbol{x}_k)c_k \mathrm{d}\boldsymbol{x}_1\mathrm{d}\boldsymbol{x}_2 \\
&\quad = \frac{1}{2}\sum_{i,j,k,l} c_i^\dagger c_j^\dagger c_l c_k \int \phi_i^*(\boldsymbol{x}_1)\phi_j^*(\boldsymbol{x}_2)\vartheta(\boldsymbol{x}_1,\boldsymbol{x}_2) \\
&\qquad \phi_k(\boldsymbol{x}_1)\phi_l(\boldsymbol{x}_2)\,\mathrm{d}\boldsymbol{x}_1\mathrm{d}\boldsymbol{x}_2 \\
&\quad = \frac{1}{2}\sum_{i,j,k,l} \langle ij|\vartheta|kl\rangle c_i^\dagger c_j^\dagger c_l c_k.
\end{aligned}$$

So, we can write

$$\begin{aligned}
\Omega^{(1)} &= \int \boldsymbol{\Psi}^\dagger(\boldsymbol{x})\eta(\boldsymbol{x})\boldsymbol{\Psi}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \\
\Omega^{(2)} &= \frac{1}{2}\int \boldsymbol{\Psi}^\dagger(\boldsymbol{x}_1)\boldsymbol{\Psi}^\dagger(\boldsymbol{x}_2)\vartheta(\boldsymbol{x}_1,\boldsymbol{x}_2) \\
&\qquad \boldsymbol{\Psi}(\boldsymbol{x}_2)\boldsymbol{\Psi}(\boldsymbol{x}_1)\,\mathrm{d}\boldsymbol{x}_1\mathrm{d}\boldsymbol{x}_2.
\end{aligned}$$

As an example, let us consider the density operator

$$\rho(\boldsymbol{x}) = \sum_{i=1}^N \delta(\boldsymbol{x}-\boldsymbol{x}_i).$$

In the occupation representation we have

$$\rho(\boldsymbol{x}) = \int \boldsymbol{\Psi}^\dagger(\boldsymbol{x}')\delta(\boldsymbol{x}-\boldsymbol{x}')\boldsymbol{\Psi}(\boldsymbol{x}')\,\mathrm{d}\boldsymbol{x}'$$

$$= \quad \boldsymbol{\Psi}^\dagger(\boldsymbol{x})\boldsymbol{\Psi}(\boldsymbol{x}) = \sum_{i,j} \phi_i^*(\boldsymbol{x})\phi_j(\boldsymbol{x})c_i^\dagger c_j.$$

4. The Problem: Stationary Solution

Our task is to find out the energy eigenstates of the stationary Hamiltonian

$$\begin{aligned} H_{\rm S} &= \sum_{i=1}^{N_e} \left[T_i + V_{\rm conf}(\boldsymbol{r}_i) + H_{{\rm SO}i} + H_{Zi} \right] + V_{\rm Coul} \\ &= \sum_{i=1}^{N_e} \frac{1}{2m} \boldsymbol{\Pi}_i^2 + \sum_{i=1}^{N_e} \frac{1}{2} m\omega_0^2 r_i^2 \\ &\quad + \sum_{i=1}^{N_e} \frac{\alpha}{\hbar} \left[\boldsymbol{\sigma} \times \boldsymbol{\Pi}_i \right]_z + \sum_{i=1}^{N_e} g\mu_B B \sigma_{zi} \\ &\quad + \frac{1}{2} \sum_{i \neq j}^{N_e} \frac{e^2}{4\pi\varepsilon\varepsilon_0 |\boldsymbol{r}_i - \boldsymbol{r}_j|} \end{aligned}$$

where the kinematic momentum $\boldsymbol{\Pi}_i$ is

$$\begin{aligned} \boldsymbol{\Pi}_i &= \boldsymbol{p}_i - e\boldsymbol{A}_i = \boldsymbol{p}_i - e\boldsymbol{A}_{Bi} \\ &= -{\rm i}\hbar\nabla_i - \frac{eB}{2}(-y_i, x_i, 0). \end{aligned}$$

4.1 Single particle spectrum

We first work out the single particle states, i.e. the eigenstates of the Hamiltonian

$$\begin{aligned} H_{\rm sp} &= T + V_{\rm conf}(\boldsymbol{r}) + H_{\rm SO} + H_Z \\ &= \frac{1}{2m} \boldsymbol{\Pi}^2 + \frac{1}{2} m\omega_0^2 r^2 \\ &\quad + \frac{\alpha}{\hbar} \left[\boldsymbol{\sigma} \times \boldsymbol{\Pi} \right]_z + g\mu_B B \sigma_z. \end{aligned}$$

These solutions are used to build up the non-interacting manybody basis for the numerical treatment of the mutual Coulomb interactions.

4.1.1 Analytic solution

There is no known way to solve the single particle problem when the Rashba SO term is present. We therefore drop it out and first figure out the eigenstates of the Hamiltonian

$$\begin{aligned} H_{\rm sp}^0 &= T + V_{\rm conf}(\boldsymbol{r}) + H_Z \\ &= \frac{1}{2m} \boldsymbol{\Pi}^2 + \frac{1}{2} m\omega_0^2 r^2 + g\mu_B B \sigma_z. \end{aligned}$$

The eigenstates of $H_{\rm sp}^0$ can be written as

$$\psi_{n\ell}(r, \theta) = g_{n\ell} \left(\frac{r^2}{a^2} \right) {\rm e}^{{\rm i}\ell\theta},$$

where, as usual the angular momentum quantum number ℓ can take only integer values. The normalized radial wave functions $g_{n\ell}(z)$ are given by

$$g_{n\ell}(z) = \frac{1}{\sqrt{\pi}a}\sqrt{\frac{n!}{(n+|\ell|)!}}\mathrm{e}^{-z/2}z^{|\ell|/2}L_n^{|\ell|}(z),$$

where $L_n^{\alpha}(z)$ stand for the (associated) Laguerre polynomials. The corresponding eigenenergies are

$$\begin{aligned}\varepsilon &= 2\hbar\omega\nu \\ \nu &= n - \frac{1}{2}\ell\kappa + \frac{1}{2}(|\ell|+1) \pm \gamma;\ n = 0,1,2,\ldots\end{aligned}$$

In the above we have introduced the shorthand notations

$$\begin{aligned}a^2 &= \frac{\hbar}{m\omega} \\ \kappa &= \frac{\omega_c}{2\omega} \\ \gamma &= \frac{g\mu_B B}{4\hbar\omega} \\ \omega^2 &= \omega_0^2 + \frac{1}{4}\omega_c^2 \\ \omega_c &= \frac{eB}{mc}.\end{aligned}$$

The solutions $\psi_{n\ell}$

- do not show any spin dependence although the Hamiltonian clearly depends on the spin via the term $g\mu_B B\sigma_z$ as do the the eigenenergies via the term $\pm\gamma$
- should be appended by a spin space factor χ. Beacause the spin dependece in our Hamiltonians is described in terms of 2×2 Pauli spin matrices we prefer to express χ as two component vectors

  $$\chi_\sigma = \begin{pmatrix}1\\0\end{pmatrix} \text{ and } \begin{pmatrix}0\\1\end{pmatrix}$$

  for the spin states $\sigma =\uparrow$ and $\sigma =\downarrow$, respectively.

In the eigenenergy the $+$-sign of the term $\pm\gamma$ corresponds to the spin-up state $\sigma =\uparrow$, and the $-$-sign to the spin-down state $\sigma =\downarrow$.

4.1.2 Rashba SO

The spin-orbit part of the single particle Hamiltonian

$$H_{\mathrm{SO}} = \frac{\alpha}{\hbar}\left[\boldsymbol{\sigma}\times(\boldsymbol{p}-e\boldsymbol{A})\right]_z = \frac{\alpha}{\hbar}\left[\boldsymbol{\sigma}\times\boldsymbol{\Pi}\right]_z$$

is written componentwise as

$$\begin{aligned} H_{\mathrm{SO}} &= \frac{\alpha}{\hbar}\left[\boldsymbol{\sigma}\times\boldsymbol{\Pi}\right]_z = \frac{\alpha}{\hbar}\left[\sigma_x\Pi_y - \sigma_y\Pi_x\right] \\ &= \frac{\alpha}{\hbar}\left[\begin{pmatrix} 0 & \Pi_y \\ \Pi_y & 0 \end{pmatrix} - \begin{pmatrix} 0 & -\mathrm{i}\Pi_x \\ \mathrm{i}\Pi_x & 0 \end{pmatrix}\right] \\ &= \frac{\alpha}{\hbar}\begin{pmatrix} 0 & \Pi_y + \mathrm{i}\Pi_x \\ \Pi_y - \mathrm{i}\Pi_x & 0 \end{pmatrix} \\ &= \mathrm{i}\,\frac{\alpha}{\hbar}\begin{pmatrix} 0 & \Pi_x - \mathrm{i}\Pi_y \\ -\Pi_x - \mathrm{i}\Pi_y & 0 \end{pmatrix}. \end{aligned}$$

Defining the *ladder operators* $\Pi_\pm$ as

$$\Pi_\pm = \Pi_x \pm \mathrm{i}\Pi_y$$

the SO term can be written compactly like

$$H_{\mathrm{SO}} = \mathrm{i}\,\frac{\alpha}{\hbar}\begin{pmatrix} 0 & \Pi_- \\ -\Pi_+ & 0 \end{pmatrix}.$$

Explicit expressions for the ladder operators read

$$\begin{aligned} \Pi_+ &= p_x + \mathrm{i}p_y - \frac{eB}{2}(\mathrm{i}x - y) \\ \Pi_- &= p_x - \mathrm{i}p_y + \frac{eB}{2}(\mathrm{i}x + y), \end{aligned}$$

where we have used the minimal coupling scheme

$$\boldsymbol{\Pi} = \boldsymbol{p} - e\boldsymbol{A} = \boldsymbol{p} - \frac{eB}{2}(-y, x, 0).$$

Expressing the operator combinations

$$\begin{aligned} p_x \pm \mathrm{i}p_y &= -\mathrm{i}\hbar\left(\frac{\partial}{\partial x} \pm \mathrm{i}\,\frac{\partial}{\partial y}\right) \\ \mathrm{i}x \mp y &= \mathrm{i}(x \pm \mathrm{i}y) \end{aligned}$$

in polar coordinates like

$$\begin{aligned} p_x \pm \mathrm{i}p_y &= -\mathrm{i}\hbar\mathrm{e}^{\pm\mathrm{i}\theta}\left(\frac{\partial}{\partial r} \pm \mathrm{i}\frac{1}{r}\,\frac{\partial}{\partial \theta}\right) \\ \mathrm{i}x \mp y &= \mathrm{i}r\mathrm{e}^{\pm\mathrm{i}\theta} \end{aligned}$$

we end up with

$$\Pi_\pm = -\mathrm{i}\hbar\mathrm{e}^{\pm\mathrm{i}\theta}\left(\frac{\partial}{\partial r} \pm \mathrm{i}\frac{1}{r}\,\frac{\partial}{\partial \theta} \pm \frac{m\omega_c}{2\hbar}\,r\right).$$

