# Nuclear Structure. Microscopical Approach

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# Hartree-Fock Method

$$H = \sum_{i=1}^{N} T(\mathbf{r}_i) + \frac{1}{2} \sum_{i \neq j = 1}^{N} V(\mathbf{r}_i, \mathbf{r}_j),$$

$$H = \sum_{k,l} \langle k|T|l\rangle a_k^\dagger a_l + \frac{1}{2} \sum_{k,l,m,n} \langle kl|V|mn\rangle a_k^\dagger a_l^\dagger a_n a_m,$$

where

$$\langle k|T|l\rangle = \int \phi_k^*(\mathbf{r}) T(\mathbf{r}) \phi_l(\mathbf{r})\, d\mathbf{r},$$

$$\langle kl|V|mn\rangle = \int \phi_k^*(\mathbf{r}_1)\phi_l^*(\mathbf{r}_2) V(\mathbf{r}_1, \mathbf{r}_2)\phi_m(\mathbf{r}_1)\phi_n(\mathbf{r}_2)\, d\mathbf{r}_1\, d\mathbf{r}_2.$$

Creation and annihilation operators

$$a_k^\dagger a_l^\dagger + a_l^\dagger a_k^\dagger = 0, \qquad a_k a_l + a_l a_k = 0, \qquad a_k a_l^\dagger + a_l^\dagger a_k = \delta_{k,l}.$$

$$|\Phi\rangle = \prod_{h=1}^{N} a_h^\dagger |0\rangle \quad \text{and} \quad a_k|0\rangle = 0 \text{ for any } k$$

$$\Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\mathbf{r}_1) & \phi_1(\mathbf{r}_2) & \ldots & \phi_1(\mathbf{r}_N) \\ \phi_2(\mathbf{r}_1) & \phi_2(\mathbf{r}_2) & \ldots & \phi_2(\mathbf{r}_N) \\ \ldots & \ldots & \ldots & \ldots \\ \phi_N(\mathbf{r}_1) & \phi_N(\mathbf{r}_2) & \ldots & \phi_N(\mathbf{r}_N) \end{vmatrix}.$$

Single-particle wave functions $\phi_k(\mathbf{r})$ are determined by

$$\delta\langle\Phi|H|\Phi\rangle = 0 \iff \begin{cases} \langle\delta\Phi|H|\Phi\rangle = 0, \\ \langle\Phi|H|\delta\Phi\rangle = 0. \end{cases}$$

$$\phi_h(\mathbf{r}) \to \phi_h(\mathbf{r}) + \eta\phi_p(\mathbf{r}) \quad \text{with } 1 \leqslant h \leqslant N \text{ and } p > N.$$

$$|\delta\Phi\rangle = \eta a_p^\dagger a_h |\Phi\rangle$$

and

$$\langle\Phi|H a_p^\dagger a_h|\Phi\rangle = 0 \quad \text{and} \quad \langle\Phi|a_h^\dagger a_p H|\Phi\rangle = 0.$$

for any pair $h$ and $p$.

## Ground state averages

$$\langle\Phi|a_h^\dagger a_p a_k^\dagger a_l|\Phi\rangle = \langle\Phi|a_h^\dagger\left(\delta_{k,p} - a_k^\dagger a_p\right)a_l|\Phi\rangle$$

$$= \delta_{k,p}\langle\Phi|a_h^\dagger a_l|\Phi\rangle - \langle\Phi|a_h^\dagger a_k^\dagger a_p a_l|\Phi\rangle = \delta_{k,p}\delta_{l,h}$$

$$\langle\Phi|a_h^\dagger a_p a_k^\dagger a_l^\dagger a_n a_m|\Phi\rangle = \langle\Phi|a_h^\dagger\left(\delta_{k,p} - a_k^\dagger a_p\right)a_l^\dagger a_n a_m|\Phi\rangle$$

$$= -\delta_{k,p}\delta_{n,h}\langle\Phi|a_l^\dagger a_m|\Phi\rangle + \delta_{l,p}\langle\Phi|a_k^\dagger a_h^\dagger a_n a_m|\Phi\rangle + \delta_{k,p}\langle\Phi|a_l^\dagger a_n a_h^\dagger a_m|\Phi\rangle$$

$$\langle\Phi|a_l^\dagger a_m|\Phi\rangle = \bar{\delta}_{l,m}, \quad \bar{\delta}_{l,m} = \begin{cases} \delta_{l,m}, & \text{if } 1 \leqslant l,m \leqslant N; \\ 0, & \text{any else} \end{cases}$$

$$= \delta_{k,p}\delta_{m,h}\bar{\delta}_{l,n} - \delta_{k,p}\delta_{n,h}\bar{\delta}_{l,m} + \delta_{l,p}\delta_{n,h}\bar{\delta}_{k,n} - \delta_{l,p}\delta_{m,h}\bar{\delta}_{k,n}$$

# Interaction part

$$\langle\Phi|a_h^\dagger a_p \sum_{k,l,m,n} \langle kl|V|mn\rangle a_k^\dagger a_l^\dagger a_n a_m|\Phi\rangle$$

$$= \sum_{g=1}^{N}\langle pg|V|hg\rangle - \sum_{g=1}^{N}\langle pg|V|gh\rangle + \sum_{g=1}^{N}\langle gp|V|gh\rangle - \sum_{g=1}^{N}\langle gp|V|hg\rangle$$

Using the definition of matrix element

$$\langle kl|V|mn\rangle = \int \phi_k^*(\mathbf{r}_1)\phi_l^*(\mathbf{r}_2)V(\mathbf{r}_1,\mathbf{r}_2)\phi_m(\mathbf{r}_1)\phi_n(\mathbf{r}_2)\, d\mathbf{r}_1\, d\mathbf{r}_2,$$

$$(k,l)(m,n)\,(r_1,r_2) \leftrightarrow (l,k)(n,m)\,(r_2,r_1) \;\Rightarrow\; \langle kl|V|mn\rangle = \langle lk|V|nm\rangle$$

$$\langle gp|V|gh\rangle - \langle gp|V|hg\rangle = \langle pg|V|hg\rangle - \langle pg|V|gh\rangle$$

$$\langle\Phi|a_h^\dagger a_p \sum_{k,l,m,n} \langle kl|V|mn\rangle a_k^\dagger a_l^\dagger a_n a_m|\Phi\rangle = 2\left[\sum_{g=1}^{N}\langle pg|V|hg\rangle - \sum_{g=1}^{N}\langle pg|V|gh\rangle\right].$$

# Stationary conditions



First equation

$$\langle\Phi|a_h^\dagger a_p H|\Phi\rangle = \langle p|T|h\rangle + \sum_{g=1}^{N}\left[\langle pg|V|hg\rangle - \langle pg|V|gh\rangle\right] = 0$$

and the second equation

$$\langle\Phi|H a_p^\dagger a_h|\Phi\rangle = \langle h|T|p\rangle + \sum_{g=1}^{N}\left[\langle hg|V|pg\rangle - \langle hg|V|gp\rangle\right] = 0$$

for any $p$ and $h$.

# HF Hamiltonian

One can define the Hamiltonian of Hartree-Fock method

$$\langle k|H_{\mathrm{HF}}|l\rangle \equiv \langle k|T|l\rangle + \sum_{g=1}^{N} [\langle kg|V|lg\rangle - \langle kg|V|gl\rangle]$$

with property

$$\langle k|H_{\mathrm{HF}}|l\rangle = 0 \quad \text{if } (1 \leqslant k \leqslant N \text{ and } l > N) \quad \text{or } (k > N \text{ and } 1 \leqslant l \leqslant N).$$

The equations to determine $\phi_k(\mathbf{r})$

$$\langle k|H_{\mathrm{HF}}|l\rangle = \varepsilon_k \delta_{k,l}$$

$$\langle k|T|l\rangle + \sum_{h=1}^{N} [\langle kh|V|lh\rangle - \langle kh|V|hl\rangle] = \varepsilon_k \delta_{k,l}$$

# Coordinate representation

In coordinate representation

$$-\frac{\hbar^2}{2m}\nabla^2\phi_k(\mathbf{r}) + \sum_{h=1}^{N}\int \phi_h^*(\mathbf{r}')V(\mathbf{r}',\mathbf{r})\phi_h(\mathbf{r}')\phi_k(\mathbf{r})\,d\mathbf{r}' - \sum_{h=1}^{N}\int \phi_h^*(\mathbf{r}')V(\mathbf{r}',\mathbf{r})\phi_h(\mathbf{r})\phi_k(\mathbf{r}')\,d\mathbf{r}' = \varepsilon_k\phi_k(\mathbf{r})$$

