Nuclear Structure Theory Notes

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Contents

LECTURE 4

Second Quantization and nuclear shell model

1. Reminder of Quantum Mechanics

1.1. The Mathematics of first quantization.

1.1.1. *Vector Space.* Quantum mechanics is a theory for the description of the statistical behavior of microscopic entities. It defines physical states in a sesquilinear form of a vector space $\mathcal{H}$ on the field of complex numbers, also known as Hilbert space. **ket** $|a\rangle \in \mathcal{H}$ or **bra** $\langle b| \in \mathcal{H}^*$ (dual space) [**1**].

Properties of vector spaces:

- addition: $|a\rangle + |b\rangle = |c\rangle$
- scalar product: $\alpha|a\rangle = |a\rangle\alpha$ with $\alpha \in \mathbb{C}$
- inner product: $\langle b|a\rangle = \alpha$ with $\alpha \in \mathbb{C}$
- the inner product is sesquilinear, in other words linear in $|a\rangle$ and anti-linear in $\langle b|$: $\langle b|a+\alpha c\rangle = \langle b|a\rangle + \alpha\langle b|c\rangle$, and $\langle b|a\rangle = \langle a|b\rangle^*$
- and doing so it defines a norm for the vector: $\langle a|a\rangle = ||a||^2 = x \geq 0$, with $x \in \mathbb{R}$

1.1.2. *Basis. orthornormal basis* $\{|n\rangle\} = \{|1\rangle, |2\rangle, \ldots, |N\rangle\}$ it is an orthonormal basis for the vector space V if $\forall|n\rangle, |m\rangle \in \{|n\rangle\} \Rightarrow |n\rangle \in V$, $\langle n|n\rangle = 1, \langle m|n\rangle = 0$ (normalized and orthogonal), and $\forall|a\rangle \in V \Rightarrow |a\rangle = \sum_{n=1}^{N} c_n|n\rangle$ (complete basis)

1.1.3. *Operators.* Mathematically operators act on a vector, mapping it from a vector space to another. In Quantum Mechanics operators are **linear** ($(X+\alpha Y)|a\rangle = X|a\rangle + \alpha Y|a\rangle$) and **associative**. In general $X|a\rangle = |b\rangle$, with $|a\rangle \in V$ and $|b\rangle \in W$,

$$X := |b\rangle\langle a|, \tag{1}$$

and if we consider a physical state $|a\rangle$ with norm 1

$$X|a\rangle = \langle a|a\rangle|b\rangle = |b\rangle. \tag{2}$$

$$\langle m|X|n\rangle := X_{mn} \in \mathbb{C} \tag{3}$$

$$X|a\rangle = |b\rangle \Leftrightarrow \langle a|X^\dagger = \langle b|, \text{ with} |b\rangle \in W and \langle b| \in W^*, \tag{4}$$

$$(X^\dagger)_{nn'} = X^*_{n'n} \tag{5}$$

$$(XY)^\dagger = Y^\dagger X^\dagger \tag{6}$$

$X|x\rangle = x|x\rangle$, $x \in \mathbb{C}$ eigenvalue, $|x\rangle \in V$ eigenvector.

Linear operators which satisfy $A^\dagger = A$ are called **Hermitian**, and have real eigenvalues.

$$A = \sum_n a_n|n\rangle\langle n|, \qquad a_n \in \mathbb{R} \tag{7}$$

Linear operators which satisfy $UU^\dagger = 1 \Rightarrow U^\dagger = U^{-1}$ are called **unitary** ($||Ua||^2 = \langle a|U^\dagger U|a\rangle = ||a||$).

Linear operators which satisfy $P^2 = P$ (idempotency) and are Hermitian, are called orthogonal **projectors**. $P_1|a\rangle = |a_1\rangle \in V_1 \subset V$ and $\langle b|P_1^\dagger(|a\rangle - P_1|a\rangle) = 0$. In the Dirac notation: $P_1 = \sum_{i=1}^{N_1} |i\rangle\langle i|$ where $i = 1 \dots N_1$ are a subset of the orthonormal basis.

If the case $V_1 \equiv V$, $P_V = \sum_{n=1}^{N} |n\rangle\langle n| \equiv \mathbb{I}$ is the identity operator.

Density operator: $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$, $p_i = |\langle\psi_i|a\rangle|^2$ probability of $|\psi_i\rangle$ in state $|a\rangle$, $|\psi_i\rangle$ is normalized and $\sum_i p_i = 1$

$$\langle A\rangle = \sum_i p_i \langle\psi_i|A|\psi_i\rangle = \mathrm{Tr}[\rho A] \tag{8}$$

1.1.4. *Tensor Products.* $|\phi\rangle_1 = \sum a_n|n\rangle \in \mathcal{H}^{\mathcal{N}}{}_1$, $|_\rangle\chi_2 = \sum c_m|m\rangle \in \mathcal{H}^{\mathcal{M}}{}_2$ Define the tensor products of spaces $|\phi_1 \otimes \chi_2\rangle := |\phi\chi\rangle_{12} = \sum_{n,m} a_n c_m |n \otimes m\rangle_{12} \in \mathcal{H}^{\mathcal{N}}{}_1 \otimes \mathcal{H}^{\mathcal{M}}{}_2$ with dimension $N \cdot M$, is the space of two interacting quantum systems.

$$\langle n \otimes m|n' \otimes m'\rangle_{12} = \delta_{m,m'}\delta_{n,n'}. \tag{9}$$

If $A|\phi_1\rangle = a|\phi_1\rangle$,

$$\Rightarrow A|\phi\chi\rangle_{12} = a|\phi\chi\rangle_{12}. \tag{10}$$

Two–body Density Matrix

$$\rho_{12} = \rho_1 \otimes \rho_2 = \sum_{i,j} p_i p_j |\phi_i\chi_j\rangle_{12}\ {}_{12}\langle\phi_i\chi_j| \tag{11}$$

$$\rho_1 = \mathrm{Tr}_2[\rho_{12}] = \sum_m \langle m|\rho_{12}|m\rangle \tag{12}$$

1.1.5. *Coordinates.* An infinite dimensional (with uncountable cardinality) Hilbert space $\mathscr{H}$, is used to represent quantum state that vary in a continuous spectrum, most importantly r and k. The inner product makes use of integrals over wavefunctions and operator which are defined in the sense of the distributions.

Coordinate $|\mathbf{r}\rangle$ and momentum $|\mathbf{k}\rangle$ representations.

$$\hat{\mathbf{r}}|\mathbf{r}\rangle = \mathbf{r}|\mathbf{r}\rangle \tag{13}$$

$$\hat{\mathbf{p}}|\mathbf{k}\rangle = \mathbf{k}|\mathbf{k}\rangle \tag{14}$$

$$\hat{\mathbf{p}}|\mathbf{r}\rangle = -i\hbar\frac{\mathrm{d}}{\mathrm{d}\mathbf{r}}|\mathbf{r}\rangle \tag{15}$$

$$\hat{\mathbf{r}}|\mathbf{k}\rangle = -\frac{1}{i\hbar}\frac{\mathrm{d}}{\mathrm{d}\mathbf{k}}|\mathbf{k}\rangle \tag{16}$$

$$\langle\mathbf{r}|\mathbf{k}\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}\mathbf{r}\cdot\mathbf{k}} \tag{17}$$

1.1.6. *Variational Principle.* Let's consider $|\psi_\lambda\rangle$ eigenvectors of $\hat{H}$, with eigenvalue λ $\hat{H}\,|\psi_\lambda\rangle = \lambda\,|\psi_\lambda\rangle$, forms an orthonormal set $\sum_{\lambda_1,\lambda_2}\langle\psi_{\lambda_1}\mid\psi_{\lambda_2}\rangle = \delta_{\lambda_1\lambda_2}$

Expectation value of h is then given by

$$\langle\psi\mid H\mid\psi\rangle = \sum_{\lambda_1,\lambda_2}\langle\psi|\psi_{\lambda_1}\rangle\,\langle\psi_{\lambda_1}|H|\psi_{\lambda_2}\rangle\,\langle\psi_{\lambda_2}|\psi\rangle \tag{18}$$

$$= \sum_{\lambda}\lambda\,|\langle\psi_\lambda\mid\psi\rangle|^2 \geq \sum_{\lambda\in\mathrm{Spec}(H)} E_0\,|\langle\psi_\lambda\mid\psi\rangle|^2 = E_0 \tag{19}$$

so if we minimize E_0 we find the exact expectation value of the Hamiltonian.

1.2. Schroedinger equation.

1.2.1. *Time dependent and independent Schroedinger Equation.*

$$\hat{H}\Psi(\mathbf{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t), \tag{20}$$

$$\left[\frac{-\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t). \tag{21}$$

If H is time independent than the time evolution and the coordinate evolution are separable.

$$\hat{H}(\mathbf{r})\Psi(\mathbf{r}) = E\Psi(\mathbf{r}), \tag{22}$$

with H defined as

$$\left[\frac{-\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r})\right]\Psi(\mathbf{r}) = E\Psi(\mathbf{r}). \tag{23}$$

1.2.2. *Solutions of time independent Schroedinger equations for notable potentials.*
Free particle Schroedinger equation.

One dimensional case $\mathbf{r}\to x$
$V(\mathbf{r}) = 0 \Rightarrow H = T$

$$\hat{H}\psi = E\psi \tag{24}$$

$$\frac{-\hbar^2}{2m}\frac{\mathrm{d}}{\mathrm{d}x}\psi(x) = E\psi(x) \tag{25}$$

$$\psi(x) = e^{ikx}; \qquad k = \frac{\sqrt{2mE}}{\hbar} \tag{26}$$

Square well.

$$V(x) = \begin{cases} -V_0 & -a/2 < x < a/2 \\ 0 & |x| > a/2 \end{cases} \tag{27}$$

if $E < 0$,

$$\psi(x) = A\sin(k_0 x) + B\cos(k_0 x); \qquad k_0 = \frac{\sqrt{2m(E+V_0)}}{\hbar} \qquad |x| < a \qquad -V_0 < E < 0 \tag{28}$$

$$\psi(x) = Ce^{kx} + De^{-kx}; \qquad k = -\frac{\sqrt{2m(E)}}{\hbar} \qquad x > a \qquad E < 0 \tag{29}$$

$$\psi(x) = Ee^{kx} + Fe^{-kx}; \qquad k = -\frac{\sqrt{2m(E)}}{\hbar} \qquad x < -a \qquad E < 0 \tag{30}$$

with $k = \sqrt{2mE}/\hbar$, and $k_0 = \sqrt{2m(E+V_0)}/\hbar$. Since $\psi(x) \in L^2$, $\Rightarrow C = F = 0$ for rinormalizability.

THEOREM 1. *If the potential is symmetric, so that $V(x) = V(-x)$, then $\psi(x)$ can be taken as either even or odd.*

for $\psi(x)$ odd $B = 0, D = -F$ $\psi(x) \in C$, so we apply matching conditions for $\psi(x)$ and $\psi'(x)$.

$$k = -\frac{k_0}{\tan(k_0 a)}. \tag{31}$$

if $E > 0$, means that also for $|x| > a$ I have positive eigenvalue, so the eigenfunction must be also trigonometric,

$$\psi(x) = A\sin(k_0 x) + B\cos(k_0 x); \qquad k_0 = \frac{\sqrt{2m(E+V_0)}}{\hbar} \qquad |x| < a/2 \qquad -V_0 < E < 0 \tag{32}$$

$$\psi(x) = C\sin(kx+\phi) + D\cos(kx+\phi); \qquad k = \frac{\sqrt{2m(E)}}{\hbar} \qquad x > a/2 \qquad E > 0 \tag{33}$$

$$\psi(x) = E\sin(kx+\phi) + F\cos(kx+\phi); \qquad k = \frac{\sqrt{2m(E)}}{\hbar} \qquad x > a/2 \qquad E > 0 \tag{34}$$

(35)

again I choose to solve the odd case, implying $B = D = F$. Note the phase factor ϕ between the solution inside and outside the well.

using the same technique of matching conditions one obtains,

$$\frac{\mathrm{tg}(ka+\phi)}{k} = \frac{\mathrm{tg}(k_0 a+\phi)}{k_0} \tag{36}$$

which has solutions for every k, thus every E defining a continuous energy spectrum. Note that, ϕ is univocally determined,

$$\phi = \mathrm{arctg}\left(\frac{k}{k_0}\mathrm{tg}(k_0 a+\phi)\right) - ka, \tag{37}$$

and is related to the *phase shift*.

Moreover considering the matching conditions at $\psi(a)$,

$$\frac{A}{E} = \frac{\sin(ka+\phi)}{\sin(k_0 a)} \tag{38}$$

implying that for $\sin(k_0 a) \to 0$, the wavefunction inside the well becomes increasingly important respect to the ones outside defining a resonance for $k_0 a = n\pi$ (Fabry-Perot cavity rule), or $E_n = \frac{(n\hbar\pi)^2}{2ma^2} - V_0$

if I put this square well in a box of length L (or infinite potential well), I have an additional boundary condition that is $\psi(\pm L) = 0$, implying

$$\Rightarrow \sin(ka + \phi) = 0 \Rightarrow E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L} + \phi\right)^2. \tag{39}$$

that is not as easy as it seems (remember that ϕ is the solution of a trascendent equation function of k and k_0), but recovers the previous solution for $L >> a$.