Changing to the dimensionless variable

$$z = \frac{r^2}{a^2}$$

the ladder operators take the form

$$\Pi_\pm = -i\frac{\hbar}{a}\mathrm{e}^{\pm\mathrm{i}\theta}\sqrt{z}\left(2\,\frac{\partial}{\partial z} \pm \mathrm{i}\frac{1}{z}\,\frac{\partial}{\partial\theta} \pm \kappa\right),$$

which will be handy when we have to operate with them on the single particle states

$$\psi_{n\ell}(r,\theta) = g_{n\ell}\left(\frac{r^2}{a^2}\right)\mathrm{e}^{\mathrm{i}\ell\theta} = g_{n\ell}(z)\mathrm{e}^{\mathrm{i}\ell\theta}.$$

Matrix elements

We now have to solve numerically the eigenproblem

$$H_{\mathrm{sp}}\Phi(\boldsymbol{r}) = E\Phi(\boldsymbol{r}),$$

where the single particle Hamiltonian is composed as

$$H_{\mathrm{sp}} = H^0_{\mathrm{sp}} + H_{\mathrm{SO}}.$$

The solutions can be written as superpositions

$$\Phi = \sum_{k=0} c_k\Phi_k.$$

We take the *basis states* Φ_k to be the eigenstates of H^0_{sp}, i.e. they satisfy

$$H^0_{\mathrm{sp}}\Phi_k = \varepsilon_k\Phi_k.$$

The superposition coefficients

$$c = \begin{pmatrix} c_0 \\ c_1 \\ \vdots \end{pmatrix}$$

satisfy the eigenvalue equation

$$\mathcal{H}c = Ec,$$

where the elements of the matrix $\mathcal{H}$ are given by

$$\begin{aligned}
\mathcal{H}_{ij} &= \langle\Phi_i|H_{\mathrm{sp}}|\Phi_j\rangle = \int \Phi_i^*(\boldsymbol{r})H_{\mathrm{sp}}\Phi_j(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} \\
&= \int \Phi_i^*(\boldsymbol{r})H^0_{\mathrm{sp}}\Phi_j(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} \\
&\quad + \int \Phi_i^*(\boldsymbol{r})H_{\mathrm{SO}}\Phi_j(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} \\
&= \varepsilon_i\delta_{ij} + \langle\Phi_i|H_{\mathrm{SO}}|\Phi_j\rangle.
\end{aligned}$$

The first term is diagonal in our basis and its contribution is known from our analytic solution. The second term is just what we called single particle matrix elements in our treatment of occupation presentation.
Obviously our analytic solutions

$$\Psi_k = \psi_{n\ell}(r,\theta) = g_{n\ell}\left(\frac{r^2}{a^2}\right)\mathrm{e}^{\mathrm{i}\ell\theta}$$

are good candidates for basis states Φ_k. However, recalling that the SO Hamiltonian was given by

$$H_{\mathrm{SO}} = \mathrm{i}\,\frac{\alpha}{\hbar}\begin{pmatrix} 0 & \Pi_- \\ -\Pi_+ & 0 \end{pmatrix},$$

we see that in fact, the eigenstates Φ of H_{sp} must actually be two component *spinors*, like

$$\Phi = \begin{pmatrix} \Phi^{\uparrow} \\ \Phi^{\downarrow} \end{pmatrix}.$$

We can, nevertheless expand this in terms of the complete set $\{\Psi_k\}$ as

$$\Phi = \begin{pmatrix} \Phi^{\uparrow} \\ \Phi^{\downarrow} \end{pmatrix} = \sum_k c_k^{\uparrow}\begin{pmatrix} \Psi_k \\ 0 \end{pmatrix} + \sum_k c_k^{\downarrow}\begin{pmatrix} 0 \\ \Psi_k \end{pmatrix}.$$

Let us now assume that we can separate the angular dependence in the spinors like

$$\Phi(\boldsymbol{r}) = \begin{pmatrix} \Phi^{\uparrow}(\boldsymbol{r}) \\ \Phi^{\downarrow}(\boldsymbol{r}) \end{pmatrix} = \begin{pmatrix} \phi^{\uparrow}(r)\mathrm{e}^{\mathrm{i}\ell^{\uparrow}\theta} \\ \phi^{\downarrow}(r)\mathrm{e}^{\mathrm{i}\ell^{\downarrow}\theta} \end{pmatrix}$$

Applying the operator

$$H_{\mathrm{SO}} = \mathrm{i}\,\frac{\alpha}{\hbar}\begin{pmatrix} 0 & \Pi_- \\ -\Pi_+ & 0 \end{pmatrix}$$

with

$$\Pi_\pm = -\mathrm{i}\hbar\mathrm{e}^{\pm\mathrm{i}\theta}\left(\frac{\partial}{\partial r} \pm \mathrm{i}\frac{1}{r}\,\frac{\partial}{\partial\theta} \pm \frac{m\omega_c}{2\hbar}\,r\right)$$

we get

$$\begin{aligned} H_{\mathrm{SO}}\Phi(\boldsymbol{r}) &= \mathrm{i}\,\frac{\alpha}{\hbar}\begin{pmatrix} 0 & \Pi_- \\ -\Pi_+ & 0 \end{pmatrix}\begin{pmatrix} \phi^{\uparrow}(r)\mathrm{e}^{\mathrm{i}\ell^{\uparrow}\theta} \\ \phi^{\downarrow}(r)\mathrm{e}^{\mathrm{i}\ell^{\downarrow}\theta} \end{pmatrix} \\ &= \mathrm{i}\,\frac{\alpha}{\hbar}\begin{pmatrix} \Pi_-\phi^{\downarrow}(r)\mathrm{e}^{\mathrm{i}\ell^{\downarrow}\theta} \\ -\Pi_+\phi^{\uparrow}(r)\mathrm{e}^{\mathrm{i}\ell^{\uparrow}\theta} \end{pmatrix} \\ &= \begin{pmatrix} \tilde{\phi}^{\downarrow}(r)\mathrm{e}^{\mathrm{i}(\ell^{\downarrow}-1)\theta} \\ -\tilde{\phi}^{\uparrow}(r)\mathrm{e}^{\mathrm{i}(\ell^{\uparrow}+1)\theta} \end{pmatrix}, \end{aligned}$$

where the functions $\tilde{\phi}^{\uparrow,\downarrow}(r)$ are obtained from the functions $\phi^{\uparrow,\downarrow}(r)$ by applying the radial part of the operators $\Pi_\pm$ on them.
Since $H^0_{\rm sp}$ depends neither on angle nor on spin it retains the angular dependence of the Ψ. Thus, for Ψ to be an eigenstate of

$$H_{\rm sp} = H^0_{\rm sp} + H^0_{\rm SO}$$

we must have

$$\begin{aligned} \ell^\downarrow - 1 &= \ell^\uparrow \\ \ell^\uparrow + 1 &= \ell^\downarrow. \end{aligned}$$

Both equation yield the same constrain

$$\ell^\downarrow = \ell^\uparrow + 1$$

implying that the spinors can in fact be written as

$$\Phi(\boldsymbol{r}) = \begin{pmatrix} \phi^\uparrow(r)\mathrm{e}^{\mathrm{i}\ell\theta} \\ \phi^\downarrow(r)\mathrm{e}^{\mathrm{i}(\ell+1)\theta} \end{pmatrix}.$$

Thus the quantum number ℓ (actually the total angular momentum $\ell + s_z$) is a conserved quantity which greatly simplifies our task. Note also, that the quantum number ℓ must be integer: going around a full circle in the configuration space we must end up with the original state.
Introducing the ket-vectors $|n\ell\rangle$ via the scalar product

$$\langle \boldsymbol{r}|n\ell\rangle = \Psi_k = \psi_{n\ell}(r,\theta) = g_{n\ell}\left(\frac{r^2}{a^2}\right)\mathrm{e}^{\mathrm{i}\ell\theta}$$

and the spinors $|n;\sigma\rangle$ like

$$\begin{aligned} |n;\uparrow\rangle &= \begin{pmatrix} |n,\ell\rangle \\ 0 \end{pmatrix} \\ |n;\downarrow\rangle &= \begin{pmatrix} 0 \\ |n,\ell+1\rangle \end{pmatrix} \end{aligned}$$

and the short hand

$$\eta^\pm = 1 \pm \kappa$$

it is straightforward (but somewhat tedious) task to figure out the matrix elements

$$\begin{aligned} \langle n';\uparrow|H_{\rm SO}|n;\uparrow\rangle &= 0 \\ \langle n';\uparrow|H_{\rm SO}|n;\downarrow\rangle &= \frac{\alpha}{a}\begin{cases} \eta^-\sqrt{n+\ell+1}\delta_{n'n} & \\ +\eta^+\sqrt{n+1}\delta_{n',n+1}; & \ell > 0 \\ -\eta^+\sqrt{n+|\ell|}\delta_{n'n} & \\ -\eta^-\sqrt{n}\delta_{n',n-1}; & \ell \le 0 \end{cases} \end{aligned}$$

$$\begin{aligned}
\langle n';\downarrow|H_{\mathrm{SO}}|n;\uparrow\rangle &= \frac{\alpha}{a}\begin{cases} \eta^-\sqrt{n+\ell+1}\delta_{n'n} & \\ +\eta^+\sqrt{n}\delta_{n',n-1}; & \ell \geq 0 \\ -\eta^+\sqrt{n+|\ell|}\delta_{n'n} & \\ -\eta^-\sqrt{n+1}\delta_{n',n+1}; & \ell < 0 \end{cases} \\
\langle n';\downarrow|H_{\mathrm{SO}}|n;\downarrow\rangle &= 0.
\end{aligned}$$

Because spin-orbit coupling H_{SO} conserves the angular momentum (total angular momentum $\ell + s_z = \ell + \frac{1}{2}$) we can construct the Hamiltonian matrices separately for each ℓ.
We take the spinors

$$\begin{aligned}
|n;\uparrow\rangle &= \begin{pmatrix} |n,\ell\rangle \\ 0 \end{pmatrix} \\
|n;\downarrow\rangle &= \begin{pmatrix} 0 \\ |n,\ell+1\rangle \end{pmatrix}
\end{aligned}$$

as our complete basis and expand the eigenstates Φ of the single particle Hamiltonian

$$H_{\mathrm{sp}} = H^0_{\mathrm{sp}} + H^0_{\mathrm{SO}}$$

in terms of them as

$$\Phi = \sum_n c^{\uparrow}_n |n;\uparrow\rangle + \sum_n c^{\downarrow}_n |n;\downarrow\rangle.$$

Because the base states $|n;\sigma\rangle$ are eigenstates of H^0_{sp} we can see that in this representation the contribution of H^0_{sp} is limited to the diagonal of the matrix.