Single-particle effective potentials:

| Direct | Exchange |
|---|---|
| $U(\mathbf{r}) \equiv \sum_{h=1}^{N}\int \phi_h^*(\mathbf{r}')V(\mathbf{r}',\mathbf{r})\phi_h(\mathbf{r}')\,d\mathbf{r}'$ | $W(\mathbf{r}',\mathbf{r}) \equiv \sum_{h=1}^{N}\phi_h^*(\mathbf{r}')V(\mathbf{r}',\mathbf{r})\phi_h(\mathbf{r})$ |

# Properties of HF potential



Effective Hartree-Fock potential

$$\left[U_{\mathrm{HF}}\phi_k\right](\mathbf{r}) \equiv U(\mathbf{r})\phi_k(\mathbf{r}) - \int W(\mathbf{r}',\mathbf{r})\phi_k(\mathbf{r}')\,d\mathbf{r}'$$

and

$$-\frac{\hbar^2}{2m}\nabla^2\phi_k(\mathbf{r}) + \left[U_{\mathrm{HF}}\phi_k\right](\mathbf{r}) = \varepsilon_k\phi_k(\mathbf{r}).$$

As $W^*(\mathbf{r}',\mathbf{r}) = W(\mathbf{r},\mathbf{r}')$

- $\varepsilon_k$ — real;
- $\phi_k(\mathbf{r})$ — normalized and mutually orthogonal .

# HF ground state energy — I



$$E_0 = \langle\Phi|H|\Phi\rangle$$

$$\langle\Phi|a_k^\dagger a_l|\Phi\rangle \neq 0, \quad \text{if } 1 \leqslant k,l \leqslant N$$
$$\langle\Phi|a_k^\dagger a_l|\Phi\rangle = \bar{\delta}_{k,l}$$

$$\langle\Phi|a_k^\dagger a_l^\dagger a_n a_m|\Phi\rangle, \neq 0 \quad \text{if } 1 \leqslant k,l,m,n \leqslant N$$
$$\langle\Phi|a_k^\dagger a_l^\dagger a_n a_m|\Phi\rangle = \langle\Phi|a_k^\dagger \left(\bar{\delta}_{l,n} - a_n a_l^\dagger\right) a_m|\Phi\rangle$$
$$= \bar{\delta}_{l,n}\langle\Phi|a_k^\dagger a_m|\Phi\rangle - \langle\Phi|a_k^\dagger a_n a_l^\dagger a_m|\Phi\rangle$$
$$= \bar{\delta}_{k,m}\bar{\delta}_{l,n} - \bar{\delta}_{k,n}\bar{\delta}_{l,n}$$
$$= \langle\Phi|a_k^\dagger a_m|\Phi\rangle\langle\Phi|a_l^\dagger a_n|\Phi\rangle - \langle\Phi|a_k^\dagger a_n|\Phi\rangle\langle\Phi|a_l^\dagger a_m|\Phi\rangle.$$

# HF ground state energy — II



$$
\begin{aligned}
E_0 = \langle\Phi|H|\Phi\rangle \quad &= \sum_{h=1}^{N}\langle h|T|h\rangle + \frac{1}{2}\sum_{h,g}\left(\langle hg|V|hg\rangle - \langle hg|V|gh\rangle\right) \\
&= \sum_{h=1}^{N}\varepsilon_h - \frac{1}{2}\sum_{h,g}\left(\langle hg|V|hg\rangle - \langle hg|V|gh\rangle\right) \\
&= \sum_{h=1}^{N}\varepsilon_h - \frac{1}{2}\sum_{h=1}^{N}\langle h|U_{\mathrm{HF}}|h\rangle
\end{aligned}
$$

# Energy of particle-hole excitation — I

$$|ph) \equiv a_p^\dagger a_h |\Phi\rangle$$

$$\begin{aligned}
(ph|H|ph) &= \langle\Phi|a_h^\dagger a_p H a_p^\dagger a_h|\Phi\rangle \\
&= \langle\Phi| \left[a_h^\dagger a_p,\, H a_p^\dagger a_h\right]_- + H a_p^\dagger a_h a_h^\dagger a_p|\Phi\rangle \\
&= \langle\Phi| \left[a_h^\dagger a_p,\, H a_p^\dagger a_h\right]_- |\Phi\rangle \\
&= \langle\Phi| \left[a_h^\dagger a_p,\, H\right]_- a_p^\dagger a_h + H \left[a_h^\dagger a_p,\, a_p^\dagger a_h\right]_- |\Phi\rangle
\end{aligned}$$

as $\left[a_h^\dagger a_p,\, a_p^\dagger a_h\right]_- = a_h^\dagger a_p a_p^\dagger a_h - a_p^\dagger a_h a_h^\dagger a_p = a_h^\dagger a_h - a_p^\dagger a_p$

$$\begin{aligned}
&= \langle\Phi| \left[a_h^\dagger a_p,\, H\right]_- a_p^\dagger a_h|\Phi\rangle + \langle\Phi|H a_h^\dagger a_h|\Phi\rangle \\
&= \langle\Phi|H|\Phi\rangle + \langle\Phi|a_p^\dagger a_h \left[a_h^\dagger a_p,\, H\right]_- + \left[\left[a_h^\dagger a_p,\, H\right]_-,\, a_p^\dagger a_h\right]_- |\Phi\rangle \\
&= E_0 + \langle\Phi| \left[\left[a_h^\dagger a_p,\, H\right]_-,\, a_p^\dagger a_h\right]_- |\Phi\rangle
\end{aligned}$$

# Energy of particle-hole excitation — II

$$\langle\Phi|\left[\left[a_h^\dagger a_p,\, H\right]_-,\, a_p^\dagger a_h\right]_- |\Phi\rangle = \langle p|T|p\rangle - \langle h|T|h\rangle$$

$$+\sum_{g=1,g\neq h}^{N}\left(\langle pg|V|pg\rangle - \langle pg|V|gp\rangle\right) - \sum_{g=1}^{N}\left(\langle hg|V|hg\rangle - \langle hg|V|gh\rangle\right)$$

But

$$\langle p|T|p\rangle + \sum_{g=1}^{N}\left(\langle pg|V|pg\rangle - \langle pg|V|gp\rangle\right) = \varepsilon_p$$

$$\langle h|T|h\rangle + \sum_{g=1}^{N}\left(\langle hg|V|hg\rangle - \langle hg|V|gh\rangle\right) = \varepsilon_h$$

# Energy of particle-hole excitation — III



$$(ph|H|ph) = E_0 + \varepsilon_p - \varepsilon_h + (\langle ph|V|ph\rangle - \langle ph|V|hp\rangle)$$

If one removes a particle infinitely far, then $\langle ph|V|ph\rangle = \langle ph|V|hp\rangle = 0$. The energy required to remove particle from the state $h$ and to put it at infinity with $\varepsilon_p = 0$, ("ionization" energy) is equal to $(-\varepsilon_h)$ (*Koopmans' theorem)*.