Harmonic Oscillator.

The 1 dimensional harmonic oscillator

$$V = \frac{1}{2}m\omega^2 x^2, \tag{40}$$

have solutions with eigenfunctions

$$\psi_n(x) = \frac{1}{\sqrt{2^n\, n!}} \cdot \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \cdot e^{-\frac{m\omega x^2}{2\hbar}} \cdot H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right), \tag{41}$$

with $H_n(x)$ are Hermite polinomials

$$H_n(z) = (-1)^n\ e^{x^2}\frac{d^n}{dx^n}\left(e^{-x^2}\right), \tag{42}$$

and eigenvalues

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \tag{43}$$

with $n = 0, 1, 2, \ldots$ the *quantum number*.

The three dimensional isotropic harmonic oscillator,

$$V = \frac{1}{2}m\omega^2 r^2 \tag{44}$$

is easy to solve considering $r^2 = x^2 + y^2 + z^2$ that gives three independent 1D harmonic oscillators, since the potential is *separable* thus the solution is *factorizable*.

Solving the system in spherical coordinates we use the angular momentum operator $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$. A central potential is separable in central and angular part, since

$$\hat{L}^2|\mathbf{r}\rangle = -\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]|\mathbf{r}\rangle \tag{45}$$

that is proportional to angular part of the Laplace operator Δ, corresponding to the operator part of $\hat{\mathbf{p}}^2$, in spherical coordinates.

$$\Rightarrow \hat{\mathbf{p}}^2 = -\hbar^2\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{\hat{L}^2}{r^2} := \hat{p}_r^2 + \frac{\hat{L}^2}{r^2} \tag{46}$$

Eigenfunctions of $\hat{L}$ are called spherical harmonics that in spherical coordinates are written as $Y_m^l(\theta, \phi)$. $\hat{L}_z|l, m\rangle = \hbar m|l, m\rangle$ and $\hat{L}^2|l, m\rangle = \hbar^2 l(l+1)|l, m\rangle$. In rotationally invariant systems energy cannot depend from L_i. For a given central interaction,

$$\Rightarrow H = \frac{\hat{p}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2} + V(r) \tag{47}$$

we have a system that is separable r and Ω (solid angle), thus its eigensolutions have to be factorized in in eigenfunctions of $\frac{\hat{p}_r^2}{2m} + V(r)$, that we call the *radial part* as $\phi(r)$, and $\frac{\hat{L}^2}{2mr^2}$ that is the *angular part* and are the spherical harmonics.

The solutions for 44 are

$$E_{nl} = \hbar\omega \left(2n + l + \frac{3}{2}\right), \tag{48}$$

and

$$\phi_{kl}(r) = N_{kl} r^l e^{-\nu r^2} L_k^{(l+\frac{1}{2})}(2\nu r^2), \tag{49}$$

with,

$$N_{kl} = \sqrt{\sqrt{\frac{2\nu^3}{\pi}} \frac{2^{k+2l+3}\ k!\ \nu^l}{(2k+2l+1)!!}} \tag{50}$$

with $\nu \equiv \frac{\mu\omega}{2\hbar}$ and ${L_k}^{(l+\frac{1}{2})}(2\nu r^2)$ are generalized Laguerre polynomials, that are the solutions to the above differential equation.

Both Hermite and Laguerre polynomials are a orthonormal basis of the Hilbert space, being complete orthogonal basis for L^2. Consequently **spherical harmonics are a basis of the Hilbert space**.

1.3. Spin and Angular momentum. $SO(3)$ is the group of rotations in 3D space, is the group of unitary orthogonal (det= 1) 3x3 matrices. $SU(2)$ is the group of rotations in 2D space, is the group of unitary *special* (det= 1) 2x2 matrices, also known as the Pauli matrices.

$$\sigma_0 = \mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{51}$$

$\hat{\sigma}$ are the spinor operators for spin 1/2 particles. $\hat{\sigma}, \hat{\mathbf{L}}$, live in different spaces, so $[\hat{\sigma}, \hat{\mathbf{L}}] = 0$. This also means that eigenvectors are factorized $|l, m\rangle \otimes |\pm\rangle$. The two possible state of spins, define a new space called *spinor space*

$$\langle \mathbf{r}|l, m\rangle \otimes |\pm\rangle = \begin{pmatrix} u_{lm}^+(\mathbf{r}) \\ u_{lm}^-(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} \psi^+(\mathbf{r}) \\ \psi^-(\mathbf{r}) \end{pmatrix} Y_m^l(\theta, \phi), \tag{52}$$

this representation of wavefunctions in factorized solutions of $\hat{\mathbf{L}}$ and $\hat{\sigma}$, considering a complete set of operators (commute each others) $\hat{L}_z, \hat{\sigma}_z, \hat{\sigma}^2, \hat{L}^2$ is called LS–coupling.

We can define the *total angular momentum*,

$$\hat{\mathbf{J}} := \hat{\sigma} + \hat{\mathbf{L}}, \tag{53}$$

we have the following set of complete operators, J^2, L^2, σ^2, J_z, which define the J–coupling scheme. Quantum number $|l - s| \leq j \leq l + s$.

1.4. Exercises.

(1) demonstrate Eq. (5) and (6).
(2) demonstrate the Schwartz inequality $|\langle a|b\rangle|^2 \leq ||a||^2 ||b||^2$.

(3) finish problem in Sect. 1.2.2, solving the even cases. Then consider the density current

$$\mathbf{j}(\mathbf{r}) = \frac{\hbar}{2im}[\psi(\mathbf{r})\boldsymbol{\nabla}\psi^*(\mathbf{r}) + \psi^*(\mathbf{r})\boldsymbol{\nabla}\psi(\mathbf{r})], \tag{54}$$

and calculate how the current density behaves inside and outside the potential well.

2. Second Quantization

2.1. The Mathematics of second quantization. We want to describe a relativistic field theory for quantum mechanics. Since in relativity there is no mass conservation, particle number and type is not conserved and has to be defined dinamically. Consequently we will introduce a formalism for many-particle systems called "second quantization"

2.1.1. *Fock Space and symmetries.* Considering Hilbert space $\mathscr{H}$ of one particle system as defined in sect. 1.1.5 we consider the hilbert space relative to A–particle systems as

$$\mathscr{H}_A = \mathscr{H} \otimes \mathscr{H} \otimes \ldots \otimes \mathscr{H} \tag{55}$$

The wavefunctions in this space are $\Phi(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_A)$.

Transposition operator $\hat{P}_{ij}$ which swaps the places of ith and jth particle.

$$\hat{P}_{ij}\Phi(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_A) = \Phi(x_1, \ldots, x_j, \ldots, x_i, \ldots, x_A). \tag{56}$$

$\hat{P}_{ij}$ an Hermitian, and unitary operator, so its an operator which eigenvalues can only be $+1$ or -1. We can then divide the space $\mathscr{H}_A$ in space composed of eigenfunctions of $\hat{P}_{ij}$ with eigenvalues $p_{ij} = \pm 1$, $\mathscr{H}_A^{(\pm)}$, and the one orthogonal to these two.

$$\mathscr{H}_A = \mathscr{H}_A^{(+)} \oplus \mathscr{H}_A^{(-)} \oplus \mathscr{H}_A' \tag{57}$$

Theorem 2 (Spin Statistic theorem). *Particles living in $\mathscr{H}_A^{(+)}$, with $\hat{P}_{ij}\Phi{=}\Phi$, have integer spin and are called bosons;*
particles living in $\mathscr{H}_A^{(-)}$, with $\hat{P}_{ij}\Phi{=}{-}\Phi$, have semi-integer spin and are called fermions.[**2**]

$\mathscr{H}_A'$ is the orthogonal complement, populated by functions that are neither symmetric nor anti-symmetric (irreducibile representation of the permutation group), but and up to now is no experimental evidence indicating a connection with physical wavefunctions.

$$\Psi \in \mathscr{H}_2^{(\pm)} \Rightarrow \Phi(x_1\mu, x_2\nu) = \frac{1}{\sqrt{2}}\left(\phi_\mu(x_{P_1})\phi_\nu(x_2) \pm \phi_\mu(x_2)\phi_\nu(x_1)\right) \tag{58}$$

When constructing the basis of A-particle states in the space $\mathscr{H}_A^{(-)}$ we similarly single-out **antisymmetric** states,

$$\Phi_{\mu_1\ldots\mu_A}(x_1, \ldots, x_A) = (A!)^{-1/2}\sum_P (-1)^P \phi_{\mu_1}(x_{i_1})\ldots\phi_{\mu_A}(x_{i_A}), \tag{59}$$

where P is the permutation of A elements, $\mathrm{P}(1, 2\ldots, A){=}(i_1, i_2, \ldots, i_A)$. The above state is called Slater determinant of single-particle states,

$$\Phi_{\mu_1\ldots\mu_A}(x_1, \ldots, x_A) = (A!)^{-1/2}\begin{vmatrix} \phi_{\mu_1}(x_1) & \phi_{\mu_2}(x_1) & \cdots & \phi_{\mu_A}(x_1) \\ \phi_{\mu_1}(x_2) & \phi_{\mu_2}(x_2) & \cdots & \phi_{\mu_A}(x_2) \\ \cdots & \cdots & \cdots & \cdots \\ \phi_{\mu_1}(x_A) & \phi_{\mu_2}(x_A) & \cdots & \phi_{\mu_A}(x_A) \end{vmatrix}. \tag{60}$$

Fock space

$$\mathcal{F}^{(\pm)} := \mathbb{C} \oplus \mathscr{H} \oplus \mathscr{H}_2^{(\pm)} \oplus \cdots \oplus \mathscr{H}_n^{(\pm)} \oplus \cdots \tag{61}$$

with functions as

$$f \in \mathcal{F}^{(\pm)} = \begin{pmatrix} f_0 & \in \mathbb{C} \\ f_1(\mathbf{r}_1\sigma_1) & \in \mathscr{H} \\ f_2(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) & \in \mathscr{H}_2^{(\pm)} \\ \vdots & \vdots \\ f_n(\mathbf{r}_1\sigma_1, \cdots, \mathbf{r}_n\sigma_n) & \in \mathscr{H}_n^{(\pm)} \\ \vdots & \vdots \end{pmatrix}. \tag{62}$$

Applying the number operator results in

$$\hat{N}\Phi = \begin{pmatrix} 0 \cdot f_0 \\ 1 \cdot f_1(\mathbf{r}_1\sigma_1) \\ 2 \cdot f_2(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) \\ \vdots \\ n \cdot f_n(\mathbf{r}_1\sigma_1, \cdots, \mathbf{r}_n\sigma_n) \\ \vdots \end{pmatrix}. \tag{63}$$

2.1.2. *Creation operators.* We define a creation operator that creates a particle in the antisymmetric Fock space, thus

$$a_\mu^+ \Phi_A(\mu_1, \cdots, \mu_A) := \begin{cases} 0 & \text{for } \mu \in \{\mu_i\}, \\ \Phi_{A+1}(\mu, \mu_1, \cdots, \mu_A) & \text{for } \mu \notin \{\mu_i\}, \end{cases} \tag{64}$$

and the annihilation operator, hermitian conjugate of the constructor, is given by

$$a_\mu \Phi_{A+1}(\mu_1, \cdots, \mu_A + 1) := \begin{cases} 0 & \text{for } \mu \notin \{\mu_i\} \\ (-1)^{i+1}\Phi_A(\mu_1, \cdots, \mu_{i-1}, \mu_{i+1}, \cdots, \mu_{A+1}) & \text{for } \mu = \mu_i \end{cases} \tag{65}$$

In $\mathcal{F}^{(-)}$, in other words for fermions, creation and annihilation rules operator obey this following anticommutation rules

$$\left\{a_\mu^+, a_\nu^+\right\} = 0, \tag{66}$$

$$\{a_\mu, a_\nu\} = 0, \tag{67}$$

$$\left\{a_\mu, a_\nu^+\right\} = \delta_{\mu,\nu}. \tag{68}$$

From these relations follows that $a_\mu^+ a_\mu^+ = 0$, that embed the Pauli principle into the properties of the creation operators.

At this point we can define a *vacuum state* such as

$$a_\mu|0\rangle = 0 \qquad \forall\mu \tag{69}$$

and every state is defined by application of constructor operators

$$|\mu_1 \cdots \mu_A\rangle := a_{\mu_1}^+ \cdots a_{\mu_A}^+|0\rangle \tag{70}$$

which defines an orthonormal set of states, correspondant to the slater determinant wavefunction in Eq. (65).