4.2 Coulomb interaction

The solutions

$$\Phi_k = |k\rangle = \sum_n c_n^{k\,\uparrow} |n;\uparrow\rangle + \sum_n c_n^{k\,\downarrow} |n;\downarrow\rangle.$$

of the eigenproblem

$$H_{\mathrm{sp}}\Phi_k = E_k\Phi_k$$

obtained in the previous section form a complete set and thus can be used to form a complete basis for multiparticle problems. In occupation representation we write these non-interacting N_e electron states as

$$\Psi = |k_1, \ldots, k_{N_e}\rangle,$$

where k_i label the occupied states Φ_{k_i}. To bring the Coulomb interaction of the many particle Hamiltonian

$$\begin{aligned}
H_{\mathrm{S}} &= \sum_{i=1}^{N_e} H_{\mathrm{sp}\,i} + V_{\mathrm{Coul}} \\
&= \sum_{i=1}^{N_e} H_{\mathrm{sp}\,i} + \frac{1}{2}\sum_{i\neq j}^{N_e} \frac{e^2}{4\pi\varepsilon\varepsilon_0|\boldsymbol{r}_i - \boldsymbol{r}_j|}
\end{aligned}$$

into the game we need to evaluate the twobody matrix elements
$\langle k_1 k_2 | e^2/(4\pi\epsilon\epsilon_0 |\boldsymbol{r}_1 - \boldsymbol{r}_2|) | k_3 k_4 \rangle$.
Since each of the states $|k_i\rangle$ involved in the twobody matrix elements is in fact a superpostion

$$\Phi_{k_i} = |k\rangle = \sum_n c_n^{k_i\uparrow} |n;\uparrow\rangle + \sum_n c_n^{k_i\downarrow} |n;\downarrow\rangle$$

and the spinors $|n;\sigma\rangle$ are composed of states $|n\ell\rangle$ like

$$\begin{aligned} |n;\uparrow\rangle &= \begin{pmatrix} |n,\ell\rangle \\ 0 \end{pmatrix} \\ |n;\downarrow\rangle &= \begin{pmatrix} 0 \\ |n,\ell+1\rangle \end{pmatrix} \end{aligned}$$

we see that we actually have to evaluate the matrix elements

$$\begin{aligned} &V_{n_1\ell_1 n_2\ell_2 n_3\ell_3 n_4\ell_4} \\ &\quad = \left\langle n_1\ell_1; n_2\ell_2 \left| \frac{e^2}{4\pi\epsilon\epsilon_0 |\boldsymbol{r}_1 - \boldsymbol{r}_2|} \right| n_3\ell_3; n_4\ell_4 \right\rangle. \end{aligned}$$

The evalutation can be performed by

- expressing the Coulomb potential $1/r$ in terms of its Fourier transform, i.e.

$$\frac{1}{r} = \frac{1}{2\pi} \int \frac{\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}}{k} \, \mathrm{d}\boldsymbol{k}$$

- using the explicit representation

$$L_n^\alpha(x) = \sum_{m=0}^{n} (-1)^m \begin{pmatrix} n+\alpha \\ n-m \end{pmatrix} \frac{x^m}{m!}$$

  for the Laguerre polynomials L_n^α appearing in the wave functions

$$\begin{aligned} \langle \boldsymbol{r} | n\ell \rangle &= \Psi_k = \psi_{n\ell}(r,\theta) = g_{n\ell} \left(\frac{r^2}{a^2} \right) \mathrm{e}^{\mathrm{i}\ell\theta} \\ &= \frac{1}{\sqrt{\pi} a} \sqrt{\frac{n!}{(n+|\ell|)!}} \mathrm{e}^{-r^2/2a^2} \\ &\qquad \times \left(\frac{r}{a} \right)^{|\ell|} L_n^{|\ell|} \left(\frac{r^2}{a^2} \right) \mathrm{e}^{\mathrm{i}\ell\theta}. \end{aligned}$$

Since the evaluation is rather lengthy we just, for the completeness' sake show the final result:

$$\begin{aligned} &V_{n_1\ell_1 n_2\ell_2 n_3\ell_3 n_4\ell_4} \\ &\quad = \delta_{\ell_1+\ell_2,\ell_3+\ell_4} \frac{\sqrt{2} e^2}{4\pi\epsilon\epsilon_0 a} \end{aligned}$$

$$
\begin{aligned}
&\times \left(\frac{n_1!}{(n_1+|\ell_1|)!}\right)\left(\frac{n_2!}{(n_2+|\ell_2|)!}\right)\\
&\times \left(\frac{n_3!}{(n_3+|\ell_3|)!}\right)\left(\frac{n_4!}{(n_4+|\ell_4|)!}\right)\\
&\times \mathcal{S}_{n_1\ell_1 n_2\ell_2 n_3\ell_3 n_4\ell_4}
\end{aligned}
$$

where $\mathcal{S}_{n_1\ell_1 n_2\ell_2 n_3\ell_3 n_4\ell_4}$ is the sixfold summation

$$
\begin{aligned}
&\mathcal{S}_{n_1\ell_1 n_2\ell_2 n_3\ell_3 n_4\ell_4}\\
&= \sum_{\kappa_1=0}^{n_1}\sum_{\kappa_2=0}^{n_2}\sum_{\kappa_3=0}^{n_3}\sum_{\kappa_4=0}^{n_4}\\
&\quad \left[\kappa_1+\kappa_4+\frac{1}{2}(|\ell_1|+|\ell_4|-k\right]!\\
&\quad \times \left[\kappa_2+\kappa_3+\frac{1}{2}(|\ell_2|+|\ell_3|-k\right]!\\
&\quad \times \frac{(-1)^{\kappa_1+\kappa_4}}{\kappa_1!\kappa_4!}\frac{(-1)^{\kappa_2+\kappa_3}}{\kappa_2!\kappa_3!}\\
&\quad \times \frac{(n_1+|\ell_1|)!(n_4+|\ell_4|)!}{(n_1-\kappa_1)!(|\ell_1|+\kappa_1)!(n_4-\kappa_4)!(|\ell_4|+\kappa_4)!}\\
&\quad \times \frac{(n_2+|\ell_2|)!(n_3+|\ell_3|)!}{(n_2-\kappa_2)!(|\ell_2|+\kappa_2)!(n_3-\kappa_3)!(|\ell_3|+\kappa_3)!}\\
&\quad \times \sum_{s=0}^{\kappa_{14}} \frac{\left[\kappa_1+\kappa_4+\frac{1}{2}(|\ell_1|+|\ell_4|+k)\right]!}{\left[\kappa_1+\kappa_4+\frac{1}{2}(|\ell_1|+|\ell_4|-k)-s\right]!(k+s)!}\\
&\quad \times \sum_{t=0}^{\kappa_{23}} \frac{\left[\kappa_2+\kappa_3+\frac{1}{2}(|\ell_2|+|\ell_3|+k)\right]!}{\left[\kappa_2+\kappa_3+\frac{1}{2}(|\ell_2|+|\ell_3|-k)-t\right]!(k+t)!}\\
&\quad \times \frac{(-1)^{s+t}}{s!t!}\,\frac{\Gamma\left(k+s+t+\frac{1}{2}\right)}{2^{k+s+t+1}}.
\end{aligned}
$$

Above we have used the notation

$$
\begin{aligned}
k &= |\ell_1-\ell_4| = |\ell_2-\ell_3|\\
\kappa_{14} &= \kappa_1+\kappa_4+\frac{1}{2}(|\ell_1|+|\ell_4|-k)\\
\kappa_{23} &= \kappa_2+\kappa_3+\frac{1}{2}(|\ell_2|+|\ell_3|-k).
\end{aligned}
$$

We should note that

- due to the Kronecker delta $\delta_{\ell_1+\ell_2,\ell_3+\ell_4}$ the total orbital angular momentum is conserved
- because the Coulomb interaction does not depend on spin the total spin and its z-component are also conserved, so

- (the z-component of) the total angular momentum is conserved and we can solve the multielectron eigenstates for each total angular momentum separately
- the numerical evaluation of the sum $\mathcal{S}$ is very unstable and requires in practice multiprecision arithmetic.

4.3 The Code

4.3.1 Base states

Base states as well as any other quantum states are represented as objects of classes derived from the abstract

```
class QuantumState {
public:
  ...
  QuantumState() : id_( 0 ) {}
  QuantumState( COUNT id ) : id_( id ) {}

  virtual ~QuantumState() {}

  virtual FLOAT ener() const = 0;
  virtual void show() const = 0;

  COUNT getID() const { return id_; }
  ...
private:
  COUNT id_;
  ...
};
```

Types `COUNT`, `FLOAT`, e.t.c. are `typedef`-defined in a header file (now as `unsigned`, `double`, ...).

Our fundamental basis consists of the spinors

$$\begin{aligned}
|n;\uparrow\rangle &= \begin{pmatrix} |n,\ell\rangle \\ 0 \end{pmatrix} \\
|n;\downarrow\rangle &= \begin{pmatrix} 0 \\ |n,\ell+1\rangle \end{pmatrix} \\
\langle \boldsymbol{r}|n\ell\rangle &= \frac{1}{\sqrt{\pi}a}\sqrt{\frac{n!}{(n+|\ell|)!}}\mathrm{e}^{-r^2/2a^2} \\
&\qquad \times \left(\frac{r}{a}\right)^{|\ell|} L_n^{|\ell|}\left(\frac{r^2}{a^2}\right)\mathrm{e}^{\mathrm{i}\ell\theta}.
\end{aligned}$$

Since we will never need the explicit wave function it suffices to represent these spinor states as

```
class BaseSpinor : public QuantumState {
public:
  ...
  BaseSpinor( int ud, int n, int m ) :
    ud_( ud ), n_( n ), m_( m )
    {}
  ...
  virtual FLOAT ener() const  // e in meV
    { return nu( n_, m_, ud_ )*keUnit_; }
  virtual void show() const;
  int udQN() const     // spin up/down: +1/-1
    { return ud_; }
  int nQN() const      // degree of L
    { return n_; }
  int mQN() const      // angular momentum
    { return m_; }
  FLOAT nu() const// energy in 2\hbar\omega
    { return nu( n_, m_, ud_ ); }
  static FLOAT nu( int n, int m, int ud )
    { return n + 0.5*(-m*kappa_
      + abs( m ) + 1.0) + ud*gamma_; }
private:
  int ud_;
  int n_;
  int m_;

  static FLOAT keUnit_;
  static FLOAT kappa_;
  static FLOAT gamma_;
  ...
};
```

We now have to construct the basis set from the base spinors. The framework expects the bases to be handed over as objects of

```
class QNumMap {
  ...
  QNumMap( QStateGenerator& qsgen, ... );
  QNumMap( QuantumState const* const* qs, ... );
  QNumMap( const QNumMap& qmap );
  ...
  virtual ~QNumMap() { zap_(); }
  ...
  COUNT count() const { return nst_; }
  QuantumState* state( COUNT i ) const
    { return state_[i]; }
  virtual void show( COUNT l, COUNT u ) const;
```

```
  ...
  QuantumState* operator[]( COUNT i ) const
    { return state_[i]; }
protected:
  QuantumState** state_;
  COUNT nst_;
  ...
private:
  ...
  void zap_();
};
```

There are several ways to construct `QNumMap`s. For example, one could collect the basis states into a vector and hand it to `QNumMap` (second constructor) or, as we will do, let `QNumMap` itself construct the vector of basis states (first constructor). For that purpose we need to derive a quantum state generator from the abstract base class

```
class QStateGenerator {
public:
  QStateGenerator() : qsf_( 0 ) {}
  QStateGenerator( const QStateFilter& qsf ) :
    qsf_( &qsf ) {}
  virtual ~QStateGenerator() {}

  virtual QuantumState* genQState() = 0;
protected:
  const QStateFilter* qsf_;
};
```

The constructor of `QNumMap` calls the method `genQState()` as long as it returns a non-zero pointer to a created `QuantumState`, this time to a `BaseSpinor`-object.