# Phenomenological approach



$$
\begin{aligned}
H &= \sum_{i=1}^{N} T(\mathbf{r}_i) + \frac{1}{2}\sum_{i\neq j=1}^{N} V(\mathbf{r}_i,\mathbf{r}_j) \\
&= \underbrace{\sum_{i=1}^{N} T(\mathbf{r}_i) + U_{\mathrm{HF}}}_{H_{\text{mean field}}} + \underbrace{\frac{1}{2}\sum_{i\neq j=1}^{N} V(\mathbf{r}_i,\mathbf{r}_j) - U_{\mathrm{HF}}}_{H_{\text{residual interaction}}}
\end{aligned}
$$

$$
\begin{aligned}
H_{\text{mean field}}(\vec{r}) &\approx -\frac{\hbar^2}{2M}\Delta + U(r) - \varkappa\frac{1}{r}\frac{d}{dr}U(r)(\mathbf{l},\mathbf{s}), \\
U(r) &= -\frac{U_0}{1+\exp[\alpha(r-R_0)]}, \\
R_0 &= r_0 A^{1/3}.
\end{aligned}
$$

# Skyrme two-body effective interactions



$$
\begin{aligned}
V_{\rm Sk}(\mathbf{r}_1,\mathbf{r}_2) = {} & t_0\big(1+x_0P_\sigma\big)\delta(\mathbf{r}_{1,2}) \\
& + \frac{t_1}{2}\big(1+x_1P_\sigma\big)\big(\mathbf{k}^{\dagger\,2}_{1,2}\delta(\mathbf{r}_{1,2})+\delta(\mathbf{r}_{1,2})\mathbf{k}^2_{1,2}\big) \\
& + t_2\big(1+x_2P_\sigma\big)\mathbf{k}^\dagger_{1,2}\delta(\mathbf{r}_{1,2})\mathbf{k}_{1,2} \\
& + \frac{t_3}{6}\big(1+x_3P_\sigma\big)\rho\Big(\frac{\mathbf{r}_1+\mathbf{r}_2}{2}\Big)\delta(\mathbf{r}_{1,2}) \\
& + it_4(\sigma_1+\sigma_2)\times\mathbf{k}^\dagger_{1,2}\cdot\delta(\mathbf{r}_{1,2})\mathbf{k}_{1,2};
\end{aligned}
$$

$$
\begin{aligned}
P_\sigma &\equiv (1+\sigma_1\cdot\sigma_2), \\
\mathbf{r}_{1,2} &\equiv \mathbf{r}_1-\mathbf{r}_2, \\
\mathbf{k}_{1,2} &\equiv -\frac{i}{2}\big(\nabla_1-\nabla_2\big)
\end{aligned}
$$

# Gogny two-body effective interactions



$$V_{\text{Gogny}}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{j=1}^{2} e^{-\left(\frac{\mathbf{r}_{1,2}}{\mu_j}\right)^2} \left(W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau\right)$$

$$+ t_3 \left(1 + x_0 P_\sigma\right) \delta(\mathbf{r}_{1,2}) \rho^\alpha \left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2}\right)$$

$$+ i W_{ls} (\sigma_1 + \sigma_2) \times \mathbf{k}^\dagger_{1,2} \cdot \delta(\mathbf{r}_{1,2}) \mathbf{k}_{1,2};$$

$$P_\tau \equiv (1 + \tau_1 \cdot \tau_2).$$

# Thouless theorem

$$|\Phi\rangle = \prod_{h=1}^{N} a_h^\dagger |0\rangle \quad \text{and} \quad a_k|0\rangle = 0 \text{ for any } k;$$

*Theorem.* Any $N$-particle Slater determinant $|\Psi\rangle$ which is not orthogonal to $|\Phi\rangle$ can written in the form

$$|\Psi\rangle = \left[\prod_{h=1}^{N}\prod_{p=N+1}^{\infty}\left(1 + C_{h,p}a_p^\dagger a_h\right)\right]|\Phi\rangle = \left[\exp\left(\sum_{h=1}^{N}\sum_{p=N+1}^{\infty} C_{h,p}a_p^\dagger a_h\right)\right]|\Phi\rangle,$$

where the coefficients $C_{h,p}$ are uniquely determined. Controversely, any wave function $|\Psi\rangle$ written in this form with $N$-particle Slater determinant $|\Phi\rangle$ is an $N$-particle Slater determinant
(D. J. Thouless, Nucl. Phys. **21** (1960) 225).

# HF Stability Condition — I



$$|\phi\rangle = \exp\Big(\sum_{p,h} \chi_{p,h}\, a_p^\dagger a_h\Big)|\Phi\rangle = \prod_{p,h}\big(1 + \chi_{p,h}\, a_p^\dagger a_h\big)|\Phi\rangle\,,$$

$$|\phi\rangle \approx \Big(1 + \sum_{p,h} \chi_{p,h}\, a_p^\dagger a_h + \frac{1}{2}\big(\sum_{p,h} \chi_{p,h}\, a_p^\dagger a_h\big)^2 + O(\chi^3)\Big)|\Phi\rangle\,,$$

$$\langle\phi|\phi\rangle \approx \langle\Phi|\Big(1 + \sum_{p,h} \chi^*_{p,h}\, a_h^\dagger a_p + \frac{1}{2}\big(\sum_{p,h} \chi^*_{p,h}\, a_h^\dagger a_p\big)^2\Big)$$

$$\times\Big(1 + \sum_{p,h} \chi_{p,h}\, a_p^\dagger a_h + \frac{1}{2}\big(\sum_{p,h} \chi_{p,h}\, a_p^\dagger a_h\big)^2\Big)|\Phi\rangle\,.$$

# HF Stability Condition — II

As

$$\langle\Phi|a_h^\dagger a_p a_{p_1}^\dagger a_{h_1}|\Phi\rangle = \delta_{p,p_1}\delta_{h,h_1}\ ,$$
$$\langle\Phi|a_h^\dagger a_p a_{h_1}^\dagger a_{p_1}|\Phi\rangle = \langle\Phi|a_p^\dagger a_h a_{p_1}^\dagger a_{h_1}|\Phi\rangle = 0$$

$$\langle\phi|\phi\rangle = \big(1 + \sum_{p,h} \chi_{p,h}^* \, \chi_{p,h}\big)\langle\Phi|\Phi\rangle\ ,\ \ \langle\Phi|\Phi\rangle = 1.$$

HF property of $\Phi$: $\langle ph|H|\Phi\rangle = 0$, with $|ph\rangle \equiv a_p^\dagger a_h|\Phi\rangle$.

$$\begin{aligned}\langle\phi|H|\phi\rangle = \langle\Phi|\big(1 + \chi_{p,h}^* \, a_h^\dagger a_p + \frac{1}{2}\chi_{p,h}^* \, \chi_{p_1,h_1}^* \, a_h^\dagger a_p a_{h_1}^\dagger a_{p_1}\big) \\ \times H\big(1 + \chi_{p,h} \, a_p^\dagger a_h + \frac{1}{2}\chi_{p,h} \, \chi_{p_1,h_1} \, a_p^\dagger a_h a_{p_1}^\dagger a_{h_1}\big)|\Phi\rangle + O(\chi^3)\end{aligned}$$

# HF Stability Condition — III



$$\langle\phi|H|\phi\rangle = \langle\Phi|H|\Phi\rangle + \frac{1}{2}\langle\Phi|H a_p^\dagger a_h a_{p_1}^\dagger a_{h_1}\big)|\Phi\rangle \chi_{p,h}\,\chi_{p_1,h_1} + \chi_{p,h}^*\,\langle\Phi|a_h^\dagger a_p H a_{p_1}^\dagger a_{h_1}|\Phi\rangle \chi_{p_1,h_1} + \frac{1}{2}\chi_{p,h}^*\,\chi_{p_1,h_1}^*\,\langle\Phi|a_h^\dagger a_p a_{h_1}^\dagger a_{p_1} H|\Phi\rangle + O(\chi^3)\,,$$

$$\frac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle} = \langle\Phi|H|\Phi\rangle\big(1-\chi_{p,h}^*\,\chi_{p,h}\big) + \frac{1}{2}\langle\Phi|H a_p^\dagger a_h a_{p_1}^\dagger a_{h_1}\big)|\Phi\rangle \chi_{p,h}\,\chi_{p_1,h_1} + \chi_{p,h}^*\,\langle\Phi|a_h^\dagger a_p H a_{p_1}^\dagger a_{h_1}|\Phi\rangle \chi_{p_1,h_1} + \frac{1}{2}\chi_{p,h}^*\,\chi_{p_1,h_1}^*\,\langle\Phi|a_h^\dagger a_p a_{h_1}^\dagger a_{p_1} H|\Phi\rangle + O(\chi^3)$$

$$\frac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle} = \langle\Phi|H|\Phi\rangle + \frac{1}{2}(\chi^\dagger\,\chi)\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} \chi \\ \chi^* \end{pmatrix} + O(\chi^3)$$

where

$$\begin{aligned} A_{ph,p_1h_1} &= \langle\Phi|a_h^\dagger a_p H a_{p_1}^\dagger a_{h_1}|\Phi\rangle - \langle\Phi|H|\Phi\rangle\delta_{p,p_1}\delta_{h,h_1} \\ &= \langle ph|H|p_1h_1\rangle - \langle\Phi|H|\Phi\rangle\delta_{p,p_1}\delta_{h,h_1}\ , \\ B_{ph,p_1h_1} &= \langle\Phi|a_h^\dagger a_p a_{h_1}^\dagger a_{p_1} H|\Phi\rangle = \langle ph,\, p_1h_1|H|\Phi\rangle\ . \end{aligned}$$

$$A^\dagger = A \text{ or } A_{ph,p_1h_1} = A^*_{p_1h_1,ph}$$
$$\tilde{B} = B \text{ or } B_{ph,p_1h_1} = B_{p_1h_1,ph}.$$

Index $q$ to label particle-hole pairs $(p,h)$: $A_{q,q_1} = A^*_{q_1,q}$

# HF Stability Condition — V



$|\Phi\rangle$ minimizes the expectation value of $H$ if $\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}$ is positive definite matrix.