2.1.3. *Operators in second-quantization.* $\hat{N}_\nu$ gives the number of fermions occupying the ν-th single-particle state,

$$\hat{N} := \sum_\nu a_\nu^+ a_\nu, \tag{71}$$

that is used to define the fermion-number operator:

$$\hat{N}|\mu_1 \dots \mu_A\rangle = A|\mu_1 \dots \mu_A\rangle. \tag{72}$$

THEOREM 3 (Second-quantization representation of operators). *In the second-quantization representation, the K-particle operator is defined by its antisymmetrized matrix elements and has the following form:*

$$\hat{F} = (K!)^{-2} \sum_{\substack{\mu_1 \dots \mu_K \\ \nu_1 \dots \nu_K}} F_{\mu_1 \dots \mu_K \nu_1 \dots \nu_K} a_{\mu_1}^+ \dots a_{\mu_K}^+ a_{\nu_K} \dots a_{\nu_1}, \tag{73}$$

that reduces to the case of one and two body operators to

$$\hat{F} = \sum_{\mu_1 \nu_1} F_{\mu_1 \nu_1} a_{\mu_1}^+ a_{\nu_1}, \tag{74}$$

$$\hat{F} = \frac{1}{4} \sum_{\mu_1 \mu_2 \nu_1 \nu_2} F_{\mu_1 \mu_2 \nu_1 \nu_2} a_{\mu_1}^+ a_{\mu_2}^+ a_{\nu_2} a_{\nu_1}. \tag{75}$$

Creation and destruction operator can also be represented in the Hilbert space (coordinate or momentum), giving the creation or destruction of a particle in a particular position or momentum.

2.1.4. *From first to second–quantized form.* Let's consider a one body operator in the second quantization form, as in Eq. (74), using the field operators as defined in the previous lecture

$$a^+(\mathbf{r}) := \sum_\mu \phi_\mu^*(\mathbf{r}) a_\mu^+, \qquad a(\mathbf{r}) := \sum_\mu \phi_\mu(\mathbf{r}) a_\mu, \tag{76}$$

we can build it from first quantization operator

$$\hat{F} = \sum_{\mu_1 \nu_1} \langle \mu | F | \nu \rangle a_\mu^+ a_\nu = \int \mathrm{d}^3 r a^+(\mathbf{r}) a(\mathbf{r}) F(\mathbf{r}) \tag{77}$$

Implying that densities ($\rho = \sum_i \rho(\mathbf{r} - \mathbf{r}_i)$) in second quantization, at a given coordinate $\mathbf{r}$ are then given by

$$\hat{\rho}(\mathbf{r}) = \hat{a}^+(\mathbf{r}) a(\mathbf{r}) \tag{78}$$

2.2. Wick Theorem. Let's consider a decomposition of A on Ψ such as

$$A = A_0 + A_+ + A_-, \tag{79}$$

with,

$$A_0 \text{ is a constant,} \tag{80}$$

$$A_-|\Psi\rangle = 0, \tag{81}$$

$$\langle \Psi | A_+ = 0. \tag{82}$$

Let then $P{=}|\Psi\rangle\langle\Psi|$ be the operator projecting on the state $|\Psi\rangle$. Thus we get the explicit form of the decomposition (79) that fullfills the rules of (80-82),

$$A_0 = \langle\Psi|A|\Psi\rangle, \tag{83}$$

$$A_- = (A - \langle\Psi|A|\Psi\rangle)\,(1-P), \tag{84}$$

$$A_+ = (1-P)AP, \tag{85}$$

with for any operator A and any state $|\Psi\rangle$.

If we want to calculate the average product of two operators

$$\langle\Psi|AB|\Psi\rangle = \langle\Psi|A|\Psi\rangle\langle\Psi|B|\Psi\rangle + \langle\Psi|A_-B_+|\Psi\rangle, \tag{86}$$

that relates to (anti–)commutator relations,

$$\begin{aligned} \langle\Psi|A_-B_+|\Psi\rangle &= \langle\Psi|\{A_-,B_+\}|\Psi\rangle = \langle\Psi|[A_-,B_+]|\Psi\rangle \\ &= \langle\Psi|\{A_-,B\}|\Psi\rangle = \langle\Psi|[A_-,B]|\Psi\rangle = \cdots \end{aligned} \tag{87}$$

We then define a contraction, and auto–contraction, for fermions as

$$\overbracket{AB} := \{A_-,B\}, \tag{88}$$

$$\overbracket{A} := 0. \tag{89}$$

To be noted that the contractions for bosons are given by commutator and the auto–contraction is a number that gives an important contribution to observables such as the total energy.

THEOREM 4 (Wick's theorem). *If all mutual contractions of pairs of operators in the product are numbers, then the average value of the product of these operators equals the linear combination of products of all possible contractions and auto-contractions.*

$$\overbracket{AD_1D_2\ldots D_kB} := c^k\overbracket{AB}D_1D_2\ldots D_k. \tag{90}$$

2.2.1. *Wick's theorem for Slater determinants.* Owing to anticommutation rules (68), fermion contractions are numbers. Can be build considering the configuration which annhilate the state on the left and right (cf. (80-82)) is called **normal ordering** $N[\cdots]$, and contractions are then defined as

$$\overbracket{AB} = AB - N[AB]. \tag{91}$$

They result in the following values,

$$\overbracket{a_\mu^+ a_\nu} = \sum_{i=1}^{A}\delta_{\mu\mu_i}\delta_{\nu\mu_i}, \tag{92}$$

$$\overbracket{a_\mu a_\nu^+} = \sum_{i=A+1}^{M}\delta_{\mu\mu_i}\delta_{\nu\mu_i}, \tag{93}$$

$$\overbracket{a_\mu^+ a_\nu^+} = \overbracket{a_\mu a_\nu} = 0, \tag{94}$$

while auto–contractions vanish:

$$\overset{\sqcap}{a}{}^{+}_{\mu} = \overset{\sqcap}{a}_{\mu} = 0. \tag{95}$$

This again is for the specific case of *naked* fermions, we will later see that in the case of other creation and annhilation in other systems contractions and autocontractions can have a different outcome, for example in the system with pairing interaction in the Bolgolybov basis (cf. Lecture 6).

2.2.2. *Calculations of matrix elements.* Calculation of one body matrix element over two body states gives,

$$\langle \alpha_1', \alpha_2' | \hat{F} | \alpha_1, \alpha_2 \rangle = \sum_{\mu_1 \mu_2 \nu_1 \nu_2} F_{\mu\nu} \langle 0 | a_{\alpha_2'} a_{\alpha_1'} a_\mu^+ a_\nu a_{\alpha_1}^+ a_{\alpha_2}^+ | 0 \rangle \tag{96}$$

$$= F_{\alpha_1'\alpha_1}\delta_{\alpha_2'\alpha_2} + F_{\alpha_2'\alpha_2}\delta_{\alpha_1'\alpha_1} - F_{\alpha_1'\alpha_2}\delta_{\alpha_2'\alpha_1} - F_{\alpha_2'\alpha_1}\delta_{\alpha_1'\alpha_2}, \tag{97}$$

making use of contractions.

2.3. Exercises.

(1) Prove that the square of a general one–body operator is equal to a sum of one– and two–body operators.
(2) Calculate the matrix elements of a two body operator Eq.(75) between two body states using Wick theorem.
(3) In nuclear physics is sometimes assumed that is possible to approximate the interaction between one nucleon and all other nucleons by a potential $V(\mathbf{r})$. The Schrödinger equation with this potential is then solved, obtaining the eigenstates $\psi_i(\mathbf{r})$ and the corresponding energies ϵ_i. An antisymmetric A–particle wavefunction can be constructed using a Slated determinant,

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_A) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_1(\mathbf{r}_1) & \phi_2(\mathbf{r}_1) & \cdots & \phi_A(\mathbf{r}_1) \\ \phi_1(\mathbf{r}_2) & \phi_2(\mathbf{r}_2) & \cdots & \phi_A(\mathbf{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{r}_A) & \phi_2(\mathbf{r}_A) & \cdots & \phi_A(\mathbf{r}_A) \end{vmatrix}. \tag{98}$$

Verify in the case of $A = 3$ that the Slater determinant is antisymmetric and that the formulation above is normalized. Show also that this implies that two (or more) particles cannot be found at the same place in this space. Note that this properties of a Slater determinant are valid also in the general $A \times A$ case and follow from the general properties of the determinant (as defined by the Leibnitz formula as the sum of possible permutations of the matrix elements with the appropriate phase).

3. The nuclear shell model

Using the second quantization, we can consider a general Hamiltonian,

$$\hat{H} = \hat{T} + \hat{U} + \hat{V}, \tag{99}$$

where T is the kinetic term, U is an eventual one–body potential, and V is a two–body interaction that in second quantization can be written as (cf. sect. 2.1.3),

$$\begin{aligned}\hat{T} &= \sum_{i=1}^{A} t(\mathbf{r}) = \sum_{\mu\nu} t_{\mu\nu} a^\dagger_\mu a_\nu \\ \hat{V} &= \sum_{i<j} V(\mathbf{r}_i, \mathbf{r}_j) = \frac{1}{2}\sum_{i\neq j} V(\mathbf{r}_i, \mathbf{r}_j) \\ &= \frac{1}{2}\sum_{\mu_1\mu_2\nu_1\nu_2} v_{\mu_1\mu_2\nu_1\nu_2} a^\dagger_{\mu_1} a^\dagger_{\mu_2} a_{\nu_2} a_{\nu_1}, \end{aligned} \tag{100}$$

where $v_{\mu_1\mu_2\nu_1\nu_2}$ is the interaction's matrix element between particles 1 and 2 in states μ_i and ν_i,

$$v_{\mu_1\mu_2\nu_1\nu_2} = \langle \mu_1\mu_2 | V | \nu_1\nu_2 \rangle. \tag{101}$$

The eigenstate of the system will be now obtained by finding eigenstates of the Hamiltonian, that is finding those states in which basis the Hamiltonian matrix is diagonal. We just solved many–body physics. Or have we not?

3.1. Two–particle system. The two–particle wavefunction, can be constructed from the slater determinant using a given angular momentum coupling scheme (cf. sect. 1.3). Considering particles coupled to good total angular momentum J, the wavefunction is,

$$\Psi(\alpha_1(1), \alpha_2(2); JM), \tag{102}$$

where α_i are all the quantum numbers relative to a particle, often $\alpha \equiv n, l, j$, (i) the coordinates of particle i, often $(i) \equiv \mathbf{r}_i, \sigma_i$, and J the total angular momentum of the two–particle system and M its projection.

The two–particle wavefunction in J–scheme can be written as,

$$\Psi(\alpha_1(1), \alpha_2(2); JM) = \sum_{m_1,m_2} \langle j_1 m_1, j_2 m_2 | JM \rangle \phi_{j_1 m_1}(1) \phi_{j_2 m_2}(2), \tag{103}$$

where $\langle j_1 m_1, j_2 m_2 | JM \rangle$ is the Clebsch–Gordan coefficient of angular momentum coupling, and ϕ the one–particle wavefunction. Furthermore, the wavefunction Ψ needs to be antsymmetric in the case of identical particles (cf. exercise) by considering the action of the Slater determinant,

$$\begin{aligned}\tilde{\Psi}(\alpha_1(1), \alpha_2(2); JM) &= \sum_{m_1,m_2} \langle j_1 m_1, j_2 m_2 | JM \rangle \begin{vmatrix} \phi_{j_1 m_1}(1) & \phi_{j_2 m_2}(1) \\ \phi_{j_1 m_1}(2) & \phi_{j_2 m_2}(2) \end{vmatrix}, \\ &= \frac{1}{\sqrt{2}} \sum_{m_1,m_2} \langle j_1 m_1, j_2 m_2 | JM \rangle (\phi_{j_1 m_1}(1)\phi_{j_2 m_2}(2) - \phi_{j_1 m_1}(2)\phi_{j_2 m_2}(1)), \\ &= \frac{1}{\sqrt{2}} \left[\Psi(\alpha_1(1), \alpha_2(2); JM) - (-1)^{j_1+j_2-J} \Psi(\alpha_2(1), \alpha_1(2); JM) \right], \end{aligned} \tag{104}$$

using the symmetry properties of the Clebsch–Gordan $\langle j_1 m_1, j_2 m_2 | JM \rangle = (-1)^{j_1+j_2-J} \langle j_2 m_2, j_1 m_1 | JM \rangle$.

Now if we consider the case of two identical particles coupled in the same j–shell $j_1 = j_2$, it follows that with the rest being equal (104) would admit only $J =$ even couplings. This is the case e.g. for ^{18}O: considering an harmonic oscillator + spin orbit basis, the two neutrons after close shell will occupy the $d_{5/2}$ shell; therefore the two neutrons can couple to $J = 0, 2, 4$, with the maximum J is given by occupying $m = \pm 5/2$ and $\pm 3/5$ states. In fact, these $J = 0^+, 2^+, 4^+$ states are the lowest

energy states for ^{18}O. Analogously the same principle can be applied to hole states, e.g. ^{54}Ni has to holes in $f_{7/2}$ shell giving the first excited states with $J = 0, 2, 4, 6$. Being this principle related to the fermion nature of the particle, it holds for both proton and neutron states (and electrons considering atomic levels).