4.3.2 SO coupling

Recall that

- we are now solving the single particle states with Rashba SO coupling included
- Rashba SO conserves total angular momentum $\ell + s_z$. Since the orbital angular momenta of up- and down-spinors were related by $\ell^{\downarrow} = \ell^{\uparrow} + 1$ it suffices to specify $\ell^{\uparrow}$, say. Hence we can solve separately the problem for each $\ell = \ell^{\uparrow}$
- Rashba SO mixes states with different principal (radial) quantum numbers.

We generate the base spinors with

```
class BaseSpGen : public QStateGenerator {
```

```
public:
  BaseSpGen( int n, int m = 0 ) : n_max_( n )
    { set( m ); }

  void set( int m )
    { m_ = m; ud_ = 1; n_ = 0; first_ = true; }

  virtual QuantumState* genQState()
    { return nextConf_() ?
    (new BaseSpinor( ud_, n_, ud_ > 0
                     ? m_ : m_ + 1 )) : 0; }
private:
  bool nextConf_();

  int n_max_; // maximum degree
  int m_; // angular momentum of spin up state
  int ud_;    // spin up/down
  int n_;     // current n_
  bool first_;
};
```

The constructor argument `n` specifies the maximum degeree of Laguerre polynomials involved in the diagonalization and `m` tells the ℓ of the up-spinor. The actual generation of configurations the `genQState()`-method uses to create `BaseSpinor`s is done by

```
bool
BaseSpGen::nextConf_()
{
  if( first_ ) {
    first_ = false;
    return true;
  }

  if( ud_ > 0 ) {
    ud_ = -1;
    return true;
  }

  if( n_ >= n_max_ )
    return false;

  n_++;
  ud_ = 1;

  return true;
}
```

We now proceed to the construction of the matrix representation of the single

particle Hamiltonian $H_{\rm sp}$. For convenience the framework acknowledges the concept of single particle Hermitian operator as

```
template<class Field>
class SBHermOperator :
   public SymmColumnArray<Field> {
public:
  SBHermOperator( const QNumMap& qmap,
          OnebodyOperator<Field>* obo,
          DiagonalOperator<Real>* dgo = 0 );

  ~SBHermOperator() { delete[] wrk_; }

  Field matElem( const Field* lft,
                 const Field* rgt );
  ...
 private:
  const QNumMap& qmap_;
  const int dim_;
  OnebodyOperator<Field>* obo_;
  DiagonalOperator<Real>* dgo_;
  Field* wrk_;
  ...
};
```

The class `SBHermOperator`

- is derived from the class `SymmColumnArray` representing symmetric matrices, and as such has a collection of typical matrix operations, including a diagonalization method
- the first argument of the constructor is the `QNumMap` consisting of the single particle basis, this time of our `BaseSpinor`s
- the second argument represents the onebody operator
- the last argument represent the diagonal operator, i.e. it takes care of matrix elements of the form $\langle i|H_{\rm sp}|i\rangle$. It is, ofcourse redundant because the second argument could handle the diagonal terms. Nevertheless, it is occasionally handy.

The actual onebody and diagonal operators are derived from

```
template<class Field>
class OnebodyOperator {
public:
  OnebodyOperator() {}
  virtual ~OnebodyOperator() {}

  virtual Field
    element( const QuantumState* lft,
```

```
            const QuantumState* rgt ) = 0;
  virtual bool
    isSymmetric() const = 0;//<i|T|j>=<j|T|i>^*?
};
```
and
```
template<class Field>
class DiagonalOperator {
public:
  DiagonalOperator() {}
  virtual ~DiagonalOperator() {}

  virtual Field
    element( const QuantumState* st ) = 0;
};
```
like
```
class SOOper : public OnebodyOperator<FLOAT> {
public:
  SOOper( FLOAT beta, FLOAT etap, FLOAT etam ) :
    beta_( beta ), etap_( etap ), etam_( etam )
    {}

  virtual FLOAT
    element( const QuantumState* lft,
             const QuantumState* rgt );
  virtual bool isSymmetric() const
    { return true; }
private:
  const FLOAT beta_;   // alpha/a
  const FLOAT etap_;   // eta^+
  const FLOAT etam_;   // eta^-
};
```
and
```
class BaseDiagOper :
   public DiagonalOperator<FLOAT> {
public:
  virtual FLOAT
    element( const QuantumState* diag )
{ return
 static_cast<const BaseSpinor*>( diag )->nu(); }
};
```
In these classes

- `element()` methods receive pointers to `QuantumState`-objects from `SBHermOperator`
- to figure out the `QuantumState`-objects to be passed `SBHermOperator` consults the `QNumMap`-object we gave to it in the construction phase.

Since this `QNumMap` contains `BaseSpinor`s we can safely cast `QuantumState*`-pointers to `BaseSpinor*`-pointers in the `element()`-methods

- `SOOperator` handles the Rashba SO
- the diagonal terms are simply the energies of our base spinors.

The `element()`-method of `SOOperaror` is a direct implementation of the onebody matrix elements $\langle n';\sigma'|H_{\rm SO}|n;\sigma\rangle$:

```
FLOAT
SOOper::element( const QuantumState* lft,
                 const QuantumState* rgt )
{
  const BaseSpinor* lst =
    static_cast<const BaseSpinor*>( lft );
  const BaseSpinor* rst =
    static_cast<const BaseSpinor*>( rgt );
  int lud = lst->udQN();
  int rud = rst->udQN();

  if( lud == rud )
    return 0.0;

  int lm = lst->mQN();
  int rm = rst->mQN();
  int ln = lst->nQN();
  int rn = rst->nQN();
  if( rud > 0 ) {
    if( lm != rm + 1 )
      return 0.0;

    if( rm >= 0 ) {
      if( ln == rn )
    return beta_*etam_*sqrt( rn + rm + 1.0 );
      if( ln == rn - 1 )
    return beta_*etap_*
      sqrt( static_cast<FLOAT>( rn ) );
      return 0.0;
    }

    if( ln == rn )
      return -beta_*etap_*
        sqrt( rn +
              fabs( static_cast<FLOAT>( rm ) ) );
    if( ln == rn + 1 )
      return -beta_*etam_*sqrt( rn +1.0 );
```

```
    return 0.0;
  }
  if( lm != rm - 1 )
    return 0.0;

  if( rm > 0 ) {
    if( ln == rn )
      return beta_*etam_*
        sqrt( static_cast<FLOAT>( rn + rm ) );
    if( ln == rn + 1 )
      return beta_*etap_*sqrt( rn + 1.0 );
    return 0.0;
  }

  if( ln == rn )
    return -beta_*etap_*
      sqrt( rn +
        fabs( static_cast<FLOAT>( rm - 1 ) ) );
  if( ln == rn - 1 )
    return -beta_*etam_*
            sqrt( static_cast<FLOAT>( rn ) );
  return 0.0;
}
```

Superposition spinors
We now have all pieces needed for the numerical solution of the single particle problem. Schematically we proceed as

1. Given the maximum degree `n_max` of the Laguerre polynomial expansion and the orbital angular momentum `ell` of the spin-up spinor we create the basis

   ```
   BaseSpGen spgen( n_max, ell );
   QNumMap base( spgen );
   COUNT dim = // size of the basis
     base.count();
   FLOAT* ener = // space for spectrum
     new FLOAT[dim];
   ```

2. We construct the onebody operators and the Hamiltonian

   ```
   SOOper soop( beta, eta_p, eta_m );
   BaseDiagOper bdiag;
   SBHermOperator<FLOAT> ham( base, &soop,
                              &bdiag );
   ```

   where `beta` stands for α/a and `eta_p`/`eta_m` for $\eta^{\pm}$

3. The diagonalization

```
ham.diag( ener );
```

returns the eigenvalues (energies) in the argument vector `ener`. The eigenvectors are stored in the columns of the matrix and can be retrieved by the method

```
Field* SymmColumnArray<Field>::
                col( int i ) const;
```

of the base class.

Let Θ_k stand for the spinors in our collection `base`, i.e. they represent either the spinor

$$\begin{pmatrix} |n,\ell\rangle \\ 0 \end{pmatrix}$$

or the spinor

$$\begin{pmatrix} 0 \\ |n,\ell+1\rangle \end{pmatrix}.$$

The spinors satisfying the Schrödinger equation

$$H_{\rm sp}\Phi = E\Phi$$

are then the superpositions

$$\Phi = \sum_k c_k \Theta_k,$$

where the coefficients c_k are the components of the eigenvector corresponding to the eigenvalue E.
Note that

- the diagonalization is done separately for each orbital angular momentum ℓ, so we have to loop over angular momenta $\ell = -\ell_{\rm max}, -\ell_{\rm max}+1, \ldots, \ell_{\rm max}$, say, to cover the interesting spectrum
- the diagonalization is a full one, i.e. for each ℓ we get `dim` eigenvalues and eigenvectors
- we will use these superposition states Φ as a basis for the multielectron computations, so we need to save them.

Superposition quantum states are so ubiquitous that they deserve their own class

```
template<class Field>
class SupposQuantumState : public QuantumState {
  SupposQuantumState( const QNumMap& qmap,
                      const Field* c, COUNT dim,
```

```
                        FLOAT cut = 0.0 );
  ...
  virtual ~SupposQuantumState();

  COUNT dim() const  // dimension of the
    { return dim_; } // full Hilbert space
  Field coef( COUNT i ) const // original
    { return c_[i]; } // i'th coefficient
  COUNT count() const // number of selected
    { return cnt_; }  // states
  Field selCoef( COUNT i ) const//i'th selected
    { return c_[isel_[i]]; } // coeffficient
  QuantumState* state( COUNT i ) const//original
    { return qmap_[i]; }         // i'th state
  QuantumState* selState( COUNT i ) const //i'th
    { return qmap_[isel_[i]]; }// selected state
  const QNumMap& qNumMap() const
    { return qmap_; }
  ...
protected:
// mapping of the states in superposition
  const QNumMap& qmap_;
//original superposition coefficients
  Field* c_;
  COUNT dim_;// number of original coefficients
  FLOAT cut_;        // |c_[i]| < cut_ rejected
  COUNT cnt_; // number of selected coefficients
  COUNT* isel_;       // and their indeces
};
```

Very often only a fraction of coefficients c_k in the expansion

$$\Phi = \sum_k c_k \Theta_k$$

differ essentially from zero. Therefore this class offers an opportunity to exclude unimportant components from the computations by tuning the cut off parameter `cut`.
The solutions of the single particle solutions are stored as `SupposQuantumState` objects.