# Random Phase Approximation

# Time Dependent Perturbation



One-body perturbation

$$W(t) = We^{-i\omega t} + Ue^{i\omega t}, \quad W^\dagger = U.$$

For the optimum Slater determinant

$$\langle \delta\Psi | H + W(t) - i\hbar \frac{\partial}{\partial t} | \Psi \rangle = 0.$$

Introducing

$$\begin{aligned} \Psi &= \phi \, e^{-iE_0 t/\hbar}, \\ E_0 &= \langle \Phi | H | \Phi \rangle, \\ i\hbar \frac{\partial}{\partial t} \Psi &= E_0 \Psi + e^{-iE_0 t/\hbar} \, i\hbar \frac{\partial}{\partial t} \phi. \end{aligned}$$

# Time Dependent HF Variational Principle I



$$\langle \delta\phi | H - E_0 + W(t) - i\hbar \frac{\partial}{\partial t} | \phi \rangle = 0.$$

Let $\phi$ be a Slater determinant

$$\begin{aligned}
\phi &= \big(1 + \chi_{p,h}\, a_p^\dagger a_h + \frac{1}{2}\chi_{p,h}\,\chi_{p_1,h_1}\, a_p^\dagger a_h a_{p_1}^\dagger a_{h_1} + O(\chi^3)\big)\Phi\,, \\
\delta\phi &= \delta\chi_{p,h}\big(a_p^\dagger a_h + \chi_{p_1,h_1}\, a_p^\dagger a_h a_{p_1}^\dagger a_{h_1} + \ldots\big)\Phi\,, \\
\langle\delta\phi| &= \delta\chi_{p,h}^*\,\langle\Phi|\big(a_h^\dagger a_p + \chi_{p_1,h_1}^*\, a_{h_1}^\dagger a_{p_1} + \ldots\big).
\end{aligned}$$

## Time Dependent HF Variational Principle II

$$\langle\delta\phi|H - E_0 + W(t) - i\hbar\frac{\partial}{\partial t}|\phi\rangle$$

$$= \delta\chi^*_{p,h}\,\langle\Phi|\big(a^\dagger_h a_p + \chi^*_{p_1,h_1}\,a^\dagger_{h_1}a_{p_1} + \ldots\big)$$

$$\times\,\big(H - E_0 + W(t) - i\hbar\frac{\partial}{\partial t}\big)\big(1 + \chi_{p_1,h_1}\,a^\dagger_{p_1}a_{h_1} + \ldots\big)|\Phi\rangle$$

$$= \delta\chi^*_q\left(\langle q|H - E_0|q_1\rangle\chi_{q_1} + \chi^*_{q_1}\langle qq_1|H|\Phi\rangle + \langle q|W(t)|\Phi\rangle - i\hbar\dot{\chi}_{q_1}\langle q|q_1\rangle\right) = 0\,.$$

Assuming that $\chi$ and $W$ are of the same order

$$A_{q,q_1}\chi_{q_1} + B_{q,q_1}\chi^*_{q_1} + W_q(t) - i\hbar\dot{\chi}_q = 0,$$

or

$$A\chi + B\chi^* + W(t) - i\hbar\dot{\chi} = 0\,,$$

# Time Dependent HF Variational Principle III



where $W(t)$ is the vector with elements:

$$W_q(t) = \langle p, h|We^{-i\omega t} + Ue^{i\omega t}|\Phi\rangle = W_q e^{-i\omega t} + U_q e^{i\omega t}.$$

Attempt solution as

$$\chi = Xe^{-i\omega t} + Y^* e^{i\omega t}$$

$$\begin{aligned} -i\hbar\dot{\chi}_q &= -\hbar\omega X_q e^{-i\omega t} + \hbar\omega Y^* e^{i\omega t}, \\ A_{q,q_1} X_{q_1} e^{-i\omega t} &+ A_{q,q_1} Y^*_{q_1} e^{i\omega t} + B_{q,q_1} X^*_{q_1} e^{i\omega t} + B_{q,q_1} Y_{q_1} e^{-i\omega t} \\ &+ W_q e^{-i\omega t} + U_q e^{i\omega t} - \hbar\omega X_q e^{-i\omega t} + \hbar\omega Y^*_q e^{i\omega t} = 0\,, \end{aligned}$$

# Inhomogeneous equations



$$\left(A_{q,q_1}X_{q_1} + B_{q,q_1}Y_{q_1} - \hbar\omega X_q + W_q\right)e^{-i\omega t}$$
$$+\left(A_{q,q_1}Y^*_{q_1} + B_{q,q_1}X^*_{q_1} + \hbar\omega Y^*_q + U_q\right)e^{i\omega t} = 0\,,$$

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} X \\ Y \end{pmatrix} - \hbar\omega\begin{pmatrix} X \\ -Y \end{pmatrix} = -\begin{pmatrix} W \\ -U^* \end{pmatrix}.$$

# Generalized Eigenvalue Problem I



The properties of solution of the eigenvalue problem:

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \lambda \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix}$$

or

$$AX + BY = \lambda Y$$
$$B^*Y + A^*Y = -\lambda Y \, ,$$

here $A$, $B$, $\hat{1}$, $\hat{0}$ are the square $m \times m$ matrices; $\hat{1}$, $\hat{0}$ are the diagonal matrices having 1 and 0 at their main diagonals, correspondingly. $X$ and $Y$ are the unknown $m \times 1$ column matrices (vectors): $\tilde{X} = (x_1, \ldots, x_m)$ and $\tilde{Y} = (y_1, \ldots, y_m)$.

The following properties of the matrices are assumed.

1. Matrix $A$ is Hermitian: $A^\dagger = A$ or $A_{i,j} = A^*_{j,i}$.
2. Matrix $B$ is symmetric: $\tilde{B} = B$ or $B_{i,j} = B_{j,i}$.

Consequence of (1) and (2). Matrix $\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}$ is Hermitian:

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}^\dagger = \begin{pmatrix} A^\dagger & B^{*\dagger} \\ B^\dagger & A^{*\dagger} \end{pmatrix} = \begin{pmatrix} A & \tilde{B} \\ \tilde{B}^* & A^* \end{pmatrix} = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}.$$

The matrix $\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}$ has the full set of eigenvectors:

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} z_k = \eta_k z_k \,,$$

$$\tilde{z}_k = (z_{1,k}, \ldots, z_{2m,k})\,, \quad (k = 1, 2, \ldots 2m)\,,$$

# Generalized Eigenvalue Problem III



$$z_k^\dagger z_l = \sum_{q=1}^{2m} z_{q,k}^* z_{q,l} = \delta_{k,l}$$

$$\sum_{k=1}^{2m} z_{q,k}\, z_{r,k}^* = \delta_{q,r} \,.$$

The eigenvalues $\eta_k$ are the real numbers.