If we consider the case of two different particles in two states of the same j, the wavefunction Ψ will not have be antisymmetrized, therefore all the possible combinations of j will be available obtaining $J = 0, \ldots, 2j$. For example in ^{30}P, the neutron and proton in the $d_{3/2}$ obtaining $J = 0^+, 1^+, 2^+, 3^+$ above a 1^+ ground state.

The energy of the states will be given by the effective interaction between the two nucleons in the different JM configurations, that is, the interaction's matrix elements. A general two–body interaction will contain effective one– and two–body terms. The effective one body terms is obtainable using contraction methods such as Hartree–Fock, and the effective two–body is the residual part left. This effective two–body interaction will act on the two particles in the j–shell determining the energies of the ground and excited states, introducing an energy shift ΔE respect to the eigenenergy of the one–body Hamiltonian. This energy shift is given by the two–body matrix element of the residual interaction,

$$\Delta E(\mu_1\mu_2;\Lambda) = v^{\Lambda}_{\mu_1\mu_2\mu_1\mu_2} = \langle \mu_1\mu_2;\Lambda|V|\mu_1\mu_2;\Lambda\rangle, \tag{105}$$

with μ_i represent the state of the particles and Λ the quantum numbers of the coupled state, and v are the matrix elements of the residual interaction.

3.2. Calculation of two–body matrix elements. To calculate the two body matrix elements of an interaction is possible to use different strategies expanding on different bases. A popular choice to calculate a central interaction is expand it in the complete set of the Legendre polynomial,

$$V\left(|\mathbf{r}_1 - \mathbf{r}_2|\right) = \sum_{l=0}^{\infty} v_l(r_1, r_2) P_l(\cos\theta_{12}), \tag{106}$$

that can be itself written in terms of the spherical harmonics, that are themselves eigenfunctions of the centrifugal term in three dimension (cf. sect. 1.2.2),

$$P_l(\cos\theta_{12}) = \frac{4\pi}{2l+1} \sum_m {Y_m^l}^*(\Omega_1) Y_m^l(\Omega_2), \tag{107}$$

where l corresponds to the angular momentum, Ω to the solid angle. Considering the matrix element between states of good total angular momentum j as in the example is section 3.1, it can be then calculated as

$$v^J_{j_1j_2j_1j_2} = \langle j_1j_2;J|V|j_1j_2;J\rangle = \sum_l \langle j_1j_2;J|v_l(r_1,r_2)\frac{4\pi}{2l+1}\sum_m {Y_m^l}^*(\Omega_1)Y_m^l(\Omega_2)|j_1j_2;J\rangle. \tag{108}$$

Since the radial and the angular part are now partially factorized, can now separate them and as usual the solution will be the product of the factors. The radial part will be given by,

$$F_l = \int \phi^*_{n_1l_1}(r_1)\phi^*_{n_2l_2}(r_1) v_l(r_1,r_2)\phi_{n_1l_1}(r_2)\phi_{n_2l_2}(r_2)\mathrm{d}r_1\mathrm{d}r_2, \tag{109}$$

where $\phi_{n_il_i}(r_i)$ are the radial wavefunctions of the basis, with n and l the principal and angular quantum numbers respectively. A popular choice of basis in nuclear physics is the 3D harmonic oscillator (sect. 1.2.2), but it can as well be a set of wavefunctions obtained after Hartree-Fock calculation to separate one–body and residual effective two–body components.

The expressions for the angular part can be calculated using reduction rules and Wigner-Eckart theorem (cf. [**3**]):

THEOREM 5 (Wigner-Eckart theorem). *The matrix elements of spherical tensor operators can be represent in a part depending on the projection quantum numbers (m), called geometrical part, and an independent part called reduced matrix element, in the following way*

$$\langle \alpha j m_j | T^l_{m_l} | \alpha' j' m'_j \rangle = \langle j' m'_j l m_l | j m_j \rangle \langle j || \hat{T}^l || j' \rangle.$$

The reduced matrix element are convenient because they simplify the sum over m, and to be calculated they often require the application of the Wigner-Eckart theorem.

obtaining in the case of spherically symmetrically basis,

$$f_l = (-1)^{j_1+j_2+J} \frac{4\pi}{2l+1} \left\{ \begin{array}{ccc} j_1 & j_2 & J \\ j_2 & j_1 & l \end{array} \right\} \langle j_1 || \hat{Y}^l || j_1 \rangle \langle j_1 || \hat{Y}^l || j_1 \rangle, \tag{110}$$

where the expression in curly brackets is known as a Wigner $6j$–symbol, and the $\langle \cdot || \bullet || \cdot \rangle$ is the *reduced* matrix element.

If needed, a similar procedure can obtain the exchange component to guarantee antisymmetrization of the matrix elements for identical particles.

4. Many–particle systems

We can now use the interaction diagonalization procedure of the nuclear shell model in cases of many–particles. It is possible to construct a basis of the Fock space using creation operators,

$$\prod_i a_i^\dagger |0\rangle, \qquad \text{or} \qquad \prod_i a_i |0\rangle, \tag{111}$$

this can be seen as filling a vector of states, e.g. $a_3^\dagger a_5^\dagger a_6^\dagger |0\rangle$ can be represented as $|001011\rangle$. Each of these states are normalized and orthogonal. All the possible combinations will then construct a basis for the Fock space. The solution of the many–body problem will be simply given by diagonalizing the Hamiltonian in the space corresponding to the given number of particles. Problem is, the number of possible slater determinants, and two–body matrix elements among them, grows with the number of possible combinations of A identical particles in the space of N states,

$$D = \left(\begin{array}{c} N \\ A \end{array} \right), \tag{112}$$

which grows exponentially with the growth of the basis and number of particles as represented in Fig. 1. Therefore, the shell model for many particles (also equivalent to Configuration Interaction) has limits in solving systems with many particles and large model spaces. To overcome the limitations in number of particles and possible number of states, the nuclear shell model often reduces the model space to few states around magic shell closure, the valence space. This is done using an effective interaction for the specific model space.

Another approach is to use the power of massive computing to treat light systems, as described in the example in the following section.

4.1. Modern Applications.

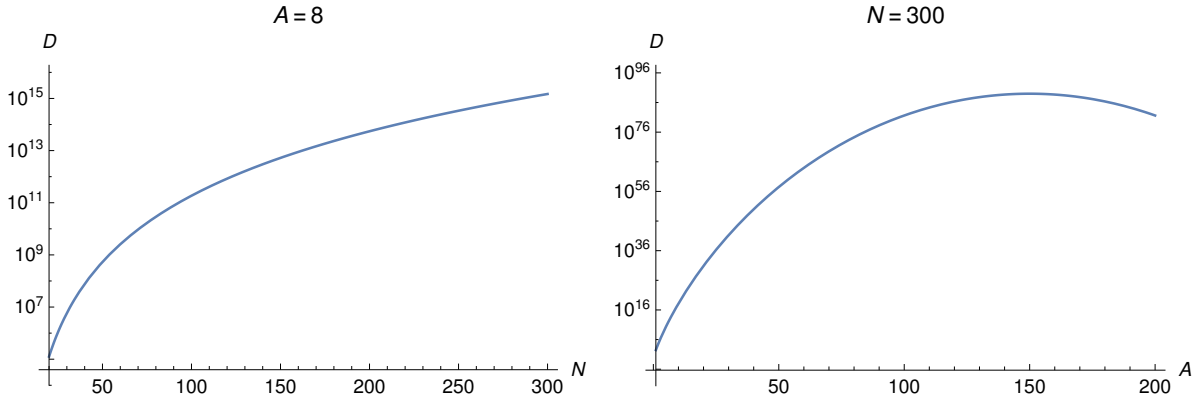

FIGURE 1. Size of the Fock space D

4.1.1. *Deuteron wavefunction and fusion reactors.* Thermonuclear reaction are crucial to understand many phenomena ranging from the modeling of the big-bang, stellar burning to the exploration of nuclear fusion as a terrestrial source of energy. In particular the fusion of a deuteron (^{2}H, or d) with a triton (^{3}H, or t),

$$d + t \rightarrow {}^4\text{He} + n + 17.6 \text{ MeV},$$

is of the most viable avenues for nuclear fusion, pursued at facilities such as ITER and NIF. Calculating a predicting the properties and cross section of such a reaction in the different configuration of initial and final states is therefore important to understand the best efficiency reachable by fusion reactors.

The deuteron is a two–particle systems. It's wavefunction is similar to the prescriptions defined in sect. 3.1, with the addition of the isospin quantum number discussed in Lecture 2. The deuteron has a spin triplet $S = 1$ isospin singlet $T = 0$ ground state. Since both nn and pp interactions are repulsive (there is no bound diproton or dineutron), matrix element (and therefore the correction to the independent particle binding energy) for the $T = 1, T_z = \pm 1$ state are positive and the $T = 1$ state is less bound than the $T = 0$ state. Since the ground state is $T = 0$, the antisymmetrization will imply,

$$|T = 0\rangle = \frac{1}{\sqrt{2}}(|pn\rangle - |np\rangle). \tag{113}$$

The rest of the properties of the ground state depends on details of the interaction and which matrix elements are more attractive or repulsive. In fact, studying the deuteron is one crucial way to gain information about the properties of the two-body sector of the nucleon-nucleon interaction. It is observed that the ground state of the deuteron is a 1^+, with $S = 1$ and a mixture of $L = 0$ and $L = 2$ [**4**], which gives an information about an important aspect of the nuclear interaction: the tensor force, binding states of different spin.

The properties of the deuteron have been thoroughly investigated, but research is still actively ongoing on the study of low–energy fusion. In particular a question regarding fusion technology is if efficiency can be improved by polarizing deuteron and tritium isotopes. Tritium is a spin 1/2 state, and is polarization implies only alignment on the reaction symmetry axis. But since the deuteron is in a spin $S = 1$ state, it can be polarized to $S_z = \pm 1$ or 0. This polarized state are difficult to study experimentally, but could be an important design feature in future fusion reactors if the spin alignment implies an increased efficiency greater than the energy necessary for the polarization.

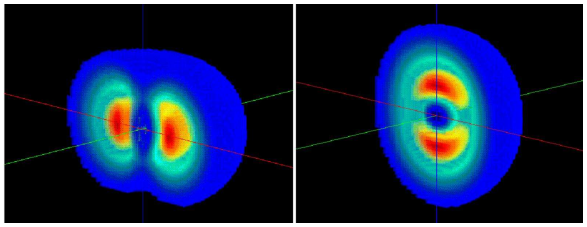

FIGURE 2. Deuteron wavefunction in $M = 0$ and $M = 1$ substate of the 1^+ ground state, from [**4**].

The state–of–the–art calculation [**5**] is very sophisticated in order to include effects of coupling to the continuum and the dynamics of reactions (cf. Lecture 8), but the basic concept of deuteron and tritium wavefunction are based on the few–particle shell model that we have seen in this lecture. This study finds that: "the reaction rate increases by about 32 % compared to the unpolarized one and, further, the same reaction rate as the unpolarized one can be achieved at $\tilde{4}5$ % lower temperature", therefore giving strong indication of the advantages of polarizing reactant in future nuclear fusion reactors.

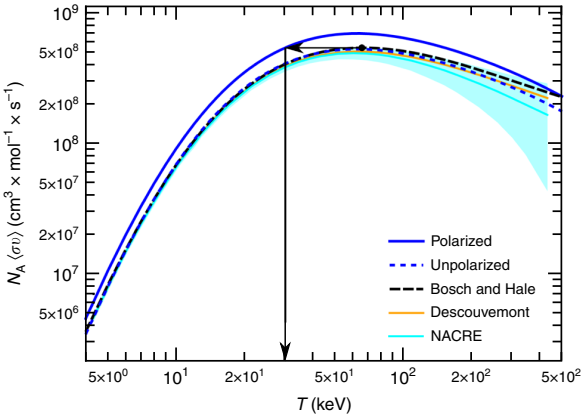

FIGURE 3. From [**5**].

4.1.2. *Nuclear transitions, Urca process and supernovae.* The shell model approach is useful to have a compact and effective description of many–nucleons systems, by considering effective interaction in a valence space. A recent work uses the description of beta–decay to shed light on the fate of dying stars [**6**]. As nuclei are fused in the core of the star, the most stable isotopes are produced in the core of the star accumulating an inert iron core. This iron core is held together against the gravitational pressure by the energy of the Pauli principle, accumulating electrons in states of higher and higher energy and forming the "electron degeneracy pressure". Once the energy of the electron state is greater than its mass and compensates for the neutron–proton mass difference and binding energy, it would be energetically favorable to capture the electron in the nucleus a undergo an inverse beta decay process. Once the depletion of electron starts, the pressure will decrease favouring a collapse of the iron core that in turn will favour electron capture, determining a catastrophic stellar process known as supernova.

The reaction rate of the electron capture transition will influence the process, and it can be calculated using the nuclear shell model and the concepts of this lecture. An interesting case is ${}^{20}_{10}\mathrm{Ne}_{10}$. With 2 protons and 2 neutrons has 2 particles above the ${}^{16}\mathrm{O}$ doubly magic close shell. ${}^{20}_{9}\mathrm{F}_{11}$ is the neighbour. The states of both nuclei can be calculated using the nuclear shell model and USDB (universal *sd* type b) effective interaction between nucleons in the *sd* valence space [**7**] and diagonalizing it in the small space of 4 particles in 3 states.