4.3.3 Coulomb interaction

Basis
We solve the stationary problem

$$\left[\sum_{i=1}^{N_e} H_{\mathrm{sp}_i} + V_{\mathrm{Coul}}\right] \Psi = E\Psi$$

by expanding the wave function Ψ in terms of the occupations

$$\Xi_k = |k_1, \ldots, k_{N_e}\rangle$$

like

$$\Psi = \sum_k C_k \Xi_k.$$

To construct the basis set $\{|k_1, \ldots, k_{N_e}\rangle\}$ we note that

- the code refers to the single particle states Φ_k comprising the Slater determinants $|k_1, \ldots, k_{N_e}\rangle$ just by numbers $0, 1, \ldots, M-1$, where M is the number of single particle states involved
- the set $\{|k_1, \ldots, k_{N_e}\rangle\}$ is constructed by picking up N_e integers out of M ones in all possible ways (order of picking doesn't matter)
- no physics (excludig the Fermi statistics) is involved in this construction process
- matrix elements $\langle k'_1, \ldots, k_{,N_e} |H_{\rm S}| k_1, \ldots, k_{N_e}\rangle$ can be non-zero only if the left and right hand sides differ by at most two occupied states. This fact is also independent of the problem
- the phases introduced when permuting the states to be destroyed to the front and the states created to the correct positions depend only on the occupations of the left and right hand sides and not the specific problem.

We see that the basis $\{|k_1, \ldots, k_{N_e}\rangle\}$, the possible nonzeros and the phases associated with the matrix elements depend only on the number (and on the numbering) of the single particle states and on the number of electrons.
In the code these notions are combined in

```
class NonIntManybodySystem {
public:
  NonIntManybodySystem( NonIntGenerator& gen,
                        ... );
  ...
  virtual ~NonIntManybodySystem() {}

  COUNT dim() const // size of the basis
    { return dim_; }
  int nPart() const // number of electrons
    { return nPart_; }
  int maxSnglQN() const // max occupied states
    { return nimbb_.maxSnglQN(); }
  L_COUNT nonZ() const // number of nonzeros
    { return opms_.count(); }

  const NonIntManybodyBase& base() const;
```

```
  const OperMasks& masks() const;
  ...
private:
  NonIntManybodyBase nimbb_;
  OperMasks opms_;
  COUNT dim_;
  int nPart_;
};
```
The non-interacting manybody basis (`NonIntManybodyBase`) itself is generated by
```
class NonIntGenerator :
  public QStateGenerator {
public:
  NonIntGenerator( int np, int nl );
  NonIntGenerator( int np, int nl,
           const NIMBSFilter& mbf );
  virtual ~NonIntGenerator() {}
  ...
  int nPart() const { return np_; }
protected:
  ...
  int np_;          // # of particles
  int nl_; // # of single particle levels
  const NIMBSFilter* mbsf_; // filter
};
```
In the simplest case only the number of electrons (`np`) and the number of single particle levels (`nl`) are needed. At this stage it is possible to incorporate some physics into the play via a `NIMBSFilter` which checks each generated occupation $|k_1, \ldots, k_{N_e}\rangle$ against some criteria. For example, we could accept only the occupations with a given total angular momentum.
A `NonIntManybodySystem` object contains also templates `OperMasks` for manybody Hamiltonian matrices. These templates

- specify the positions of possible nonzero elements
- list the differing occuppied single particle states for each possible nonzero matrix element
- give the phase associated with the one- and twobody matrix elements.

Because, in many cases these `NonIntManybodySystem`s do not depend on the specific problem it is possible to construct and store them in advance, and retrieve them when needed.

Twobody matrix elements
To construct the manybody Hamiltonian matrix we have to implement the one- and twobody matrix elements. The onebody matrix elements are trivial

since our single particle basis states were eigenstates of the single particle part of the Hamiltonian.
The implementation of the twobody matrix elements begins with the implementation of the known matrix elements $V_{n_1\ell_1 n_2\ell_2 n_3\ell_3 n_4\ell_4}$. This is done by deriving from the base class

```
template<class Field>
class TwobodyOperator {
public:
  TwobodyOperator() {}
  virtual ~TwobodyOperator() {}
  virtual Field element(
             const QuantumState* lft1,
             const QuantumState* lft2,
             const QuantumState* rgt1,
             const QuantumState* rgt2 ) = 0;
        // V(r_1,r_2)=V(r_2,r_1)?
  virtual bool isSymmetric() const = 0;
};
```

The implementation means the implementation of the `element()` method and involves

- realizing the fact that the `QuantumState` objects passed to the method are two component spinors $\Theta_k = |n;\sigma\rangle$ and that the Coulomb interaction conserves the spin
- checking for conserved total angular momentum
- multiple precision arithmetic
- tabulation of partial sums

is rather lengthy and is not shown here.
We should note that we just implemented the twobody matrix elements in the case of the single particle states Θ_k whereas the single particle states in our manybody Hamiltonian are in fact superpositions

$$\Phi = \sum_k c_k \Theta_k.$$

Since evaluation of one- and twobody matrix elements for superposition states when the elements for the components of the superposition are known is a common task the framework recognizes

```
template<class Field>
class SupposTwobodyOperator :
  public TwobodyOperator<Field> {
public:
  SupposTwobodyOperator(
         TwobodyOperator<Field>& basop,
```

```
        ... );
  virtual Field element(
             const QuantumState* lft1,
             const QuantumState* lft2,
             const QuantumState* rgt1,
             const QuantumState* rgt2 );
  virtual bool isSymmetric() const
    { return basop_.isSymmetric(); }
private:
  TwobodyOperator<Field>& basop_;
  ...
};
```

This time

- the `QuantumState` objects of the `element()` method are of the type `SupposQuantumState`
- each of these objects contains as a member a `QNumMap` which tells to the `SupposTwobodyOperator` what are the components of the superpositions
- these component states are then passed by the `element()` method to the twobody operator specified in the construction, in our case to the operator responsible of the evaluation of the matrix elements $V_{n_1\ell_1 n_2\ell_2 n_3\ell_3 n_4\ell_4}$.

Manybody Hamiltonian

Manybody Hamiltonians are derived from the base class

```
template<typename HOP, typename Meth>
class MBHamilton_ : public HOP {
public:
  typedef typename HOP::FieldT FieldT;
  MBHamilton_( const NonIntManybodySystem& mbs,
           const QNumMap& snglMap,
           OnebodyOperator<FieldT>* obo,
           TwobodyOperator<FieldT>* tbo,
           DiagonalOperator<FLOAT>* dgo,
           ... );
  virtual ~MBHamilton_() { delete meth_; }
  void setMaxIt( COUNT maxit ) const
    { meth_->setMaxIt( maxit ); }
  void setEps( FLOAT eps ) const
    { meth_->setEps( eps ); }
  ...
  FLOAT eigen( COUNT i ) const
    { return meth_->eigen( i ); }
  void getEigVec( FieldT* vec, COUNT i ) const
```

```
    { meth_->getEigVec( vec, i ); }
protected:
  Meth* meth_;
};
```

The Hamiltonian

- is derived from the base class specified by the first template parameter. This base class must recognize operations typical for sparse Hermitian manybody operators
- uses the method specified by the second template parameter to diagonalize the base Hermitian operator
- member method names and number depend on the diagonalization method.

Currently all implemented many particle Hamiltonians use either conjugate gradient or Davidson-Liu diagonalization, of which the latter one is more efficient although not quite as robust as the former one.

5. Periodic Hamiltonian

5.1 Trivial time dependence

Suppose that our Hamiltonian $\mathcal{H}$ can be written as

$$\mathcal{H}(t) = f(t) + H(t),$$

where the scalar function $f(t)$ depends only on time t (and not on positions, momenta, ...) so that it commutes with $H(t)$. We denote the time dependent state vectors by kets like $|\psi;t\rangle$. To eliminate the trivial time dependence from the problem

$$\mathcal{H}(t)|\Psi;t\rangle = \mathrm{i}\hbar\,\frac{\partial}{\partial t}|\Psi;t\rangle$$

we try the product

$$|\Psi;t\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int^t f(t')\,\mathrm{d}t'}|\psi;t\rangle.$$

The substitution to the Schrödinger equation leads to

$$\begin{aligned}
\mathrm{i}\hbar\,\frac{\partial}{\partial t}|\Psi;t\rangle &= i\hbar\,\frac{\partial}{\partial t}\left(\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int^t f(t')\,\mathrm{d}t'}|\psi;t\rangle\right)\\
&= f(t)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int^t f(t')\,\mathrm{d}t'}|\psi;t\rangle\\
&\quad +i\hbar\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int^t f(t')\,\mathrm{d}t'}\frac{\partial}{\partial t}|\psi;t\rangle\\
&= \mathcal{H}|\Psi;t\rangle\\
&= f(t)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int^t f(t')\,\mathrm{d}t'}|\psi;t\rangle\\
&\quad +H(t)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int^t f(t')\,\mathrm{d}t'}|\psi;t\rangle\\
&= f(t)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int^t f(t')\,\mathrm{d}t'}|\psi;t\rangle\\
&\quad +\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int^t f(t')\,\mathrm{d}t'}H(t)|\psi;t\rangle,
\end{aligned}$$

where the last equality follows from the assumption that $f(t)$ commutes with $H(t)$. This yields the equation

$$\mathrm{i}\hbar\,\frac{\partial}{\partial t}|\psi;t\rangle = H(t)|\psi;t\rangle.$$

We assume that the remaining non-trivial Hamiltonian H is a periodic function of time, i.e.

$$H(t+T_0) = H(t)$$

where T_0 is the period. The corresponding angular velocity Ω is then

$$\Omega = \frac{2\pi}{T_0}.$$

This periodicity allows us to write H as the Fourier series

$$H(t) = \sum_{n=-\infty}^{\infty} H^n \mathrm{e}^{\mathrm{i}n\Omega t},$$

where the Fourier components H^n are given by

$$H^n = \frac{1}{T_0}\int_0^{T_0} \mathrm{d}t\, \mathrm{e}^{-\mathrm{i}n\Omega t} H(t)$$

5.2 Floquet theory

Floquet theory claims that *the solutions of the time dependent Schrödinger equation*

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi;t\rangle = H(t)|\psi;t\rangle.$$

can be expanded as

$$|\psi;t\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t}\sum_n\sum_\alpha F_{n\alpha}\mathrm{e}^{\mathrm{i}n\Omega t}|\alpha\rangle,$$

where the set $\{|\alpha\rangle\}$ is an (arbitrary) complete orthonormal basis for the Hilbert space of the periodic Hamiltonian H.