3. Matrix $\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}$ is the positive definite matrix, or $\eta_k > 0$.

# Generalized Eigenvalue Problem IV



The Hermitian matrix $F$ exists, such

$$F^2 = F \cdot F = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} .$$

The eigenvectors $x_k$ form the full set in the $2m$-dimension vector space

$$\sum_{k=1}^{2m} z_{q,k}\, z^*_{r,k} = \delta_{q,r} \,,$$

$$\sum_{k=1}^{2m} \eta_k\, z_{q,k}\, z^*_{r,k} = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}_{q,r} \,,$$

$$F_{q,r} = \sum_{k=1}^{2m} \sqrt{\eta_k}\, z_{q,k}\, z^*_{r,k} \,.$$

# Generalized Eigenvalue Problem V



$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \lambda \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} ,$$

$$\begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} F \cdot F \begin{pmatrix} X \\ Y \end{pmatrix} = \lambda \begin{pmatrix} X \\ Y \end{pmatrix} ,$$

$$F \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} F \left[ F \begin{pmatrix} X \\ Y \end{pmatrix} \right] = \lambda \left[ F \begin{pmatrix} X \\ Y \end{pmatrix} \right] .$$

The matrix $F \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} F$ is Hermitian matrix, and vector $z = F \begin{pmatrix} X \\ Y \end{pmatrix}$ is the solution of standard eigenvalue problem :

$$\left[ F \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} F \right] z_i = \lambda_i z_i .$$

# Generalized Eigenvalue Problem VI



$$\det\left[F\begin{pmatrix}\hat{1} & \hat{0}\\ \hat{0} & -\hat{1}\end{pmatrix}F\right] = \det\begin{pmatrix}A & B\\ B^* & A^*\end{pmatrix}\ \det\begin{pmatrix}\hat{1} & \hat{0}\\ \hat{0} & -\hat{1}\end{pmatrix} \neq 0\,,$$

1. There are $2m$ non-zero eigenvalues $\lambda_i$ and eigenvectors $z_i$ corresponding to them;
2. $z_i^\dagger z_k = 0$ if $i \neq k$;
3. it is possible to normalize eigenvectors: $z_i^\dagger z_i = 1$.

# Projection matrices



$$E_i \equiv z_i z_i^\dagger \text{ with } z_i^\dagger z_i = 1$$

$$E_i E_j = \left[z_i z_i^\dagger\right]\left[z_j z_j^\dagger\right] = z_i \left[z_i^\dagger z_j\right] z_j^\dagger = \delta_{i,j} E_j \;,$$

$$\sum_{i=1}^{2m} E_i = \hat{I},$$

$$\sum_{i=1}^{2m} \lambda^k E_i = \left[F \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} F\right]^k \text{ for any integer } k \,.$$

# In terms of initial problem



$$
\begin{aligned}
\delta_{i,k} = z_i^\dagger z_k &= \\
&= \begin{pmatrix} X_i^\dagger Y_i^\dagger \end{pmatrix} \; F^\dagger F \; \begin{pmatrix} X_k \\ Y_k \end{pmatrix} \\
&= \begin{pmatrix} X_i^\dagger Y_i^\dagger \end{pmatrix} \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X_k \\ Y_k \end{pmatrix} \\
&= \lambda_i \begin{pmatrix} X_i^\dagger Y_i^\dagger \end{pmatrix} \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} \begin{pmatrix} X_k \\ Y_k \end{pmatrix} \\
&= \lambda_i \big( X_i^\dagger X_k - Y_i^\dagger Y_k \big).
\end{aligned}
$$

As $\lambda_i \neq 0$, for any $i \neq k$ $\big( X_i^\dagger X_k - Y_i^\dagger Y_k \big) = 0.$

## Solutions come in pairs



Norm: $\lambda_i(X_i^\dagger X_i - Y_i^\dagger Y_i) = 1.$

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X_k \\ Y_k \end{pmatrix} = \lambda_k \begin{pmatrix} X_k \\ -Y_k \end{pmatrix}.$$

$$AY_k^* + BX_k^* = -\lambda_k Y_k^*$$
$$B^*Y_k^* + A^*X_k^* = \lambda_k X_k^*,$$

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} Y_k^* \\ X_k^* \end{pmatrix} = -\lambda_k \begin{pmatrix} Y_k^* \\ -X_k^* \end{pmatrix}.$$

For any solution $(\tilde{X}, \tilde{Y})$ with $\lambda_i > 0$ exists solution $(Y^\dagger, X^\dagger)$ with negative eigenvalue, $(-\lambda_i)$ These two eigenvectors are mutually orthogonal due to trivial cancellation $X_i^\dagger Y_i^* - Y_i^\dagger X_i^* = \tilde{Y}_i X_i - \tilde{X}_i Y_i = 0\,.$

# Another normalization



$$X_i^\dagger X_i - Y_i^\dagger Y_i = \mathrm{sign}(\lambda_i) = \frac{\lambda_i}{|\lambda_i|}\,.$$

And for $z$-vectors: $z_i^\dagger z_i = \mathrm{abs}(\lambda_i)$.

# Completeness relations



For $z_i^\dagger z_i = 1$

$$F \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} F = \sum_{i=1}^{2m} \lambda_i \, z_i \, z_i^\dagger$$
$$= F \left[ \sum_{i=1}^{2m} \lambda_i \begin{pmatrix} X_i \\ Y_i \end{pmatrix} \begin{pmatrix} X_i^\dagger Y_i^\dagger \end{pmatrix} \right] F \,,$$

as $\det F \neq 0$

$$\sum_{i=1}^{2m} \begin{pmatrix} \lambda_i X_i X_i^\dagger & \lambda_i X_i Y_i^\dagger \\ \lambda_i Y_i X_i^\dagger & \lambda_i Y_i Y_i^\dagger \end{pmatrix} = \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} .$$

# With positive eigenvalues



As the eigenvalues appear by the pairs $\pm\lambda_i$

$$\sum_{i:\,\lambda_i>0} \begin{pmatrix} \lambda_i\big(X_i X_i^\dagger - Y_i^* \tilde{Y}_i\big) & \lambda_i\big(X_i Y_i^\dagger - Y_i^* \tilde{X}_i\big) \\ \lambda_i\big(Y_i X_i^\dagger - X_i^* \tilde{Y}_i\big) & \lambda_i\big(Y_i Y_i^\dagger - X_i^* \tilde{X}_i\big) \end{pmatrix} = \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix}.$$

And finally the closure relation for the positive energy solutions only

$$\sum_{i:\,\lambda_i>0} \lambda_i\big(X_i X_i^\dagger - Y_i^* \tilde{Y}_i\big) = \hat{1},$$

$$\sum_{i:\,\lambda_i>0} \lambda_i\big(X_i Y_i^\dagger - Y_i^* \tilde{X}_i\big) = \hat{0}.$$

# Another norm



With the norms $z_i^\dagger z_i = \lambda_i$ ($\lambda_i$ are positive numbers here) and $X_i^\dagger X_i - Y_i^\dagger Y_i = 1$ these relations will be

$$\sum_{i:\,\lambda_i>0} \left(X_i X_i^\dagger - Y_i^* \tilde{Y_i}\right) = \hat{1},$$

$$\sum_{i:\,\lambda_i>0} \left(X_i Y_i^\dagger - Y_i^* \tilde{X_i}\right) = \hat{0}.$$

# Some identities (a)



For any integer $k$ (with $z_i^\dagger z_i = 1$)

$$\begin{aligned}
\sum_{i=1}^{2m} \lambda_i^k \, z_i \, z_i^\dagger &= \left[ F \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} F \right]^k \\
&= F \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} F \, F \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} F \ldots F \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} F \\
&= F \left[ \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} F^2 \right]^{k-1} \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} F \\
&= F \left[ \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \right]^{k-1} \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} F \\
&= F \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}^{k-1} \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} F \, .
\end{aligned}$$

# Some identities (b)



The transition to another normalization $(z_i^\dagger z_i = \mathrm{sign}(\lambda_i)\lambda_i)$ can be done by substitution of the

$$\sum_{i=1}^{2m} \mathrm{sign}(\lambda_i)\lambda_i^{k-1}\, z_i\, z_i^\dagger \text{ instead of } \sum_{i=1}^{2m} \lambda_i^k\, z_i\, z_i^\dagger$$

as the factor $\mathrm{sign}(\lambda_i)\lambda_i$ is used to change the normalization of $z_i$:

$$\sum_{i=1}^{2m} \mathrm{sign}(\lambda_i)\lambda_i^{k-1}\, z_i\, z_i^\dagger = F \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}^{k-1} \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} F\,.$$

# Some identities (c)



For $X_i$ and $Y_i$, normalized by $X_i^\dagger X_i - Y_i^\dagger Y_i = \mathrm{sign}(\lambda_i)$,

$$\sum_{i=1}^{2m} \mathrm{sign}(\lambda_i)\lambda_i^k\, F \begin{pmatrix} X_i \\ Y_i \end{pmatrix} \begin{pmatrix} X_i^\dagger & Y_i^\dagger \end{pmatrix} F = F \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}^k \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} F\,,$$