The beta decay transition ${}^{20}\mathrm{F}\to {}^{20}\mathrm{Ne}+e^- +\bar{\nu}_e$ is then guided by the Gamow–Teller matrix element,

$$\langle {}^{20}\mathrm{Ne}(0^+)|G_A\hat{\sigma}\hat{\tau}|{}^{20}\mathrm{F}(0^+)\rangle, \tag{114}$$

where G_A is the axial coupling constant that defines the interaction. This process is naturally occurring in the lab and nature with an half-life of $16s$. The inverse process can happen if the electron pressure is high enough, such as in the dense environment of the onset of supernova.

In the case the temperature is high enough, it might trigger the so–called Urca process. Named after a casino (*cassino de Urca* in Rio de Jainero) because it depletes the supernova of energy as fast as a casino depletes the money of its patrons, it consists of a rapid cycle of electron–capture and β–decay, that generates a vast amount of neutrinos that are the main cooling source of a supernova.

The delicate balance of heat, density pressure, electron capture and beta decay transition rates, determines the destiny of stars. That is, if they undergo supernova leaving a neutron star or black hole remnant, or end their life in a thermonuclear explosion, shedding the exterior layers and leaving the electron–degenerate core behind in the form of white dwarf.

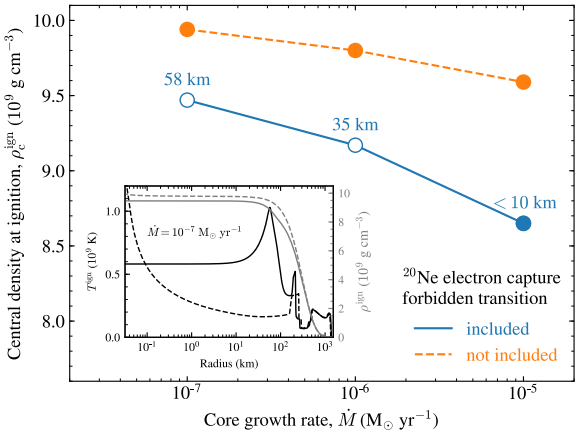

FIGURE 4. From [**6**].

4.2. Exercises.

(1) Predict the level scheme of the first excitations of ${}^{50}\mathrm{Ti}$ and ${}^{14}\mathrm{N}$ and compare them to experiment on `https://www.nndc.bnl.gov/`.

(2) Derive Eq. (110) from Wigner-Eckart theorem and the rules of angular momentum coupling.

LECTURE 11

Green's function formalism

Green's functions are a powerful tool to solve differential equations, and have been extensively used to investigate the properties of interacting many–body systems. Considering an arbitrary linear differential equation,

$$\hat{L}\phi(x) = f(x), \tag{115}$$

where $\hat{L}$ is the differential operator relating the *field* $\phi(x)$ to the *source* $f(x)$. This differential equation can be solved considering the solution to a point–like source $\delta(x)$,

$$\hat{L}G(x, x') = \delta(x - x'), \tag{116}$$

$G(x, x')$ is a particular solution to the differential operator $\hat{L}$ that is called Green's function, and assumes the role of a distribution that can be applied to the source term to obtain the solution

$$\phi(x) = \int G(x, x')f(x')\mathrm{d}x', \tag{117}$$

in an analogous way to the way the δ distribution acts on a function. The Green's function can be then considered a inverse in the sense of the distribution to the differential operator $\hat{L}$. In the case we consider as differential operator $\hat{L}$ an Hamiltonian of a many–particle system and consider the differential equation as the Schroedinger equation, we get the analogous many–body Green's functions.

We will not prove the analogy, but for this reason Green's functions are a useful tool for a systematic perturbative treatment of many–particle systems. The Green's function is a useful representation of the state of a particles and physical processes mainly affecting that state. Techniques of interacting Green's function can be used to perturbatively calculate the solution to the Schroedinger equation to the potentially exact solution.

We derive the Green's function from the formalism of second-quantization (cf. Sect. 2). Field operators $\widehat{\psi}_m(\mathbf{x}, t)$ are a set of creation (and annihilation) operators weighted over the possible single-particle wavefunctions,

$$\widehat{\psi}_m(\mathbf{x}, t) = \sum_i \psi_{m,i}(\mathbf{x}, t)a_i, \tag{118}$$

where a_i is the annihilator operator over a basis $\{i\}$, and $\psi_{m,i}(\mathbf{x}, t)$ the single time–dependent wave-function characterized by a set of quantum numbers m represented over that basis.

In other words in a system described in the $\mathcal{H}_\pm(N)$ (or $\mathcal{F}_\pm$) space, considering an Hamiltionan H and the corresponding ground state $|\psi_0\rangle$, the field operator (that is eventually a vector field of m components, e.g. the spin $\pm$ of fermions) create (and annihilate) particles. This is the description of the Hamiltonian itself, in the second quantization representation.

With this prescription, we can define the Green's function corresponding to this interacting system as,

$$iG_{m,m'}(\mathbf{x}t,\mathbf{x}'t') = \langle\psi_0|\mathcal{T}[\widehat{\psi}_{Hm}(\mathbf{x},t)\widehat{\psi}^{\dagger}_{Hm'}(\mathbf{x}',t')]|\psi_0\rangle, \tag{119}$$

where the subscript H stands for Heisenberg representation of the time–dependence,

$$\psi_{Hm}(\mathbf{x},t) = e^{iHt/\hbar}\psi_m(\mathbf{x})e^{-iHt/\hbar}, \tag{120}$$

with H the Hamiltonian, and $\mathcal{T}[...]$ is the time ordering product.

The Green's function description comes useful in many ways. Considering the properties of the second-quantization representation the expectation value of any single-particle operator is bracketed over a creation and an annihilation field operators and so the Green's function becomes a natural way to consider the expectation value of a single-particle operator in the ground state of the system, and therefore

The one particle Green's function has all the information of the ground state of a single-particle Hamiltonian; being the expectation value of the field in the ground state for a given $\mathbf{x}t,\mathbf{x}'t'$ it makes it possible to calculate the expectation value of every single-particle operator that is, in II^{nd} quantization, a linear combination of one-creator and one-annihilator operators. Green's functions are like field-testing on a given spacetime interval during which they perturb the "vacuum" of the ground state.

With the explicit time ordering, the Green's function becomes

$$\begin{aligned} iG_{m,m'}(\mathbf{x}t,\mathbf{x}'t') = &\langle\psi_0|\widehat{\psi}_{Hm}(\mathbf{x},t)\widehat{\psi}^{\dagger}_{Hm'}(\mathbf{x}',t')|\psi_0\rangle\Theta(t-t') \\ &\pm\langle\psi_0|\widehat{\psi}^{\dagger}_{Hm'}(\mathbf{x}',t')\widehat{\psi}_{Hm}(\mathbf{x},t)|\psi_0\rangle\Theta(t'-t), \end{aligned} \tag{121}$$

where the $\pm$ sign is consequence of the Hilbert (Fock) space chosen to be symmetrical or anti-symmetrical, in order to describe bosons or fermions. These two components of the Green's function, are also known as the "retarded" and "advanced" part and sometimes used independently to describe the time evolution of the system. But here we will consider the full time–ordered Green's function. Time dependence can be written explicitly in the Heisenberg representation (120) and so remembering that $|\psi_0\rangle$ is an eigenstate of the Hamiltonian it follows that $e^{-\frac{i}{\hbar}Ht'}|\psi_0\rangle = e^{-\frac{i}{\hbar}\omega_0 t'}|\psi_0\rangle$ with $\hbar\omega_0$ eigenvalue energy of the ground state, and can be carried out of the the bracket since is a number.

$$\begin{aligned} iG_{m,m'}(\mathbf{x}t,\mathbf{x}'t') =&e^{i\omega_0(t-t')}\langle\psi_0|\widehat{\psi}_m(\mathbf{x})e^{-\frac{i}{\hbar}H(t-t')}\widehat{\psi}^{\dagger}_{m'}(\mathbf{x}')|\psi_0\rangle\Theta(t-t')\pm \\ &e^{i\omega_0(t'-t)}\langle\psi_0|\widehat{\psi}^{\dagger}_{m'}(\mathbf{x}')e^{-\frac{i}{\hbar}H(t'-t)}\widehat{\psi}_m(\mathbf{x})|\psi_0\rangle\Theta(t'-t), \end{aligned} \tag{122}$$

introducing a resolution of identity summing over all the possible excited states, $\sum_n|\psi_n\rangle\langle\psi_n|$,

$$\begin{aligned} iG_{m,m'}(\mathbf{x}t,\mathbf{x}'t') =&\sum_n e^{i\omega_0(t-t')}\langle\psi_0|\widehat{\psi}_m(\mathbf{x})e^{-\frac{i}{\hbar}H(t-t')}|\psi_n\rangle\langle\psi_n|\widehat{\psi}^{\dagger}_{m'}(\mathbf{x}')|\psi_0\rangle\Theta(t-t')\pm \\ &\sum_{n'} e^{i\omega_0(t'-t)}\langle\psi_0|\widehat{\psi}^{\dagger}_{m'}(\mathbf{x}')e^{-\frac{i}{\hbar}H(t'-t)}|\psi_{n'}\rangle\langle\psi_{n'}|\widehat{\psi}_m(\mathbf{x})|\psi_0\rangle\Theta(t'-t) = \\ =&\sum_n e^{i\omega_0(t-t')}e^{-i\omega_n(t-t')}\langle\psi_0|\widehat{\psi}_m(\mathbf{x})|\psi_n\rangle\langle\psi_n|\widehat{\psi}^{\dagger}_{m'}(\mathbf{x}')|\psi_0\rangle\Theta(t-t')\pm \\ &\sum_n e^{i\omega_0(t'-t)}e^{-i\omega_n(t'-t)}\langle\psi_0|\widehat{\psi}^{\dagger}_{m'}(\mathbf{x}')|\psi_{n'}\rangle\langle\psi_{n'}|\widehat{\psi}_m(\mathbf{x})|\psi_0\rangle\Theta(t'-t), \end{aligned} \tag{123}$$

which yields,

$$iG_{m,m'}(\mathbf{x}t,\mathbf{x}'t') = \sum_n e^{i(\omega_0-\omega_n)(t-t')}\langle\psi_0|\widehat{\psi}_m(\mathbf{x})|\psi_n\rangle\langle\psi_n|\widehat{\psi}^\dagger_{m'}(\mathbf{x}')|\psi_0\rangle\Theta(t-t')\pm$$
$$\sum_{n'} e^{i(\omega_0-\omega_n)(t'-t)}\langle\psi_0|\widehat{\psi}^\dagger_{m'}(\mathbf{x}')|\psi_{n'}\rangle\langle\psi_{n'}|\widehat{\psi}_m(\mathbf{x})|\psi_0\rangle\Theta(t'-t), \tag{124}$$

that contains explicitly the $t-t'$ exponential. Since $\langle\psi_0|\widehat{\psi}_m|\psi_n\rangle$ must be non-zero for the first term, $|\psi_n\rangle$ is the state corresponding to the system with $N+1$ particles due to the destructor operator between the ground state and the intermediate state. The same happens for the second term, where $|\psi_{n'}\rangle$ must represent the system with $N-1$ particles in order to have the matrix element $\langle\psi_0|\widehat{\psi}^\dagger_{m'}|n'\rangle$ non-zero. ω_0 represents the energy frequency associated to the ground state $|\psi_0\rangle$ with N particles, while ω_n and $\omega_{n'}$ represent the energy frequency of the intermediate excited states $|\psi_n\rangle$ and $|\psi_{n'}\rangle$, with $N+1$ and $N-1$ particles respectively.