To see the validity of the claim we substitute the expansion into the Schrödinger equation and get

$$\begin{aligned}
\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi;t\rangle &= \mathrm{i}\hbar\frac{\partial}{\partial t}\left[\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t}\sum_{n\alpha}F_{n\alpha}\mathrm{e}^{\mathrm{i}n\Omega t}|\alpha\rangle\right]\\
&= \varepsilon\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t}\sum_{n\alpha}F_{n\alpha}\mathrm{e}^{\mathrm{i}n\Omega t}|\alpha\rangle\\
&\quad +\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t}\mathrm{i}\hbar\sum_{n\alpha}F_{n\alpha}\mathrm{i}n\Omega\mathrm{e}^{\mathrm{i}n\Omega t}|\alpha\rangle\\
&= \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t}\sum_{n\alpha}F_{n\alpha}\mathrm{e}^{\mathrm{i}n\Omega t}\left(\varepsilon - n\hbar\Omega\right)|\alpha\rangle\\
&= \sum_m H^m\mathrm{e}^{\mathrm{i}m\Omega t}\left[\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t}\sum_{n\alpha}F_{n\alpha}\mathrm{e}^{\mathrm{i}n\Omega t}|\alpha\rangle\right]\\
&= \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t}\sum_{nm\alpha}F_{n\alpha}\mathrm{e}^{\mathrm{i}(n+m)\Omega t}H^m|\alpha\rangle.
\end{aligned}$$

We now make a series of summation index changes as

$$\begin{aligned}
&\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t}\sum_{nm\alpha}F_{n\alpha}\mathrm{e}^{\mathrm{i}(n+m)\Omega t}H^m|\alpha\rangle\\
&= \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t}\sum_{ij\alpha}F_{n\alpha}\mathrm{e}^{\mathrm{i}i\Omega t}H^{i-j}|\alpha\rangle\Bigg|_{\substack{n+m=i\\ n=j\\ m=i-j}}\\
&= \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t}\sum_{nm\alpha}F_{n\alpha}\mathrm{e}^{\mathrm{i}n\Omega t}H^{n-m}|\alpha\rangle\Bigg|_{\substack{n=i\\ m=j,}}
\end{aligned}$$

which allows us to read the equation

$$\begin{aligned}&\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t}\sum_{n\alpha}F_{n\alpha}\mathrm{e}^{\mathrm{i}n\Omega t}\left(\varepsilon-n\hbar\Omega\right)|\alpha\rangle\\&\quad=\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t}\sum_{nm\alpha}F_{n\alpha}\mathrm{e}^{\mathrm{i}n\Omega t}H^{n-m}|\alpha\rangle.\end{aligned}$$

Noting that the exponentials $\left\{\mathrm{e}^{\mathrm{i}n\Omega t}\right\}$ form an orthogonal set on the time interval $[0,T_0]$ and that the basis $\{|\alpha\rangle\}$ was assumed to be an orthonormal one we can deduce the equality

$$\sum_{\beta}F_{n\beta}\left(\varepsilon-n\hbar\Omega\right)|\beta\rangle=\sum_{m\beta}F_{m\beta}H^{n-m}|\beta\rangle,$$

or, taking the scalar product from the left with $\langle\alpha|$,

$$(\varepsilon-n\hbar\Omega)F_{n\alpha}=\sum_{m\beta}\langle\alpha|H^{n-m}|\beta\rangle F_{m\beta}.$$

Defining the matrix elements $H^n_{\alpha\beta}$ as

$$H^n_{\alpha\beta}=\langle\alpha|H^n|\beta\rangle$$

and the matrix elements $\Gamma_{n\alpha;m\beta}$ as

$$\Gamma_{n\alpha;m\beta}=H^{n-m}_{\alpha\beta}+n\hbar\Omega\delta_{nm}\delta_{\alpha\beta}$$

we can rewrite this as the eigenvalue problem

$$\sum_{m\beta}\Gamma_{n\alpha;m\beta}F_{m\beta}=\varepsilon F_{n\alpha},$$

or, in the matrix form

$$\Gamma F=\varepsilon F.$$

Using the property

$$\begin{aligned}H^{-n}_{\beta\alpha}&=\langle\beta|H^{-n}|\alpha\rangle\\&=\frac{1}{T_0}\int_0^{T_0}\mathrm{e}^{\mathrm{i}n\Omega t}\langle\beta|H(t)|\alpha\rangle\,\mathrm{d}t\\&=\frac{1}{T_0}\int_0^{T_0}\mathrm{e}^{\mathrm{i}n\Omega t}\langle\alpha|H^\dagger(t)|\beta\rangle^*\,\mathrm{d}t\\&=\left[\frac{1}{T_0}\int_0^{T_0}\mathrm{e}^{-\mathrm{i}n\Omega t}\langle\alpha|H(t)|\beta\rangle\,\mathrm{d}t\right]^*\\&=H^n_{\alpha\beta}{}^*\end{aligned}$$

it is easy to see that

$$\Gamma_{n\alpha;m\beta}=\Gamma^*_{m\beta;n\alpha}$$

and hence the matrix Γ is Hermitian.
Due to the Hermiticity of Γ

- the eigenvalue problem $\Gamma F = \varepsilon F$ has a solution
- the eigenvalues ε are real
- the eigenvectors F form a complete (orthonormal) basis.

Obviously we can deduce that $|\psi;t\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t}\sum_{n\alpha} F_{n\alpha}\mathrm{e}^{\mathrm{i}n\Omega t}|\alpha\rangle$ indeed solves the time dependent problem.
The eigenvectors F are something like

$$F = \begin{pmatrix} F_{n\alpha} \end{pmatrix} = \begin{pmatrix} \vdots \\ F_{-1,0} \\ F_{-1,1} \\ \vdots \\ F_{0,0} \\ F_{0,1} \\ \vdots \\ F_{1,0} \\ F_{1,1} \\ \vdots \end{pmatrix},$$

that is, the Fourier component labels n run through all integers.
We now show that there exists a relation between the Fourier components. For that purpose we look at what happens if we shifted the eigenvalue by a multiple of $\hbar\Omega$. From the expression

$$\Gamma_{n\alpha;m\beta} = H^{n-m}_{\alpha\beta} + n\hbar\Omega\delta_{nm}\delta_{\alpha\beta}$$

it is clear that

$$\begin{aligned}
&\Gamma_{n\alpha;m\beta} + k\hbar\Omega\delta_{nm}\delta_{\alpha\beta} \\
&\quad = H^{n-m}_{\alpha\beta} + n\hbar\Omega\delta_{nm}\delta_{\alpha\beta} + k\hbar\Omega\delta_{nm}\delta_{\alpha\beta} \\
&\quad = H^{(n+k)-(m+k)}_{\alpha\beta} + (n+k)\hbar\Omega\delta_{n+k,m+k}\delta_{\alpha\beta} \\
&\quad = \Gamma_{n+k,\alpha;m+k,\beta}.
\end{aligned}$$

Using the component expression

$$\sum_{m\beta}\Gamma_{n\alpha;m\beta}F_{m\beta} = \varepsilon F_{n\alpha}$$

we get

$$\begin{aligned}
&(\varepsilon + k\hbar\Omega)\,F_{n\alpha} \\
&\quad = \sum_{m\beta}\left(\Gamma_{n\alpha;m\beta} + k\hbar\Omega\delta_{nm}\delta_{\alpha\beta}\right)F_{m\beta} \\
&\quad = \sum_{m\beta}\Gamma_{n+k,\alpha;m+k,\beta}F_{m\beta} = \sum_{m\beta}\Gamma_{n+k,\alpha;m\beta}F_{m-k,\beta},
\end{aligned}$$

where in the last expression we have substituted $m + k \to m$.
We now have the equation

$$(\varepsilon + k\hbar\Omega)\, F_{n\alpha} = \sum_{m\beta} \Gamma_{n+k,\alpha;m\beta} F_{m-k,\beta},$$

from which by the replacement $n + k \to n$ we get

$$(\varepsilon + k\hbar\Omega)\, F_{n-k,\alpha} = \sum_{m\beta} \Gamma_{n,\alpha;m\beta} F_{m-k,\beta}.$$

This means that the eigenvector F corresponding to the eigenvalue ε is related to the eigenvector F^k corresponding to the eigenvalue $\varepsilon + k\hbar\Omega$ by

$$F^k_{n\alpha} = F_{n-k,\alpha}.$$

Recall that the time dependent solutions related to the eigenvalue ε are

$$|\psi; t\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t} \sum_{n\alpha} F_{n\alpha} \mathrm{e}^{\mathrm{i}n\Omega t} |\alpha\rangle.$$

Correspondingly the solutions $|\psi'; t\rangle$ related to the shifted eigenvalue $\varepsilon + k\hbar\Omega$ would be

$$\begin{aligned}
|\psi'; t\rangle &= \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(\varepsilon + k\hbar\Omega)t} \sum_{n\alpha} F^k_{n\alpha} \mathrm{e}^{\mathrm{i}n\Omega t} |\alpha\rangle \\
&= \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t} \sum_{n\alpha} F^k_{n\alpha} \mathrm{e}^{\mathrm{i}(n-k)\Omega t} |\alpha\rangle \\
&= \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t} \sum_{n\alpha} F^k_{n+k,\alpha} \mathrm{e}^{\mathrm{i}n\Omega t} |\alpha\rangle \\
&= \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t} \sum_{n\alpha} F_{n\alpha} \mathrm{e}^{\mathrm{i}n\Omega t} |\alpha\rangle \\
&= |\psi; t\rangle.
\end{aligned}$$

We see that we can shift all eigenvalues ε to an interval of width $\hbar\Omega$. As the solution of the eigenvalue problem

$$\Gamma F = \varepsilon F$$

we get an infinite set eigenvalues and eigenvectors. When we label them as

$$\Gamma F^\lambda = \varepsilon_\lambda F^\lambda$$

it is thus sufficient to look at, for example only the spectral set

$$\Lambda = \left\{ \lambda \,\middle|\, -\frac{\hbar}{2}\Omega \le \varepsilon_\lambda < \frac{\hbar}{2}\Omega \right\}$$

and the corresponding set

$$|\lambda;t\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon_\lambda t}\sum_{n\alpha} F^\lambda_{n\alpha}\mathrm{e}^{\mathrm{i}n\Omega t}|\alpha\rangle,\ \lambda\in\Lambda$$

of time dependent quantum states. Due to the linear independence of the eigenvectors F^λ it is easy to see that the states $|\lambda;t\rangle$ form a complete linearly independent set of solutions for the time dependent problem. Any given state in the relevant Hilbert space, e.g. any initial state can be expressed as a linear combination of these states.
It is worthwhile to notice the beauty of the Floquet approach. It reduces time dependent problems to static ones, that is to time independent eigenvalue problems

$$\Gamma F = \varepsilon F.$$

If you happen to have a computer code for static problems in occupation representation formalism the time dependent problems are easily adapted:

- obtain a complete basis $\{|\alpha\rangle\}$ for the relevant Hilbert space, for example by solving a static problem (possibly a manybody one)
- construct a fictitious *single* particle basis $\{|m;\alpha\rangle\}$ representing the set of products $|\alpha\rangle\mathrm{e}^{\mathrm{i}\hbar m\Omega t}$
- construct a fictitious onebody operator $\mathcal{O}$ with matrix elements

$$\langle n;\alpha|\mathcal{O}|m;\beta\rangle = H^{n-m}_{\alpha\beta} + n\hbar\Omega\delta_{nm}\delta_{\alpha\beta}$$

- feed the fictitious basis and the fictitious onebody operator to your code, and solve the fictitious static onebody problem and you are done!