# Some identities (d)



$F$ is non-degenerate matrix

$$\sum_{i=1}^{2m} \operatorname{sign}(\lambda_i)\lambda_i^k \begin{pmatrix} X_i \\ Y_i \end{pmatrix} \begin{pmatrix} X_i^\dagger & Y_i^\dagger \end{pmatrix}$$

$$= \sum_{i:\,\lambda_i>0} \lambda_i^k \begin{pmatrix} X_i X_i^\dagger - (-1)^k Y_i^* \tilde{Y}_i & X_i Y_i^\dagger - (-1)^k Y_i^* \tilde{X}_i \\ Y_i X_i^\dagger - (-1)^k X_i^* \tilde{Y}_i & Y_i Y_i^\dagger - (-1)^k X_i^* \tilde{X}_i \end{pmatrix}$$

$$= \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}^k \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix}.$$

# Homogeneous equations



$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X_\alpha \\ Y_\alpha \end{pmatrix} = E_\alpha \begin{pmatrix} X_\alpha \\ -Y_\alpha \end{pmatrix}$$

If $\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}$ is positive definite all $E_\alpha \neq 0$; and the eigenvectors form a complete set;

$$\begin{pmatrix} X \\ Y \end{pmatrix} = \sum_\alpha c_\alpha \begin{pmatrix} X_\alpha \\ Y_\alpha \end{pmatrix} .$$

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} - \hbar\omega \begin{pmatrix} X \\ Y \end{pmatrix}$$

$$= \sum_\beta c_\beta (E_\beta - \hbar\omega) \begin{pmatrix} X_\beta \\ Y_\beta \end{pmatrix} = - \begin{pmatrix} W \\ -U^* \end{pmatrix} .$$

Using the orthogonality conditions

$$X_\alpha^\dagger X_\beta - Y_\alpha^\dagger Y_\beta = \frac{E_\alpha}{|E_\alpha|}\delta_{\alpha,\beta} = \mathrm{sign}(E_\alpha)\delta_{\alpha,\beta},$$

$$\sum_\beta c_\beta (E_\beta - \hbar\omega)\big(X_\alpha^\dagger \; Y_\alpha^\dagger\big)\begin{pmatrix} X_\beta \\ Y_\beta \end{pmatrix} = -\big(X_\alpha^\dagger \; Y_\alpha^\dagger\big)\begin{pmatrix} W \\ U^* \end{pmatrix},$$

$$c_\alpha = -\mathrm{sign}(E_\alpha)\frac{X_\alpha^\dagger W + Y_\alpha^\dagger U^*}{E_\alpha - \hbar\omega},$$

$$\begin{pmatrix} X \\ Y \end{pmatrix} = -\sum_\alpha \mathrm{sign}(E_\alpha)\frac{X_\alpha^\dagger W + Y_\alpha^\dagger U^*}{E_\alpha - \hbar\omega}\begin{pmatrix} X_\alpha \\ Y_\alpha \end{pmatrix}$$

If $E_\alpha, (\tilde{X} \; \tilde{Y})$ with $E_\alpha > 0$ is the solution of homogeneous system, then $(-E_\alpha), (Y^\dagger \; X^\dagger)$ is a solution too.

# Solutions II



$$\begin{pmatrix} X \\ Y \end{pmatrix} = \sum_{\alpha:\, E_\alpha > 0} \left\{ \frac{X_\alpha^\dagger W + Y_\alpha^\dagger U^*}{\hbar\omega - E_\alpha} \begin{pmatrix} X_\alpha \\ Y_\alpha \end{pmatrix} - \frac{\tilde{Y}_\alpha W + \tilde{X}_\alpha U^*}{E_\alpha + \hbar\omega} \begin{pmatrix} Y_\alpha^* \\ X_\alpha^* \end{pmatrix} \right\}$$

Lets introduce

$$W_\alpha \equiv X_\alpha^\dagger W + Y_\alpha^\dagger U^*,$$

then

$$\begin{aligned} W_\alpha^* &= \tilde{X}_\alpha W^* + \tilde{Y}_\alpha U, \\ U_\alpha &\equiv X_\alpha^\dagger U + Y_\alpha^\dagger W^*, \\ U_\alpha^* &= \tilde{X}_\alpha U^* + \tilde{Y}_\alpha W \,. \end{aligned}$$

$$\begin{pmatrix} X \\ Y \end{pmatrix} = \sum_{\alpha:\, E_\alpha > 0} \left\{ \frac{W_\alpha}{\hbar\omega - E_\alpha} \begin{pmatrix} X_\alpha \\ Y_\alpha \end{pmatrix} - \frac{U_\alpha^*}{\hbar\omega + E_\alpha} \begin{pmatrix} Y_\alpha^* \\ X_\alpha^* \end{pmatrix} \right\}.$$

# Solutions III



$$|\phi\rangle = \Big(1 + \sum_{p,h} \chi_{p,h}\, a_p^\dagger a_h\Big)|\Phi\rangle, \quad \chi_{p,h} = X_{p,h} e^{-i\omega t} + Y^*_{p,h} e^{i\omega t}$$

$$\begin{aligned}\langle\phi|W(t)|\phi\rangle &= \langle\Phi|\Big(1 + \sum_{p,h} \chi^*_{p,h}\, a_h^\dagger a_p\Big) W \Big(1 + \sum_{p,h} \chi_{p,h}\, a_p^\dagger a_h\Big)|\Phi\rangle \\ &= \sum_{p,h}\Big(\chi^*_{p,h}\,\langle p,h|W(t)|\Phi\rangle + \chi_{p,h}\langle\Phi|W(t)|p,h\rangle\Big) \\ &= \sum_q \Big[\chi_q^*(t)\Big(W_q e^{-i\omega t} + U_q e^{i\omega t}\Big) \\ &\quad + \Big(W_q^* e^{i\omega t} + U_q^* e^{-i\omega t}\Big)\chi_q(t)\Big].\end{aligned}$$

# Solutions IV



$$\langle\phi|W(t)|\phi\rangle = \sum_{\alpha:\, E_\alpha>0}\left(\frac{2|W_\alpha|^2 + e^{i2\omega t}W_\alpha^* U_\alpha + e^{-i2\omega t}W_\alpha U_\alpha^*}{\hbar\omega - E_\alpha} - \frac{2|U_\alpha|^2 + e^{i2\omega t}W_\alpha^* U_\alpha + e^{-i2\omega t}W_\alpha U_\alpha^*}{\hbar\omega + E_\alpha}\right).$$

We will

$$\begin{aligned} \text{interpret} \quad E_\alpha \quad \text{as an} \quad & \langle\alpha|H|\alpha\rangle_{\text{RPA}} - \langle 0|H|0\rangle_{\text{RPA}}\,, \\ \text{and} \quad W_\alpha \quad \text{as an} \quad & \langle\alpha|W|0\rangle_{\text{RPA}}\,. \end{aligned}$$

*The agreement establishes the recipe to calculate the excitation energy and the one-body transition operator matrix elements, There is no explicit calculations of wave functions of the ground and the excited states.*

# Sum Rules



Any quantum mechanical system

$$H\psi_\alpha = E_\alpha \psi_\alpha,$$

$R, S$ — transitional operators.

$$\sum_\beta \Big( \langle\alpha|R|\beta\rangle\langle\beta|S|\alpha\rangle - \langle\alpha|S|\beta\rangle\langle\beta|R|\alpha\rangle \Big)$$

$$= \langle\alpha|RS - SR|\alpha\rangle = \langle\alpha|[R,\, S]_-|\alpha\rangle;$$

$$\sum_\beta (E_\beta - E_\alpha) \Big( \langle\alpha|R|\beta\rangle\langle\beta|S|\alpha\rangle + \langle\alpha|S|\beta\rangle\langle\beta|R|\alpha\rangle \Big)$$

$$= \langle\alpha|[R,\, [H,\, S]_-]_-|\alpha\rangle$$

# Sum Rule I a



$$\sum_{\alpha:\, E_\alpha > 0} \Big( \langle 0|R|\alpha\rangle\langle\alpha|S|0\rangle - \langle 0|S|\alpha\rangle\langle\alpha|R|0\rangle \Big) = \langle\Phi|[R,\, S]_-|\Phi\rangle$$

for any one-body operators $R$ and $S$, where all matrix elements are RPA matrix elements:

$$\langle\alpha|S|0\rangle \equiv \sum_q \left(X^*_{q,\alpha} S_q + Y^*_{q,\alpha} S^{+\,*}_q\right) = X^\dagger_\alpha S + Y^\dagger_\alpha S^{+\,*},$$

$$\langle 0|S|\alpha\rangle = \langle\alpha|S^\dagger|0\rangle^* = \left(X^\dagger_\alpha S^+ + Y^\dagger_\alpha S^*\right)^* = \tilde{X}_\alpha S^{+\,*} + \tilde{Y}_\alpha S\,,$$

here $S^+_q$ are the matrix elements of the operator Hermite conjugated to operator $S$.