We can now consider the Fourier transform of the Green function, to recover a time–independent and frequency–dependent formulation. The matrix elements are time–independent and therefore are $\mathbb{C}$–numbers for the purpose of the Fourier transform. So keeping into account the Fourier transform of the imaginary exponential and the Heaviside theta [1], the frequency representation of the Green's function, we have to

$$\mathcal{F}[G_{m,m'}(\mathbf{x}t,\mathbf{x}'t')] = G_{m,m'}(\omega) = \lim_{\eta\to 0}\sum_n \frac{\langle\psi_0|\widehat{\psi}_m|n\rangle\langle n|\widehat{\psi}^\dagger_{m'}|\psi_0\rangle}{\omega-(\omega_n-\omega_0)+i\eta} \pm \sum_{n'}\frac{\langle\psi_0|\widehat{\psi}^\dagger_{m'}|n'\rangle\langle n'|\widehat{\psi}_m|\psi_0\rangle}{\omega+(\omega_{n'}-\omega_0)-i\eta}. \tag{125}$$

In the following we will omit the limit for simplicity. The denominator can be rewritten considering $\omega_n(N+1)-\omega_0(N) = \omega_n(N+1)-\omega_0(N+1)+\omega_0(N+1)-\omega_0(N)$, that becomes $\epsilon_n+\epsilon_F$, where $\omega_0(N+1)-\omega_0(N)$ the minimum energy required to add a particle to the N particle system, known as Fermi energy (ϵ_F) or chemical potential (μ); while $\omega_n(N+1)-\omega_0(N+1)$ the excitation energy of the $N+1$ particle system, that are the single-particle excitations states. Doing this substitutions analogously for the excitations of the $N-1$ system in the second term, we obtain the denominator as $\epsilon_{n'}-\epsilon_F$, with $\epsilon_{n'}$ as the single–hole states. Finally, we obtain the so-called **Källén–Lehmann representation** of Green's functions,

$$G_{m,m'}(\omega) = V\sum_n \frac{\langle\psi_0|\widehat{\psi}_m|n\rangle\langle n|\widehat{\psi}^\dagger_{m'}|\psi_0\rangle}{\omega-\epsilon_F-\epsilon_n+i\eta} + \sum_{n'}\frac{\langle\psi_0|\widehat{\psi}^\dagger_{m'}|n'\rangle\langle n'|\widehat{\psi}_m|\psi_0\rangle}{\omega-\epsilon_F+\epsilon_{n'}-i\eta}, \tag{126}$$

where $\sum_n$ runs over the particles and $\sum_{n'}$ over the hole states.

[1] We recall that the transform of the $\theta(t)$,

$$\theta(\omega) = \int_{-\infty}^{\infty} e^{i\omega t}\theta(t)\mathrm{d}t = \int_0^\infty e^{i\omega t}\mathrm{d}t = \frac{1}{i\omega} \qquad \text{for } \omega\neq 0,$$

that can be also be derived considering the Heaviside theta as the antiderivative of the Dirac delta. However, for $\omega=0$ the integral does not evaluate to a finite value. Therefore, the solution is usually to regularize the expression by introducing an imaginary frequency η and taking the limit for it to go to zero,

$$\theta(\omega) = \lim_{\eta\to 0}\int_0^\infty e^{i\omega t-\eta t}\mathrm{d}t = \lim_{\eta\to 0}\frac{-i}{\omega+i\eta}.$$

The Green's functions are conveniently represented in the Källén–Lehmann representation also because they can be associated to particle lines in Feynman diagrams, allowing to think diagrammatically, thus representing perturbation processes and interactions in an intuitive and graphical way.

1. Green's function and Feynman diagrams

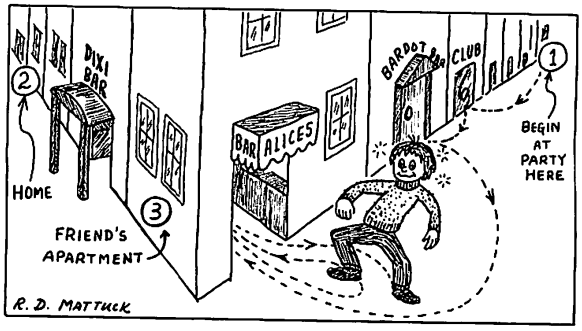

FIGURE 1. The propagator of a Drunken Man. From [**8**].

Feynman Diagrams enable us to think about processes in many–body systems using a compact and graphical representation. For a comprehensive treatment of Feynman diagrams in many-body physics cf. [**8, 9**]. The propagators and related diagrams can be written also about classical processes without loss of generality. For example, to describe the trajectory of the drunken man in Fig. 1 and the probability for him to come home, we can consider all his possible trajectories weighted with the respective probabilities. That is, the probability of going from 1 (bar) to 2 (home) $P(2,1)$ is given by the sum of the probability of all the possible trajectories that go directly $P_0(2,1)$ or by stopping in bars $A, B \ldots$,

$$\begin{aligned} P(2,1) =& P_0(2,1) + P_0(2,A)P(A)P_0(A,1) + P_0(2,B)P(B)P_0(B,1) \\ &+ P_0(2,B)P_0(B)P_0(B,A)P(A)P_0(A,1) + \ldots \ , \end{aligned}$$

and this can be represented in graphical form as in Fig. 2. The direct trajectories P_0 are referred to as "bare" propagators and this operation of considering all possible trajectories and related probabilities is referred to as "dressing" or "renormalization" of the bare properties.

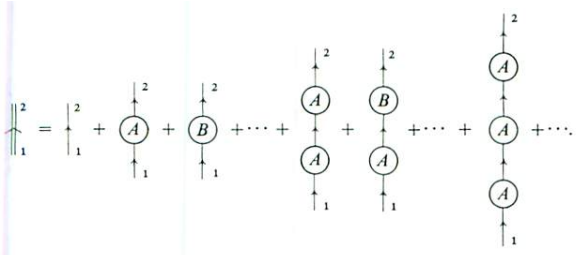

FIGURE 2. The propagator of a Drunken Man. From [**8**].

The main difference between this classical propagator and the quantum propagator we are interested in, stems from the fact that classical probabilities are real values, but in quantum mechanics

probabilities are amplitudes in the complex fields. Therefore, probabilities amplitudes do not simply multiply but also interfere.

In order to familiarize with the Feynman diagrams representations and prescriptions, we can consider the case of a system of free-fermions. In this case the Green's function G^0 of a one–body Hamiltonian H_0,

$$H_0 = \sum_\nu \epsilon^0_\nu a^\dagger_\nu a_\nu, \tag{127}$$

where ϵ^0_ν are the single–particle energies of the one–body Hamiltonian, for example in the case of the free particle $\frac{k^2_\nu}{2m}$. The solution of this Hamiltonian generates the following Green's function in the Lehmann representation (126),

$$G^0(\nu,\omega) = \sum_\mu \frac{1}{\omega - \epsilon^0_\mu + i\eta} + \frac{1}{\omega + \epsilon^0_\mu - i\eta}, \tag{128}$$

where G^0 and is defined as the "bare" Green's function that is a pure one–particle object. In the following, since we start from these diagonal elements of the Hamiltonian, we will consider particles interacting locally. That is, the general $G_{m,m'}(\omega)$ in 126 will be simplified as $G(\nu,\omega)$ for simplicity. To note that this is not the general case, and for a general Hamiltonian both indexes have to be carried on in the formalism (e.g. HFB).

Adding a two–body interaction in the Hamiltonian, makes it possible for the "bare" particle G^0 to interact with other particles and be "dressed" by the possible processes that can influence the wavefunction of the particle. The interaction can be in turn "bare" one, like the the Coulomb interaction between charged particles (e.g. electrons in metal) or the nucleon–nucleon interaction, or an "effective" one that acts within the medium (e.g. the Skyrme interaction in nuclei). Introducing the interaction between the particles, several processes that define the propagator of the particle i can now take place. Since we are calculating the dressed propagator of the particle i, we have to consider the possible . The propagator of these processes can be calculated with the help of Feynman rules, that relate individual propagators with each other. Feynman rules are derived from the field/second quantization explicit description of the bare propagator and processes [].

At the lowest order, there are three possible contributions:

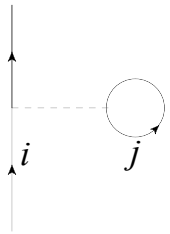

FIGURE 3. This diagram represents the interaction of the bare particle $G^0(i)$ with an average distribution of the other particles, that, in this language, is represented by the loop of $G^0(j)$.

(1) The bare particle can interact with the average density of particles in the background once the interaction is considered. The propagator of this process in Fig. 3 is particularly useful to illustrate Feynman rules and given by,

$$
\begin{array}{ccccccc}
iG^0(k) & (-i) & (-1) & \sum_{spin}\int \frac{d_4k'}{(2\pi)^4}\langle k,k'|v|k,k'\rangle & iG^0(k') & iG^0(k) \\
\text{I particle line} & \text{I interaction line} & \text{I loop} & \text{interaction I part. lines w loop} & \text{loop part line} & \text{II part line}
\end{array}
\tag{129}
$$

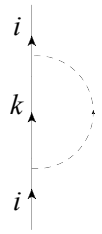

FIGURE 4. This diagram represents the bare particle i that interacts by changing in an intermediate state k.

(2) Another possible process of the same order (1 particle line, 1 interaction line) and has initial and final state i is the change of the particle to an intermediate state k by the means of the interaction v. The corresponding diagram in Fig. 4 and its contribution is then given by,

$$
iG^0(k)(-1)\sum_{spin}\int \frac{d_4k'}{(2\pi)^4}\langle k',k|v|k,k'\rangle iG^0(k')iG^0(k), \tag{130}
$$

the difference with 1) is that the interaction v brings $i \to k$ and vice versa. This contribution coming from the bare interaction and is intimately related to the Pauli principle. This relation can be seen noticing that the diagram above (Fig. 4)is equivalent topologically with Fig. 6(a). That is, the Pauli exchange between the antisymmetrized state of a particle i and another one in the same state i coming from a virtual particle-hole excitation of the vacuum (Fig. 6(b)).

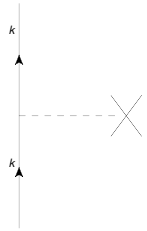

FIGURE 5. This diagram represent the interaction with a one body (external) mean field.

(3) Finally, in the case the interaction has a one–body component $\widetilde{U}$, instead of the interacting with another particle, the particle can also interact with the field $\widetilde{U}$. Therefore, instead of integrating along the dummy variable k' there is a definite matrix element,

$$
iG^0(k)\langle k|\widetilde{U}|k\rangle iG^0(k). \tag{131}
$$

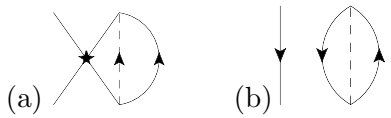

FIGURE 6. Topological equivalent of Fig. 4 (left) that comes from the exchange of hole line k with anothe one in the vacuum excitation (right).

These three contributions are taken into account in the Hartree Fock approximation: the first one, that average the contributions from all the particles k', is called Hartree term. The second one that considers the Pauli exchange principle and the anti-simmetrization of the wavefunctions, is the Fock term. The third one is an (eventual) external one body correction (eg. background of Jellium). This approach, making use of the one body Green's functions, approximate the two body interaction v with a one body mean field, in a way equivalent to other Hartree-Fock (plus eventually external field) formulations.

2. Dressed Green's function and Dyson equation

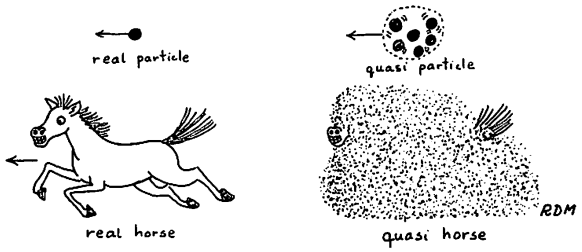

FIGURE 7. Quasiparticle and quasihorse concepts. From [**8**].

Direct nucleon-nucleon interaction, in the form of "bare" (same as vacuum) or "effective" (fitted to reproduce experimental results in finite nuclei) force, is not the only mean for a particle to interact with another one, or itself. A nucleon can interact not only via an interaction but also making use of other degrees of freedom of the system, namely collective states. In other words building block of the coupling in Feynman diagrams are vertexes, there can be particle-interaction vertexes, linking nucleons with the corresponding interaction, but also particle-vibration ones where nucleons scatters exciting or reabsorbing a vibration of the system.

The collective excitations of the system can be calculated with various methods, one of the most used in nuclear structure theory is (Quasiparticle) Random Phase Approximation, (Q)RPA. This framework consider all the correlated particle-hole excitations in order to represents the dynamical deformation of the system. This can be perturbatevly represented with Feynman diagrams as in Fig. 8. The treatment of QRPA is out of the aim of the present work, but many comprehensive studies can be found in literature [**10**].

In other words, for a given multipolarity λ, parity π (e.g. a 2^+ state, representing the quadrupolar vibration of the system), the phonons spectrum $\omega_{\lambda^\pi_\nu}$ is calculated within (Q)RPA framework. The spectrum is then used to determine the "bare" phonon's Green's function that, considering its boson

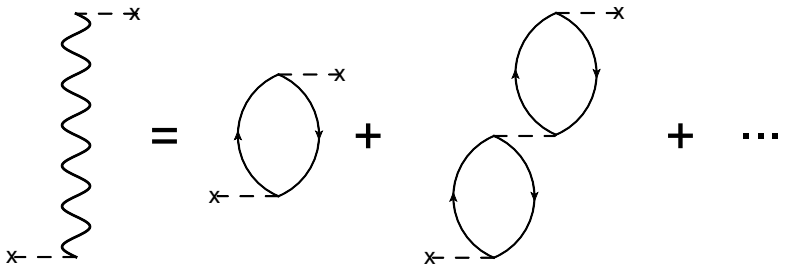

FIGURE 8. Phonons arise from correlated particle-hole excitations in the RPA framework here represented diagrammatically.

nature, is

$$D^0_{\lambda^\pi}(\omega) = \sum_n \frac{1}{\omega - \omega_{\lambda^\pi\, n} + i\delta} - \frac{1}{\omega + \omega_{\lambda^\pi\, n} - i\delta}, \tag{132}$$

that is symmetric respect to ω ($D^0_{\lambda^\pi}(\omega) = D^0_{\lambda^\pi}(-\omega)$).