5.3 Transition rates

Suppose that our system is initially at $t=0$ in the state $|\alpha\rangle$. That is, using the notation

$$|\lambda;t\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon_\lambda t}\sum_{n\alpha} F^\lambda_{n\alpha}\mathrm{e}^{\mathrm{i}n\Omega t}|\alpha\rangle$$

we require that the superposition

$$|\psi;t\rangle = \sum_\lambda x^\alpha_\lambda|\lambda;t\rangle = \sum_\lambda x^\alpha_\lambda \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon_\lambda t}\sum_{n\gamma} F^\lambda_{n\gamma}\mathrm{e}^{\mathrm{i}n\Omega t}|\gamma\rangle$$

satisfies the condition

$$|\psi;t=0\rangle = |\alpha\rangle.$$

Written explicitly this condition reads

$$\sum_\lambda x^\alpha_\lambda \sum_{n\gamma} F^\lambda_{n\gamma}|\gamma\rangle = |\alpha\rangle,$$

or taking scalar products on both sides with $\langle\gamma|$

$$\sum_\lambda x_\lambda^\alpha \sum_m F_{m\gamma}^\lambda = \delta_{\alpha\gamma},$$

from which we can solve the coefficients x_λ^α (note that the vectors x^α form the inverse of the matrix $\sum_m F_{m\alpha}^\lambda$).
The probability amplitude to find the state $|\psi;t\rangle$ at time t in the state $|\beta\rangle$ is

$$\eta_{\beta\alpha}(t) = \langle\beta|\psi;t\rangle = \sum_\lambda x_\lambda^\alpha \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon_\lambda t} \sum_n F_{n\beta}^\lambda \mathrm{e}^{\mathrm{i}n\Omega t}.$$

The corresponding transition probability is then

$$\begin{aligned} P_{\beta\alpha}(t) &= |\eta_{\beta\alpha}|^2 \\ &= \sum_{\lambda\lambda'} x_{\lambda'}^{\alpha\,*} x_\lambda^\alpha \sum_{nm} F_{m\beta}^{\lambda'\,*} F_{n\beta}^\lambda \mathrm{e}^{\mathrm{i}(\frac{1}{\hbar}(\varepsilon_{\lambda'}-\varepsilon_\lambda)t+(n-m)\Omega t)}. \end{aligned}$$

Time averaged transition probability is then

$$\bar{P}_{\beta\alpha} = \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathrm{d}t\, P_{\beta\alpha}(t).$$

It is easy to see that the integral vanishes unless

$$\frac{1}{\hbar}(\varepsilon_{\lambda'} - \varepsilon_\lambda) + (n-m)\Omega = 0.$$

Recalling, that the eigenvalues ε_λ were restricted to the interval $-\Omega/2 < \varepsilon_\lambda \leq \Omega/2$ we can conclude that we must have $n - m = 0$. Forgetting the accidental degeneracies $\varepsilon_\lambda = \varepsilon_{\lambda'}$ $(\lambda' \neq \lambda)$ we have also the condition $\lambda = \lambda'$. The time averaged transition probability reads now

$$\bar{P}_{\beta\alpha} = \sum_\lambda |x_\lambda^\alpha|^2 \sum_n |F_{m\beta}^\lambda|^2.$$

Occasionally we are interested in the time evolution of the transition probability or, equivalently how the transition probability oscillates when time goes on. For that purpose we return to the general case and define the frequency dependent transition probability $P_{\beta\alpha}(\omega)$ via

$$P_{\beta\alpha}(t) = \int \mathrm{d}\omega\, \mathrm{e}^{\mathrm{i}\omega t} P_{\beta\alpha}(\omega).$$

We see that the transition probability corresponding to the frequency ω is

$$\begin{aligned} P_{\beta\alpha}(\omega) &= \frac{1}{2\pi} \int \mathrm{d}t\, \mathrm{e}^{-\mathrm{i}\omega t} P_{\beta\alpha}(t) \\ &= \sum_{\lambda\lambda'} x_{\lambda'}^{\alpha\,*} x_\lambda^\alpha \sum_{nm} F_{m\beta}^{\lambda'\,*} F_{n\beta}^\lambda \\ &\quad \times\delta(\frac{1}{\hbar}(\varepsilon_{\lambda'} - \varepsilon_\lambda) + (n-m)\Omega - \omega). \end{aligned}$$

Using the notations

$$\Delta_{\lambda'\lambda} = \varepsilon_{\lambda'} - \varepsilon_{\lambda}$$

and

$$P_{\beta}^{\lambda'\lambda}(\omega) = \sum_{nm} {F_{m\beta}^{\lambda'}}^{*} F_{n\beta}^{\lambda} \delta(\frac{1}{\hbar}\Delta_{\lambda'\lambda} + (n-m)\Omega - \omega)$$

the total probability can be written as

$$P_{\beta\alpha}(\omega) = \sum_{\lambda\lambda'} {x_{\lambda'}^{\alpha}}^{*} x_{\lambda}^{\alpha} P_{\beta}^{\lambda'\lambda}(\omega).$$

Noting that for given frequency ω the difference $n-m$ in must be constant we can rewrite $P_{\beta}^{\lambda'\lambda}(\omega)$ as

$$P_{\beta}^{\lambda'\lambda}(\omega) = \sum_{m} {F_{m\beta}^{\lambda'}}^{*} F_{M+m,\beta}^{\lambda}$$

where now $\omega = \frac{1}{\hbar}\Delta_{\lambda'\lambda} + M\Omega$ and $M = n-m$.
We define convolution vectors C as

$$C_{m\alpha}^{\lambda'\lambda} = \sum_{n} {F_{n\alpha}^{\lambda'}}^{*} F_{m+n,\alpha}^{\lambda}.$$

We can see that we have

$$\begin{aligned} \left(C_{m\alpha}^{\lambda'\lambda}\right)^{*} &= \sum_{n} F_{n\alpha}^{\lambda'} {F_{m+n,\alpha}^{\lambda}}^{*} = \sum_{k} {F_{k\alpha}^{\lambda}}^{*} F_{-m+k,\alpha}^{\lambda'} \\ &= C_{-m,\alpha}^{\lambda\lambda'} \end{aligned}$$

and, consequently the convolutions obey the relation

$$C_{m\alpha}^{\lambda\lambda'} = \left(C_{-m\alpha}^{\lambda'\lambda}\right)^{*}.$$

In terms of the convolutions the transition probability can be rewritten as

$$P_{\alpha\beta}(\omega) = \sum_{\lambda\lambda' m} {x_{\lambda'}^{\beta}}^{*} x_{\lambda}^{\beta} C_{m\alpha}^{\lambda'\lambda} \delta\left(\frac{1}{\hbar}\Delta_{\lambda'\lambda} + m\Omega - \omega\right).$$

5.4 An example: Two state system

To see how the Floquet theory works in practice we look at the simplest possible system, a system consisting of two states. We assume that the static Hamiltonian H_0 satisfies the Schrödinger equation

$$H_0|\alpha\rangle = \lambda_{\alpha}|\alpha\rangle; \alpha = 0, 1,$$

with the eigenvalues

$$\lambda_0 = 0 \text{ and } \lambda_1 = \lambda.$$

We take the time dependent part $\mathcal{V}(t)$ of the Hamiltonian to be

$$\mathcal{V}(t) = V\left[\mathrm{e}^{-\mathrm{i}\Omega t}|1\rangle\langle 0| + \mathrm{e}^{\mathrm{i}\Omega t}|0\rangle\langle 1|\right],$$

so that the complete Hamiltonian is

$$H = \lambda|1\rangle\langle 1| + V\mathrm{e}^{-\mathrm{i}\Omega t}|1\rangle\langle 0| + V\mathrm{e}^{\mathrm{i}\Omega t}|0\rangle\langle 1|.$$

We proceed first to solve the time dependent problem directly and then to compare the results with the Floquet model. To this end we write the solution of the full Schrödinger equation

$$H|\psi\rangle = \mathrm{i}\hbar\frac{\partial}{\partial t}|\psi\rangle$$

as

$$|\psi\rangle = a_0(t)|0\rangle + a_1(t)|1\rangle.$$

We have

$$\begin{aligned}\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi\rangle &= \mathrm{i}\hbar\dot{a}_0|0\rangle + \mathrm{i}\hbar\dot{a}_1|1\rangle = H|\psi\rangle \\ &= \lambda a_1|1\rangle + V\mathrm{e}^{-\mathrm{i}\Omega t}|1\rangle a_0 + V\mathrm{e}^{\mathrm{i}\Omega t}|0\rangle a_1.\end{aligned}$$

From this we can read the system of differential equations

$$\begin{aligned}\mathrm{i}\hbar\dot{a}_0 &= V\mathrm{e}^{\mathrm{i}\Omega t}a_1 \\ \mathrm{i}\hbar\dot{a}_1 &= \lambda a_1 + V\mathrm{e}^{-\mathrm{i}\Omega t}a_0.\end{aligned}$$

Setting

$$\begin{aligned}t &= \frac{\hbar}{V}\tau \\ \nu &= \frac{\hbar\Omega}{V} \\ \gamma &= \frac{\lambda}{V}\end{aligned}$$

we end up with the equations

$$\begin{aligned}\mathrm{i}\dot{a}_0 &= \mathrm{e}^{\mathrm{i}\nu\tau}a_1 \\ \mathrm{i}\dot{a}_1 &= \gamma a_1 + \mathrm{e}^{-\mathrm{i}\nu\tau}a_0.\end{aligned}$$

In the spirit of Floquet we try solutions of the form

$$a_i(t) = \mathrm{e}^{-\mathrm{i}\epsilon\tau}\sum_n c_n^i\mathrm{e}^{\mathrm{i}n\nu\tau}.$$

Substituting this to the wave function $|\psi\rangle$ we get

$$\begin{aligned}|\psi\rangle &= a_0(t)|0\rangle + a_1(t)|1\rangle \\ &= \mathrm{e}^{-\mathrm{i}\epsilon\tau}\sum_n c_n^0\mathrm{e}^{\mathrm{i}n\nu\tau}|0\rangle + \mathrm{e}^{-\mathrm{i}\epsilon\tau}\sum_n c_n^1\mathrm{e}^{\mathrm{i}n\nu\tau}|1\rangle \\ &= \mathrm{e}^{-\mathrm{i}\epsilon\tau}\sum_{n\alpha} c_n^\alpha\mathrm{e}^{\mathrm{i}n\nu\tau}|\alpha\rangle.\end{aligned}$$

Comparing this with the Floquet expansion

$$\begin{aligned}|\psi\rangle &= \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon t}\sum_{n\alpha}F_{n\alpha}\mathrm{e}^{\mathrm{i}n\Omega t}|\alpha\rangle \\ &= \mathrm{e}^{-\mathrm{i}\,\frac{\varepsilon}{V}\tau}\sum_{n\alpha}F_{n\alpha}\mathrm{e}^{\mathrm{i}n\frac{\hbar\Omega}{V}\tau}|\alpha\rangle \\ &= \mathrm{e}^{-\mathrm{i}\,\frac{\varepsilon}{V}\tau}\sum_{n\alpha}F_{n\alpha}\mathrm{e}^{\mathrm{i}n\nu\tau}|\alpha\rangle,\end{aligned}$$

we can read the relations

$$\begin{aligned}\varepsilon &= V\epsilon \\ F_{n\alpha} &= c_n^\alpha.\end{aligned}$$

For the time derivatives of the coefficients we get

$$\begin{aligned}\dot{a}_i &= -\mathrm{i}\epsilon\mathrm{e}^{-\mathrm{i}\epsilon\tau}\sum_n c_n^i\mathrm{e}^{\mathrm{i}n\nu\tau} + \mathrm{i}\mathrm{e}^{-\mathrm{i}\epsilon\tau}\sum_n n\nu c_n^i\mathrm{e}^{\mathrm{i}n\nu\tau} \\ &= -\mathrm{i}\mathrm{e}^{-\mathrm{i}\epsilon\tau}\sum_n(\epsilon-n\nu)c_n^i\mathrm{e}^{\mathrm{i}n\nu\tau}.\end{aligned}$$