## Sum Rule I b

$$\sum_{\alpha:\,E_\alpha>0}\Big(\langle 0|R|\alpha\rangle\langle\alpha|S|0\rangle-\langle 0|S|\alpha\rangle\langle\alpha|R|0\rangle\Big)$$

$$=\sum_{\alpha:\,E_\alpha>0}\Big[\big(\tilde{X}_\alpha R^{+*}+\tilde{Y}_\alpha R\big)\big(X_\alpha^\dagger S+Y_\alpha^\dagger S^{+*}\big)-\big(\tilde{X}_\alpha S^{+*}+\tilde{Y}_\alpha S\big)\big(X_\alpha^\dagger R+Y_\alpha^\dagger R^{+*}\big)\Big]$$

$$=\sum_{\alpha:\,E_\alpha>0}\sum_{q,q_1}\big(R_q^{+*}X_{q,\alpha}X^*_{q_1,\alpha}S_{q_1}$$

$$-S_{q_1}Y_{q_1,\alpha}Y^*_{q,\alpha}R_q^{+*}+R_q^{+*}X_{q,\alpha}Y^*_{q_1,\alpha}S_{q_1}^{+*}-S_{q_1}^{+*}X_{q_1,\alpha}Y^*_{q,\alpha}R_q^{+*}$$

$$+R_qY_{q,\alpha}X^*_{q_1,\alpha}S_{q_1}-S_{q_1}Y_{q_1,\alpha}X^*_{q,\alpha}R_q+R_qY_{q,\alpha}Y^*_{q_1,\alpha}S_{q_1}^{+*}-S_{q_1}^{+*}X_{q_1,\alpha}X^*_{q,\alpha}R_q\big)$$

$$=\sum_{q,q_1}\sum_{\alpha:\,E_\alpha>0}\Big[R_q^{+*}\big(X_{q,\alpha}X^*_{q_1,\alpha}-Y^*_{q,\alpha}Y_{q_1,\alpha}\big)S_{q_1}$$

$$+R_q^{+*}\big(X_{q,\alpha}Y^*_{q_1,\alpha}-Y^*_{q,\alpha}X_{q_1,\alpha}\big)S_{q_1}^{+*}$$

$$+R_q\big(Y_{q,\alpha}X^*_{q_1,\alpha}-X^*_{q,\alpha}Y_{q_1,\alpha}\big)S_{q_1}+R_q\big(Y_{q,\alpha}Y^*_{q_1,\alpha}-X^*_{q,\alpha}X_{q_1,\alpha}\big)S_{q_1}^{+*}\Big]$$

# Sum Rule I c

$$\sum_{\alpha:\, E_\alpha > 0} \left( X_{q,\alpha} X^*_{q_1,\alpha} - Y^*_{q,\alpha} Y_{q_1,\alpha} \right) = \delta_{q,q_1} \,, \qquad \sum_{\alpha:\, E_\alpha > 0} \left( X_{q,\alpha} Y^*_{q_1,\alpha} - Y^*_{q,\alpha} X_{q_1,\alpha} \right) = 0.$$

$$\begin{aligned}
&\sum_{\alpha:\, E_\alpha > 0} \big( \langle 0|R|\alpha\rangle\langle\alpha|S|0\rangle - \langle 0|S|\alpha\rangle\langle\alpha|R|0\rangle \big) \\
&= \sum_q \big( R_q^{+*} S_q - R_q S_q^{+*} \big) \\
&= \sum_q \big( \langle q|R^\dagger|\Phi\rangle^* \langle q|S|\Phi\rangle - \langle q|R|\Phi\rangle \langle q|S^\dagger|\Phi\rangle^* \big) \\
&= \sum_q \big( \langle \Phi|R|q\rangle \langle q|S|\Phi\rangle - \langle \Phi|S|q\rangle \langle q|R|\Phi\rangle \big) \\
&= \langle\Phi|RS|\Phi\rangle - \langle\Phi|SR|\Phi\rangle = \langle\Phi|[R,\, S]_-|\Phi\rangle \,,
\end{aligned}$$

# Sum Rule II



$$\sum_{\alpha E_\alpha > 0} E_\alpha \big( \langle 0|R|\alpha\rangle\langle\alpha|S|0\rangle + \langle 0|S|\alpha\rangle\langle\alpha|R|0\rangle \big) = \langle\Phi|[R,\, [H,\, S]_-]_-|\Phi\rangle$$

With help of

$$\sum_{\alpha:\, E_\alpha > 0} E_\alpha \big( X_{q,\alpha} X^*_{q_1,\alpha} + Y^*_{q,\alpha} Y_{q_1,\alpha} \big) = A_{q,q_1} \,,$$

$$\sum_{\alpha:\, E_\alpha > 0} E_\alpha \big( X^*_{q,\alpha} X_{q_1,\alpha} + Y_{q,\alpha} Y^*_{q_1,\alpha} \big) = A^*_{q,q_1} \,,$$

$$\sum_{\alpha:\, E_\alpha > 0} E_\alpha \big( X_{q,\alpha} Y^*_{q_1,\alpha} + Y^*_{q,\alpha} X_{q_1,\alpha} \big) = -B_{q,q_1} \,,$$

$$\sum_{\alpha:\, E_\alpha > 0} E_\alpha \big( X^*_{q,\alpha} Y_{q_1,\alpha} + Y_{q,\alpha} X^*_{q_1,\alpha} \big) = -B^*_{q,q_1}$$

# Sum Rule II b



$$
\begin{gathered}
\langle\Phi|RHS|\Phi\rangle - \langle\Phi|H|\Phi\rangle\langle\Phi|RS|\Phi\rangle \\
+\langle\Phi|SHR|\Phi\rangle - \langle\Phi|H|\Phi\rangle\langle\Phi|SR|\Phi\rangle \\
-\langle\Phi|H|q,q_1\rangle\langle q|R|\Phi\rangle\langle q_1|S|\Phi\rangle \\
-\langle\Phi|R|q\rangle\langle\Phi|S|q_1\rangle\langle q,q_1|H|\Phi\rangle \\
= \langle\Phi|RHS + SHR|\Phi\rangle \\
-\big(\langle\Phi|H|q_1,q\rangle\langle q_1|S|\Phi\rangle\langle q|R|\Phi\rangle + \langle\Phi|H|\Phi\rangle\langle\Phi|SR|\Phi\rangle\big) \\
-\big(\langle\Phi|R|q\rangle\langle\Phi|S|q_1\rangle\langle q,q_1|H|\Phi\rangle + \langle\Phi|RS|\Phi\rangle\langle\Phi|H|\Phi\rangle\big) \\
= \langle\Phi|RHS - RSH + SHR - HSR|\Phi\rangle \\
= \langle\Phi|[R,\,[H,\,S]_-]_-|\Phi\rangle.
\end{gathered}
$$

## Sum Rule II c

$$\text{For} \quad R = S = P \equiv \sum_{k=1}^{A} P_k$$

$$\sum_{\alpha\colon E_\alpha > 0} E_\alpha |\langle \alpha | P | 0 \rangle_{\mathrm{RPA}}|^2 = \frac{1}{2} \langle \Phi | [P,\, [H,\, P]_-]_- | \Phi \rangle .$$

$$\sum_\alpha \mathrm{sign}(E_\alpha)\, E_\alpha^k \begin{pmatrix} X_\alpha \\ Y_\alpha \end{pmatrix} \left( X_\alpha^\dagger\, Y_\alpha^\dagger \right) = \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}^k \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix}$$

$$\sum_{\alpha\colon E_\alpha > 0} E_\alpha^k \left( |W_\alpha|^2 - (-1)^k |W_\alpha^+|^2 \right) = \left( W^\dagger\, \tilde{W}^+ \right) \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}^k \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} \begin{pmatrix} W \\ W^{+*} \end{pmatrix} .$$