Now we will use the phonon propagator and the particle propagator to construct a theory of particle–phonon propagation at infinite order, using Green's functions. The Feynman element necessary is the particle–phonon coupling vertex in Fig. 1,

$$h(ij;\lambda^\pi_\nu) = \langle \lambda^\pi_\nu | k_{\lambda^\pi} a^\dagger_{\lambda^\pi_\nu} | 0 \rangle \langle j | F^\dagger_{\lambda^\pi_\nu} | i \rangle, \tag{133}$$

where $\hat{F}$ couples states i and j and $a^\dagger_{\lambda^\pi_\nu}$ creates a phonon ν with a given multipolarity λ and parity π. This vertex and the nature of operators $\hat{F}$ and a, can be calculated in several ways. Consistently using RPA with the residual two–body interaction, or phenomenologically coupling in the collective vibrating potential model (cf. App. A, and [**10**] chapt. 4).

2.1. Dyson equation. After having illustrated the particle-phonon coupling matrix-element/vertex we have to consider its contributions to the renormalization of particle properties. The only process that can give contribution combining particle and phonon Green's functions G and D^0, from whose treated in section 1, is the rainbow type, similar to the one in Fig. 4. The equivalent to the process in Fig. 3 cannot take place because, in order to have momentum conservation, the loop vertex need a $q = 0$ phonon that is a zero-energy phonon (dispersion relation for acustic phonons $\omega(k) \sim 2\omega_0 \sin(ka)$).

A very convenient way to go beyond the first order in perturbation theory, in order to take into account many type of processes, is grouping similar type of contribution and let the presence of the dressed Green function iterate diagrams of the same type. For example in Fig. 9 the "dressed" Green's function G receives contributions from the "rainbow type" diagrams at the first (first contribution), second (from the second to the fourth contribution) and the latter is one of the third order in perturbation theory. This renormalization processes considered in Fig. 9 can be represented making use of the dressed Green's function itself: if G is as represented in Fig. 9, one can see that the second order of perturbation is given by the first order rainbow applied over (or after) itself, the third order is given by the first order rainbow applied over (or after) the second order contributions, and so on. This suggests that the series can be written making use of the building block in Fig. 10, defined to be the "proper Self-Energy" Σ^* ($D^0(\omega - \omega')$ is chosen to have ω as the total energy of the self energy process). The diagram in Fig. 10, is called *skeleton* diagram, and it includes all the *reducible* contributions of this type of diagram. That is, consecutive and nested iteration of the same diagrammatic configuration as

in Fig. 9. This can be understood also in terms of Graph theory, and the Dyson equation includes all *simply connected* types of graphs.

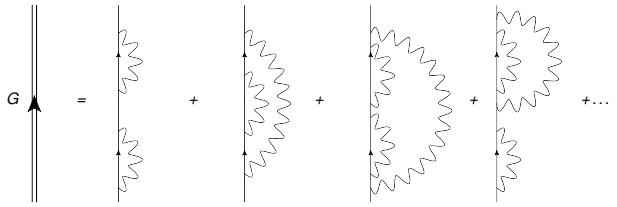

FIGURE 9. Dressed Green's Function G is given by the unperturbed G^0 perturbed by the sum of self energy processes. The self energy processes considered in the Dyson equation are the ones of the so-called "rainbow series", so the ones involving Σ- (self-interaction)-type of diagrams.

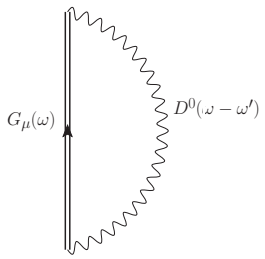

FIGURE 10. Feynman representation of the proper self energy considered, building block of the Dyson equation (Fig. 12), made by the dressed Green's function G and the unpertubed phonon D^0.

However, not all the possible second order diagrams are included in Fig. 9. The diagram in Fig. 11 is missing. These types of crossing-lines diagrams at all orders are neglected in this approximation. Therefore, we can see the iteration of the Dyson equation not as an order–by–order expansion, as in many–body perturbation theory, but as process–by–process.

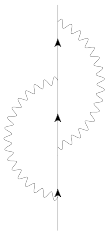

FIGURE 11. This type of diagrams are not included in the Dyson equation treatment. Eventually can be added as *vertex correction*.

This finally leads to the Dyson equation (cf. Fig. 12), which reads

$$G = G^0 + G^0 \Sigma^* G, \tag{134}$$

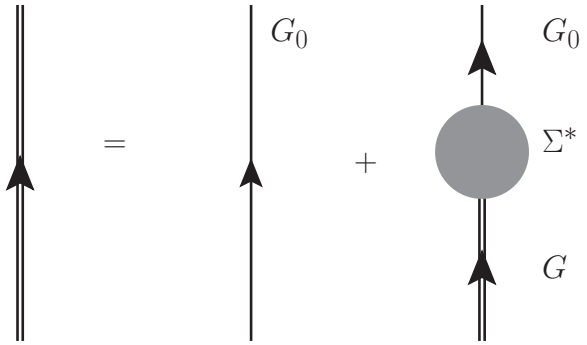

FIGURE 12. Representation of the Dyson equation, that, considering as the proper Self Energy Σ^* the one in Fig. 10, is a compact and efficient way to write the expansion 9.

making use of a self-consistency of dressed G in order to take into account infinite order of perturbation. Dyson equation in the form (134) can be multiplied on the right by G^{-1} giving

$$1 = G^{-1}G^0 + G^0\Sigma^*, \tag{135}$$

and then multiplied on the left by $(G^0)^{-1}$ giving the more compact writing

$$G^{-1} = G^0)^{-1} - \Sigma^*. \tag{136}$$

2.2. Self energy calculation. We proceed with the calculation of the proper self energy (cf. Fig. 10) Σ, as it is the building block of the Dyson equation. So following the prescriptions of sect. 1, we calculate

$$\hbar\Sigma(a,\omega) = -i\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\sum_{b\lambda_\nu^\pi}\langle\lambda_\nu^\pi|k_{\lambda^\pi}a^\dagger_{\lambda_\nu^\pi}|0\rangle\langle b|F^\dagger_{\lambda_\nu^\pi}|a\rangle$$

$$iG(b,\omega')iD^0_{\lambda_\nu^\pi}(\omega-\omega')\langle 0|k^*_{\lambda^\pi}a_{\lambda_\nu^\pi}|\lambda_\nu^\pi\rangle\langle a|F^\dagger_{\lambda_\nu^\pi}|b\rangle, \tag{137}$$

that, commuting c-numbers and c-functions, leads to

$$\hbar\Sigma(a,\omega) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\sum_{b\lambda_\nu^\pi}|\langle\lambda_\nu^\pi|k_{\lambda^\pi}a^\dagger_{\lambda_\nu^\pi}|0\rangle|^2|\langle b|F^\dagger_{\lambda_\nu^\pi}|a\rangle|^2G(b,\omega')iD^0_{\lambda_\nu^\pi}(\omega-\omega'), \tag{138}$$

and defining the vertex $|\langle\lambda_\nu^\pi|k_{\lambda^\pi}a^\dagger_{\lambda_\nu^\pi}|0\rangle|^2|\langle b|F^\dagger_{\lambda_\nu^\pi}|a\rangle|^2$ generally as the matrix element $h^2(a,b;\lambda_\nu^\pi)$,

$$\hbar\Sigma(a,\omega) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\sum_{b\lambda_\nu^\pi}G(b,\omega')iD^0_{\lambda_\nu^\pi}(\omega-\omega')h^2(a,b;\lambda_\nu^\pi). \tag{139}$$

If we want to account perturbatively for the coupling of the particles to phonons, it is very convenient to recall the definition of the Lehmann representation in eq. (126), that is very suited for iterating in a perturbative fashion due to its the integral nature based on the definition of strength function.

The Self-Energy is given by

$$\Sigma(a,\omega) = \sum_{b\lambda_\nu^\pi}h^2(a,b,\lambda^\pi)\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\int_0^{\infty}d\omega''\left[\frac{A(b,\omega'')}{\omega'-\omega''+i\eta}+\frac{B(b,\omega'')}{\omega'+\omega''-i\eta}\right]$$

$$i\left[\frac{1}{\omega-\omega'-\omega_{\lambda_\nu^\pi}+i\delta}+\frac{1}{\omega'-\omega-\omega_{\lambda_\nu^\pi}+i\delta}\right], \tag{140}$$

where $A(b,\omega)$ and $B(b,\omega)$ are called strength functions and are the energy–dependent generalization of the matrix element $h^2(a,b,\lambda_\nu^\pi)$, obtained by integrating convoluting with the dressed propagator $G(a,\omega)$.

To compute this integral in the complex plane, we have to consider the ω' variable as complex, then use the prescriptions of the Cauchy integral formula integrating over a closed path like the one in Fig. 13 and then subtracting the arc contribution,

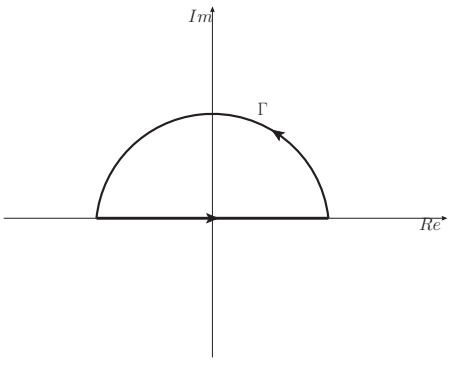

FIGURE 13.

$$\int_{-\infty}^{+\infty} = \oint_C - \int_{arc}, \tag{141}$$

where in our case we can safely assume that we don't have singularity at infinity (being the strength functions A and B related to the spectroscopic response, they must go to zero at high energy) since the integrand $(G_{a,a} \cdot D^0)$ goes to zero as $1/\omega'^2$ and so the upper bound of $\int_{arc}$ is the length of the arc itself (that goes as $\pi\omega'$), its contribution is $\leq \frac{\pi\omega'}{\omega'^2} \xrightarrow[\omega' \to \inf]{} 0$. So the integration over $\int_{-\infty}^{+\infty}$ can be replaced by the contour integration in the upper half plane, so the results will be the sum of the residues of the poles in the upper half plane.

There are four components of the functions in the integral:

- $\frac{A(b,\omega'')}{\omega'-\omega''+i\eta} \equiv G^-$, which has first order poles $\omega' = \omega'' - i\eta$, so only in the lower-half plane (fourth quadrant).
- $\frac{B(b,\omega'')}{\omega'+\omega''-i\eta} \equiv G^+$, which has first order poles $\omega' = -\omega'' + i\eta$, so only in the upper-half plane (second quadrant).
- $\frac{1}{\omega'-\omega-\omega_{\lambda_\nu^\pi}+i\delta} \equiv D^-$, which has first order poles $\omega' = \omega + \omega_{\lambda_\nu^\pi} - i\delta$, so only in the lower-half plane.
- $\frac{1}{\omega-\omega'-\omega_{\lambda_\nu^\pi}+i\delta} \equiv D^+$, which has first order poles $\omega' = \omega - \omega_{\lambda_\nu^\pi} + i\delta$, so only in the upper-half plane.