Substitutions to the first differential equation yield

$$\begin{aligned}\mathrm{e}^{-\mathrm{i}\epsilon\tau}\sum_n(\epsilon-n\nu)c_n^0\mathrm{e}^{\mathrm{i}n\nu\tau} &= \mathrm{e}^{-\mathrm{i}\epsilon\tau}\mathrm{e}^{\mathrm{i}\nu\tau}\sum_n c_n^1\mathrm{e}^{\mathrm{i}n\nu\tau} \\ &= \mathrm{e}^{-\mathrm{i}\epsilon\tau}\sum_n c_{n-1}^1\mathrm{e}^{\mathrm{i}n\nu\tau},\end{aligned}$$

and to the second one

$$\begin{aligned}&\mathrm{e}^{-\mathrm{i}\epsilon\tau}\sum_n(\epsilon-n\nu)c_n^1\mathrm{e}^{\mathrm{i}n\nu\tau} \\ &= \gamma\mathrm{e}^{-\mathrm{i}\epsilon\tau}\sum_n c_n^1\mathrm{e}^{\mathrm{i}n\nu\tau} + \mathrm{e}^{-\mathrm{i}\epsilon\tau}\mathrm{e}^{-\mathrm{i}\nu\tau}\sum_n c_n^0\mathrm{e}^{\mathrm{i}n\nu\tau} \\ &= \mathrm{e}^{-\mathrm{i}\epsilon\tau}\sum_n\gamma c_n^1\mathrm{e}^{\mathrm{i}n\nu\tau} + \mathrm{e}^{-\mathrm{i}\epsilon\tau}\sum_n c_{n+1}^0\mathrm{e}^{\mathrm{i}n\nu\tau}.\end{aligned}$$

From these we can read the equations

$$\begin{aligned}(\epsilon-n\nu)c_n^0 &= c_{n-1}^1 \\ (\epsilon-n\nu)c_n^1 &= \gamma c_n^1 + c_{n+1}^0,\end{aligned}$$

or, rearranging a little bit

$$\begin{aligned}n\nu c_n^0 + c_{n-1}^1 &= \epsilon c_n^0 \\ (n\nu+\gamma)c_n^1 + c_{n+1}^0 &= \epsilon c_n^1.\end{aligned}$$

This is clearly an eigenvalue problem related to the matrix

	$(n-1,1)$	$(n,0)$	$(n,1)$	$(n+1,0)$	
	$\ddots$ $\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$(n-1,1)$	$\cdots(n-1)\nu+\gamma$	1	0	0	$\cdots$
$(n,0)$	$\cdots$ 1	$n\nu$	0	0	$\cdots$
$(n,1)$	$\cdots$ 0	0	$n\nu+\gamma$	1	$\cdots$
$(n+1,0)$	$\cdots$ 0	0	1	$(n+1)\nu$	$\cdots$
	$\vdots$ $\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$

where the row and column labels (n,α) correspond to the coefficients c_n^α. We see that the matrix is in block diagonal form so it is sufficient to look only at one block, say

$$B = \begin{pmatrix} (n-1)\nu+\gamma & 1 \\ 1 & n\nu \end{pmatrix}.$$

The components of the eigenvectors are then labeled as $\begin{pmatrix} c_{n-1}^1 \\ c_n^0 \end{pmatrix}$.
Let's see how this fits to the general Floquet formalism. From the Hamiltonian

$$H = \lambda|1\rangle\langle 1| + V\mathrm{e}^{-\mathrm{i}\Omega t}|1\rangle\langle 0| + V\mathrm{e}^{\mathrm{i}\Omega t}|0\rangle\langle 1|$$

we can readily read the Fourier components

$$H^0 = \lambda|1\rangle\langle 1|,\ H^{-1} = V|0\rangle\langle 1|,\ H^1 = V|1\rangle\langle 0|.$$

From these one can directly read the matrix elements $H^n_{\alpha\beta}$ as

$$H^0_{11} = \lambda,\ H^{-1}_{01} = H^1_{10} = 0$$

all other matrix element vanishing. The components of the matrix

$$\Gamma_{n\alpha;m\beta} = H^{n-m}_{\alpha\beta} + n\hbar\Omega\delta_{nm}\delta_{\alpha\beta}$$

are then

$$\begin{aligned}
\Gamma_{n0:m0} &= H^{n-m}_{00} + n\hbar\Omega\delta_{nm} = n\hbar\Omega\delta_{nm} = Vn\nu \\
\Gamma_{n1;m1} &= (\lambda + n\hbar\Omega)\delta_{nm} = V(\gamma + n\nu) \\
\Gamma_{n0;m1} &= H^{n-m}_{01} = V\delta_{n,m-1} \\
\Gamma_{n1;m0} &= H^{n-m}_{10} = V\delta_{n,m+1}.
\end{aligned}$$

Arranging the rows and columns of Γ in the order $(n0)$, $(n1)$, $(n+1,0)$, ... clearly gives us the previous matrix multiplied by V which would yield the same eigenvectors. The eigenvalues would be multiplied by V which is perfectly OK ($\varepsilon = V\epsilon$).

The characteristic equation of the block is

$$\begin{aligned}
&[(n-1)\nu+\gamma-\epsilon][n\nu-\epsilon]-1\\
&\quad=[(n-1)\nu+\gamma]n\nu-[(n-1)\nu+\gamma]\epsilon\\
&\qquad-n\nu\epsilon+\epsilon^2-1\\
&\quad=\epsilon^2-\left(2(n-1)\nu+\nu+\gamma\right)\epsilon\\
&\qquad+[(n-1)\nu+\gamma]n\nu-1\\
&\quad=0.
\end{aligned}$$

Its solutions are

$$\begin{aligned}
\epsilon &= \frac{1}{2}\left[2(n-1)\nu+\nu+\gamma\pm\sqrt{D}\right]\\
&= \frac{1}{2}\left[2n\nu+(\gamma-\nu)\pm\sqrt{D}\right],
\end{aligned}$$

where

$$\begin{aligned}
D &= \left(2(n-1)\nu+\nu+\gamma\right)^2\\
&\qquad-4n\nu\left((n-1)\nu+\gamma\right)+4\\
&= (\gamma-\nu)^2+4.
\end{aligned}$$

The eigenvalues can now be written as

$$\epsilon_{\pm}^{n}=n\nu+\frac{1}{2}(\gamma-\nu)\pm\sqrt{\left(\frac{\gamma-\nu}{2}\right)^2+1}.$$

Let us now choose the block related to the coefficients c_{-1}^{1} and c_{0}^{0}, i.e. the one whose eigenvalues are $\epsilon_{\pm}^{0}$,

$$\epsilon_{\pm}=\epsilon_{\pm}^{0}=\frac{1}{2}(\gamma-\nu)\pm\sqrt{\left(\frac{\gamma-\nu}{2}\right)^2+1}. \tag{5.1}$$

The coefficients satisfy the equations

$$\begin{aligned}
(\gamma-\nu)c_{-1}^{1}+c_{0}^{0} &= \epsilon_{\pm}c_{-1}^{1}\\
c_{-1}^{1} &= \epsilon_{\pm}c_{0}^{0}.
\end{aligned}$$

So, the normalized eigenvectors can be written, for example using the latter equation as

$$\begin{pmatrix} c_{-1}^{1}\\ c_{0}^{0}\end{pmatrix}=\frac{1}{\sqrt{1+(\epsilon_{\pm})^2}}\begin{pmatrix}\epsilon_{\pm}\\ 1\end{pmatrix},$$

which are clearly linearly independent ($\epsilon_{+}\neq\epsilon_{-}$).

The former equation would yield the eigenvectors $\begin{pmatrix} 1 \\ \epsilon_\pm - (\gamma - \nu) \end{pmatrix}$. At first sight it looks like as if we had too many eigenvectors. However, using the properties

$$\begin{aligned} \epsilon_+ + \epsilon_- &= \gamma - \nu \\ \epsilon_+ \epsilon_- &= -1 \end{aligned}$$

readable from the characteristic equation

$$\epsilon^2 - (\gamma - \nu)\epsilon - 1 = 0$$

we can readily see that the eigenvectors

$$\begin{pmatrix} \epsilon_\pm \\ 1 \end{pmatrix}$$

are linearly dependent on the eigenvectors

$$\begin{aligned} \begin{pmatrix} 1 \\ \epsilon_\pm - (\gamma - \nu) \end{pmatrix} &= \begin{pmatrix} 1 \\ \epsilon_\pm - (\epsilon_+ + \epsilon_-) \end{pmatrix} \\ &= \begin{pmatrix} 1 \\ -\epsilon_\mp \end{pmatrix} \\ &= -\epsilon_\mp \begin{pmatrix} \epsilon_\pm \\ 1 \end{pmatrix}. \end{aligned}$$

In the general case the coefficients satisfy the equations

$$\begin{aligned} ((n-1)\nu + \gamma)\, c^1_{n-1} + c^0_n &= \epsilon^n_\pm c^1_{n-1} \\ n\nu c^0_n + c^1_{n-1} &= \epsilon^n_\pm c^0_n, \end{aligned}$$

from which we can read the normalized eigenvectors

$$\begin{pmatrix} c^1_{n-1} \\ c^0_n \end{pmatrix} = \frac{1}{\sqrt{1 + \left(\epsilon^n_\pm - n\nu\right)^2}} \begin{pmatrix} \epsilon^n_\pm - n\nu \\ 1 \end{pmatrix}.$$

The corresponding eigenvalues are

$$\epsilon^n_\pm = n\nu + \frac{1}{2}(\gamma - \nu) \pm \sqrt{\left(\frac{\gamma - \nu}{2}\right)^2 + 1}.$$

Returning to the general Floquet expansion the identifications

$$\begin{aligned} \varepsilon &= V\epsilon \\ F_{n\alpha} &= c^\alpha_n. \end{aligned}$$

yield

$$
\begin{aligned}
\epsilon_{\pm}^{n} &= n\nu + \frac{1}{2}(\gamma-\nu) \pm \sqrt{\left(\frac{\gamma-\nu}{2}\right)^{2}+1} \\
\varepsilon_{\pm}^{n} &= V\epsilon_{\pm}^{n} \\
&= V\left[n\nu + \frac{1}{2}(\gamma-\nu) \pm \sqrt{\left(\frac{\gamma-\nu}{2}\right)^{2}+1}\right] \\
F_{n-1,1}^{\varepsilon_{\pm}^{n}} &= c_{n-1}^{\varepsilon_{\pm}^{n},1} = c\left[\epsilon_{\pm}^{n} - n\nu\right] \\
&= \frac{c}{2}\left[\gamma-\nu \pm \sqrt{(\gamma-\nu)^{2}+4}\right] \\
F_{n0}^{\varepsilon_{\pm}^{n}} &= c_{n}^{\varepsilon_{\pm}^{n},0} = c \\
c &= \frac{1}{\sqrt{1+\left(\epsilon_{\pm}^{n} - n\nu\right)^{2}}}.
\end{aligned}
$$