The contribution given by G^-D^- vanishes, because it has no poles in the upper-half plane, thus no residues. The contribution of G^+D^+ also vanishes,

$$\begin{aligned}
&\oint_C G^+D^+ih^2(\cdot) = \\
&= \oint_C \frac{d\omega'}{2\pi} \sum_{n\lambda_\nu^\pi} \int_0^\infty d\omega'' ih^2(a,b,\lambda_\nu^\pi) \frac{B(b,\omega'')}{\omega'+\omega''-i\eta} \frac{1}{\omega-\omega'-\omega_{\lambda_\nu^\pi}+i\delta} = \\
&= \text{cost} 2\pi i \text{Res}\{G^+D^+\} = \\
&= \text{cost} \left\{ \left[\frac{\partial}{\partial\omega'} (\omega'+\omega''-i\eta)(\omega-\omega'-\omega_{\lambda_\nu^\pi}+i\delta) \Big|_{\omega'=-\omega''+i\eta} \right]^{-1} + \right. \\
&\quad \left. + \left[\frac{\partial}{\partial\omega'} (\omega'+\omega''-i\eta)(\omega-\omega'-\omega_{\lambda_\nu^\pi}+i\delta) \Big|_{\omega'=\omega-\omega'-\omega_{\lambda_\nu^\pi}+i\delta} \right]^{-1} \right\} = \\
&= \text{cost} \left[\frac{1}{\omega-\omega''-2\omega'-\omega_{\lambda_\nu^\pi}+i\delta+i\eta} \Big|_{\omega'=-\omega''+i\eta} + \right. \\
&\quad \left. + \frac{1}{\omega-\omega''-2\omega'-\omega_{\lambda_\nu^\pi}+i\delta+i\eta} \Big|_{\omega'=\omega-\omega_{\lambda_\nu^\pi}+i\delta} \right] = \\
&= \text{cost} \left[\frac{1}{\omega+\omega''-\omega_{\lambda_\nu^\pi}+i\delta-i\eta} + \frac{1}{-\omega-\omega''+\omega_{\lambda_\nu^\pi}-i\delta+i\eta} \right] = \\
&= 0,
\end{aligned} \tag{142}$$

because the two residues are opposite and cancel each other. The residues that give contribution in that contour are the ones from G^+D^-,

$$\begin{aligned}
&\oint_C G^+D^- ih^2(\cdot) = \\
&= \oint_C \frac{d\omega'}{2\pi} \sum_{b\lambda_\nu^\pi} \int_0^\infty d\omega'' ih^2(a,b,\lambda_\nu^\pi) \frac{B(b,\omega'')}{\omega'+\omega''-i\eta} \frac{1}{\omega'-\omega-\omega_{\lambda_\nu^\pi}+i\delta} = \\
&= \text{cost} 2\pi i \text{Res}\{G^+D^-\} = \\
&= 2\pi i \sum_{n\lambda_\nu^\pi} \frac{ih^2(a,b,\lambda_\nu^\pi)}{2\pi} \int_0^\infty d\omega'' B(b,\omega'') \left[\frac{\partial}{\partial\omega'} (\omega'+\omega''-i\eta)(\omega'-\omega-\omega_{\lambda_\nu^\pi}+i\delta) \Big|_{\omega'=-\omega''+i\eta} \right]^{-1} = \\
&= -\sum_{b\lambda_\nu^\pi} h^2(\mu,n,\lambda_\nu^\pi) \int_0^\infty d\omega'' \frac{B(b,\omega'')}{2\omega'+\omega''-\omega-\omega_{\lambda_\nu^\pi}+i\delta-i\eta} \Big|_{\omega'=-\omega''+i\eta} = \\
&= \sum_{b\lambda_\nu^\pi} h^2(a,b,\lambda_\nu^\pi) \int_0^\infty d\omega'' \frac{B(b,\omega'')}{\omega+\omega''+\omega_{\lambda_\nu^\pi}-i\delta-i\eta}, \qquad (143)
\end{aligned}$$

and the other one from G^-D^+ that, following the same prescriptions used above, gives

$$\oint_C G^+D^- ih^2(\cdot) = \sum_{b\lambda_\nu^\pi} h^2(a,b,\lambda_\nu^\pi) \int_0^\infty d\omega'' \frac{A(b,\omega'')}{\omega-\omega''-\omega_{\lambda_\nu^\pi}+i\delta+i\eta}, \qquad (144)$$

leading finally to the result for the proper self-energy function,

$$\Sigma(a,\omega) = \sum_{b\lambda_\nu^\pi} h^2(a,b,\lambda_\nu^\pi) \int_0^\infty d\omega'' \frac{A(n,\omega'')}{\omega-\omega''-\omega_{\lambda_\nu^\pi}+i\delta+i\eta} + \frac{B(b,\omega'')}{\omega+\omega''+\omega_{\lambda_\nu^\pi}-i\delta-i\eta}. \qquad (145)$$

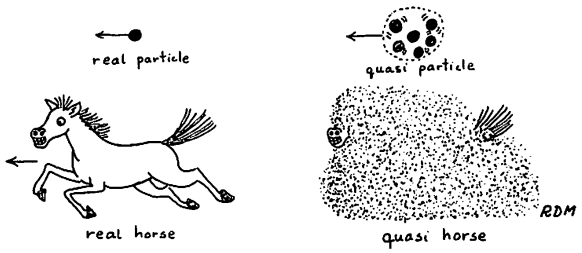

FIGURE 14. Quasiparticle and quasihorse concepts. From [**8**].

2.3. Dressed Green's function. The exact form G and the value of the total solution of eigenvector and eigenvalues are then given by the solution of the Dyson equation explained in section 2.1, which is,

$$G(a,\omega+i\eta) = \left[(G^0(a,\omega))^{-1} - \Sigma^*(a,\omega+i\eta) \right]^{-1} \qquad (146)$$

where G^0 is the Green's function of the unperturbed system, thus giving

$$G^0(a,\omega) = \sum_n \frac{|p_n\rangle\langle p_n|}{\omega-\lambda-\varepsilon_{\hat{T}_n}+i\eta} + \sum_{n'} \frac{|h_{n'}\rangle\langle h_{n'}|}{\omega-\lambda+\varepsilon_{\hat{T}_{n'}}-i\eta} \qquad (147)$$

where $\varepsilon_{\hat{T}_n}$ represent, by definition (126), the eigenvalue of the hamiltonian of the system the Green's function is describing, and since G^0 is the unperturbed Green's function of the free particle, the hamiltonian under consideration is the kinetic term $\hat{T}_n$. λ is the energy needed to add or remove a single particle on the system, and is the so-called chemical potential, or the Fermi energy $\lambda = -\varepsilon_F$. Were the terms with momenta $|k|$ or $-|k|$ in Eq. (126) in the nuclear case are particles p_n and holes $h_{n'}$ respectively. $|p_n\rangle\langle p_n|$ and $|h_{n'}\rangle\langle h_{n'}|$ are the matrix of eigenvectors of $\hat{T}$, which is diagonal being the two-body, of diagonal, contributions forbidden. Thus the inverse of G^0 is

$$(G^0(a,\omega))^{-1} = \sum_n |p_n\rangle\langle p_n|(\omega - \lambda - \varepsilon_{\hat{T}_n} + i\eta) + \sum_{n'} |h_{n'}\rangle\langle h_{n'}|(\omega - \lambda + (\varepsilon_{\hat{T}_{n'}}) - i\eta)$$

$$= \sum_n \omega \pm i\eta - \lambda - \hat{T}|a_n\rangle\langle a_n| \tag{148}$$

where we made use of the fact that the inverse of the diagonal matrix is equal to the matrix itself, and that $\hat{T}|p_n\rangle\langle p_n| = \varepsilon_{\hat{T}_n}|p_n\rangle\langle p_n|$ and $\hat{T}|h_n\rangle\langle h_n| = -\varepsilon_{\hat{T}_n}|p_n\rangle\langle p_n|$. In the end, considering Dyson equation (136), the proper Self Energy Σ^*, containing all the interaction of the system and so the two body V_{a_n,a_n}, the pairing $\Delta_{\bar{a}_n,a_n}$ and the phonon exchange $\hat{\Sigma}(a,\omega)$ described above, adding the kinetic term and the Fermi energy parameter $-\varepsilon_F$ we obtain the following equation for the dressed Green's function,

$$\hat{G}(a,\omega+i\eta) = \Big[\omega + i\eta - \hat{H}_0 - \hat{\Sigma}(a,\omega+i\eta)\Big]^{-1} \tag{149}$$

where $\hat{H}_0$ is the one–body Hamiltonian that generates the basis (that can be an HFB basis). In essence, the Green's function is a way to calculate and represent a many–body solution for a complete Hamiltonian by the means of a perturbative expansion and the related set of equations.

2.4. Exercises.

(1) Find which of these diagrams are topologically equivalent

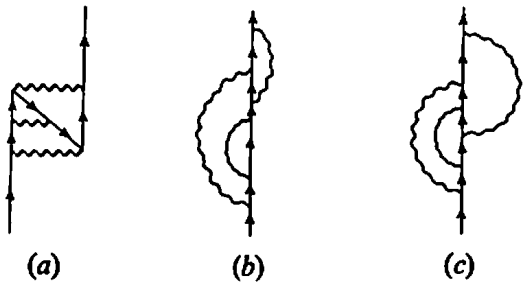

FIGURE 15.

(2) Show that the diagrammatic Hartree–Fock formulation given in sect. 1 corresponds to either the first– or second–quantization formulation seen in Lect. 3 and Hand–in exercise 2 respectively.

APPENDIX A

Particle Vibration Coupling with Separable Interaction

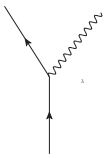

FIGURE 1. Particle-Vibration scattering vertex, the building block of the renormalization.

In this Appendix we give the basic expressions needed to compute the particle-vibration coupling vertex according to the collective model of Bohr and Mottelson [**11**]. This formalism is especially suitable to deal with the coupling of (quasi)–particles with low-lying collective density modes, making use of the experimental energies and transition strength.

The QRPA calculation will be carried out with the separable force

$$V(\vec{r}_1,\vec{r}_2) = -\kappa_{self}\; r_1\frac{\partial U}{\partial r_1} r_2\frac{\partial U}{\partial r_2}\sum_{\lambda\mu}\chi_\lambda Y^*_{\lambda\mu}(\theta_1)Y_{\lambda\mu}(\theta_2) \tag{150}$$

where $U(r)$ is a potential that gives a good reproduction of the experimental levels. In practice, one can adopt a Woods-Saxon parametrization (e.g. [**12**], cf. eq. (2-182)), with an eventual empirical pairing coupling constant adjusted to reproduce the pairing gap deduced from the experimental odd-even mass difference. The parameters χ_λ are determined so as to get a good agreement with the observed properties (energy and transition strength) of the low-lying surface modes with a (Q)RPA calculation.

This scheme then reduces to the collective particle-shape vibration (phonon) coupling scheme given by Bohr and Mottelson [**11**] (cf. Eqs. 6-207- 6-209). In fact, neglecting the exchange terms (cf. on this point [**10**], Eq. (14.54) and Chap.16), the particle-hole matrix elements are given by

$$F(abcd\lambda) = -\kappa_{self}\chi_\lambda < ab\lambda\mu|r_1\frac{\partial U}{\partial r_1}Y^*_{\lambda\mu}(\theta_1)|0 >< 0|r_2\frac{\partial U}{\partial r_2}Y^*_{\lambda\mu}(\theta_2)|cd\lambda\mu > \tag{151}$$

where μ is any of the z-projections of the angular momentum λ. In this expression the QRPA-like single-particle indices (c,d) and the scattered particle indices (a,b) appear in separated factors, so that one gets the angular momentum reordering property $F(abdc\lambda) = (-1)^{j_c-j_d+\lambda}F(abcd\lambda) = (-1)^{j_a-j_b+\lambda}F(bacd\lambda)$, and

$$\begin{aligned} V(ab\lambda\nu) &= -\kappa_{self}\chi_\lambda(u_au_b - v_av_b) < ab\lambda\mu|r_1\frac{\partial U}{\partial r_1}Y^*_{\lambda\mu}(\theta_1)|0 > \left[\frac{2\lambda+1}{2j_a+1}\right]^{1/2} \\ &\times\sum_{c\le d}(1+\delta_{cd})^{-1/2}\left[(X_{cd}(\lambda\nu)+Y_{cd}(\lambda\nu))(u_cv_d+v_cv_d) < 0|r_2\frac{\partial U}{\partial r_2}Y^*_{\lambda\mu}(\theta_2)|cd\lambda\mu >\right] \end{aligned} \tag{152}$$

The quantity in the summation is precisely the transition amplitude $M(\lambda\nu)$ of the $\hat{M} = r_2 \frac{\partial U}{\partial r_2} Y^*_{\lambda\mu}(\theta_2)$ operator, which is usually expressed in terms of the so-called collective deformation parameter as $M(\lambda\nu) = \alpha^o_{\lambda\nu}/\kappa_{self}$, assuming a collectively deformed density $\delta\rho = -r\frac{\partial\rho}{\partial r}\sum_{\lambda\mu} Y^*_{\lambda\mu}(\theta)\alpha_{\lambda\mu}$

In this way we can write

$$V(ab\lambda\nu) = -\chi_\lambda(u_a u_b - v_a v_b) < ab\lambda\mu|r_1\frac{\partial U}{\partial r_1}Y^*_{\lambda\mu}(\theta_1)|0> \left[\frac{2\lambda+1}{2j_a+1}\right]^{1/2}\alpha^o_{\lambda\nu}. \tag{153}$$

Finally, following the notation in [**11**], Eqs.(6-207 to 6-209) using the reduced matrix element $< j_b||Y_\lambda||j_a >= (-1)^{j_a-j_b} < j_a j_b;\lambda\mu|Y_{\lambda\mu}|0 > \sqrt{2\lambda+1}$ and the relation $\alpha^o_{\lambda\nu} = \beta_{\lambda\nu}/\sqrt{2\lambda+1}$, we can write

$$V(ab\lambda\nu) = h(ab\lambda\nu)(u_a u_b - v_a v_b), \tag{154}$$

where

$$h(ab\lambda\nu) = -(-1)^{j_a-j_b}\beta^{eff}_{\lambda\nu} < a|r_1\frac{\partial U}{\partial r_1}|b >< j_b||Y_\lambda||j_a > \left[\frac{1}{(2j_a+1)(2\lambda+1)}\right]^{1/2}, \tag{155}$$

which is the basic vertex in [**11**] corrected by our effective deformation parameter $\beta^{eff}_\lambda = \chi_{\lambda\nu}\beta_{\lambda\nu}$. Analogously one finds

$$W(ab\lambda\nu) = h(ab\lambda\nu)(u_a v_b + v_a u_b). \tag{156}$$

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