# RPA Phonons I



For any one-body operator $W$

$$W_\alpha = \langle \alpha | W | 0 \rangle_{\mathrm{RPA}} = X^\dagger W + Y^\dagger W^{+*},$$
$$W_\alpha^\dagger = \langle \alpha | W^\dagger | 0 \rangle_{\mathrm{RPA}} = X^\dagger W^{+} + Y^\dagger W^{*},$$

with

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X_\alpha \\ Y_\alpha \end{pmatrix} = E_\alpha \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & -\hat{1} \end{pmatrix} \begin{pmatrix} X_\alpha \\ Y_\alpha \end{pmatrix},$$
$$X_\alpha^\dagger X_\beta - Y_\alpha^\dagger Y_\beta = \mathrm{sign}\,(E_\alpha)\,\delta_{\alpha,\beta}.$$

Positive-energy solution. Let $W = a_p^\dagger a_h$

$$W_{q_1} = \langle p_1 h_1 | a_p^\dagger a_h | \Phi \rangle = \langle \Phi | a_{h_1}^\dagger a_{p_1} a_p^\dagger a_h | \Phi \rangle = \delta_{p,p_1} \delta_{h,h_1}\,,$$
$$W_{q_1}^{+} = \langle p_1 h_1 | a_h^\dagger a_p | \Phi \rangle = \langle \Phi | a_{h_1}^\dagger a_{p_1} a_h^\dagger a_p | \Phi \rangle = 0\,,$$

# RPA Phonons II



$$\langle \alpha | a_p^\dagger a_h | 0 \rangle_{\mathrm{RPA}} = X^*_{ph,\alpha},$$
$$\langle \alpha | a_h^\dagger a_p | 0 \rangle_{\mathrm{RPA}} = Y^*_{ph,\alpha}.$$

Definition of phonon operators:

$$O_\alpha^\dagger = \sum_{ph} \big( X_{ph,\alpha} a_p^\dagger a_h - Y_{ph,\alpha} a_h^\dagger a_p \big),$$
$$O_\alpha = \sum_{ph} \big( X^*_{ph,\alpha} a_h^\dagger a_p - Y^*_{ph,\alpha} a_p^\dagger a_h \big).$$

Inverse transformation:

$$a_p^\dagger a_h = \sum_{\alpha} \big( X^*_{ph,\alpha} O_\alpha^\dagger + Y_{ph,\alpha} O_\alpha \big),$$
$$a_h^\dagger a_p = \sum_{\alpha} \big( X_{ph,\alpha} O_\alpha + Y^*_{ph,\alpha} O_\alpha^\dagger \big).$$

$$
\begin{aligned}
&\sum_{\alpha}\big(X^*_{ph,\alpha}O^\dagger_\alpha + Y_{ph,\alpha}O_\alpha\big)\\
&= \sum_{p_1h_1}\sum_{\alpha}\Big[\big(X^*_{ph,\alpha}X_{p_1h_1,\alpha} - Y_{ph,\alpha}Y^*_{p_1h_1,\alpha}\big)a^\dagger_{p_1}a_{h_1}\\
&+\big(Y_{ph,\alpha}X^*_{p_1h_1,\alpha} - X^*_{ph,\alpha}Y_{p_1h_1,\alpha}\big)a^\dagger_h a_p\Big] = a^\dagger_p a_h\,.
\end{aligned}
$$

Main advantage:

$$
\begin{aligned}
\langle\beta|O^\dagger_\alpha|0\rangle_{\mathrm{RPA}} &= \sum_{ph}\big(X_{ph,\alpha}\langle\beta|a^\dagger_p a_h|0\rangle - Y_{ph,\alpha}\langle\beta|a^\dagger_h a_p|0\rangle\big)\\
&= \sum_{ph}\big(X_{ph,\alpha}X^*_{ph,\beta} - Y_{ph,\alpha}Y^*_{ph,\beta}\big) = \delta_{\alpha,\beta}\,,\\
\langle\beta|O_\alpha|0\rangle_{\mathrm{RPA}} &= 0\,.
\end{aligned}
$$

# RPA Phonons IV

$$
\begin{aligned}
\langle \alpha | R | 0 \rangle_{\mathrm{RPA}} &= \sum_{ph} \Big( X^*_{ph,\alpha} \langle ph | R | \Phi \rangle + \langle \Phi | R | ph \rangle Y^*_{ph,\alpha} \Big), \\
\langle \Phi | O_\alpha | ph \rangle &= \sum_{p_1 h_1} \Big( X^*_{p_1 h_1,\alpha} \langle \Phi | a^\dagger_{h_1} a_{p_1} a^\dagger_p a_h | \Phi \rangle - Y^*_{p_1 h_1,\alpha} \langle \Phi | a^\dagger_{p_1} a_{h_1} a^\dagger_p a_h | \Phi \rangle \Big) \\
&= \sum_{p_1 h_1} X^*_{p_1 h_1,\alpha} \delta_{p,p_1} \delta_{h,h_1} = X^*_{ph,\alpha} \,, \\
\langle ph | O_\alpha | \Phi \rangle &= \sum_{p_1 h_1} \Big( X^*_{p_1 h_1,\alpha} \langle \Phi | a^\dagger_h a_p a^\dagger_{h_1} a_{p_1} | \Phi \rangle - Y^*_{p_1 h_1,\alpha} \langle \Phi | a^\dagger_h a_p a^\dagger_{p_1} a_{h_1} | \Phi \rangle \Big) \\
&= - \sum_{p_1 h_1} Y^*_{p_1 h_1,\alpha} \delta_{p,p_1} \delta_{h,h_1} = - Y^*_{ph,\alpha} \,, \\
\langle \alpha | R | 0 \rangle_{\mathrm{RPA}} &= \sum_{ph} \Big( \langle \Phi | O_\alpha | ph \rangle \langle ph | R | \Phi \rangle - \langle \Phi | R | ph \rangle \langle ph | O_\alpha | \Phi \rangle \Big) \\
&= \langle \Phi | O_\alpha R - R O_\alpha | \Phi \rangle = \langle \Phi | [O_\alpha, R]_- | \Phi \rangle .
\end{aligned}
$$

# RPA Phonons V



Phonon operators as boson ones.

$$\text{For } R = O_\beta^\dagger : \quad \langle\Phi|\big[O_\alpha, O_\beta^\dagger\big]_-|\Phi\rangle = \langle\alpha|O_\beta^\dagger|0\rangle_{\text{RPA}} = \delta_{\alpha,\beta},$$
$$\langle\Phi|\big[O_\alpha, O_\beta\big]_-|\Phi\rangle = \langle\alpha|O_\beta|0\rangle_{\text{RPA}} = 0.$$

$$E_\alpha\langle\alpha|R|0\rangle_{\text{RPA}} = E_\alpha\big(X_\alpha^\dagger R + Y_\alpha^\dagger R^{+*}\big),$$
$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} X_\alpha \\ Y_\alpha \end{pmatrix} = E_\alpha\begin{pmatrix} X_\alpha \\ -Y_\alpha \end{pmatrix},$$
$$(X_\alpha^\dagger, Y_\alpha^\dagger)\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}^\dagger = E_\alpha(X_\alpha^\dagger, -Y_\alpha^\dagger),$$
$$E_\alpha X_\alpha^\dagger = X_\alpha^\dagger A + Y_\alpha^\dagger B^*,$$
$$E_\alpha Y_\alpha^\dagger = -\big(X_\alpha^\dagger B + Y_\alpha^\dagger A^*\big)$$

# RPA Phonons VI



$$
\begin{aligned}
E_\alpha \langle \alpha | R | 0 \rangle_{\mathrm{RPA}} &= \left( X_\alpha^\dagger A + Y_\alpha^\dagger B^* \right) R - \left( X_\alpha^\dagger B + Y_\alpha^\dagger A^* \right) R^{+*} \\
&= \langle \Phi | \left( O_\alpha H - H O_\alpha \right) R + R \left( H O_\alpha - O_\alpha H \right) | \Phi \rangle \\
&= \langle \Phi | \left[ [O_\alpha, H]_-, R \right]_- | \Phi \rangle .
\end{aligned}
$$

## Formal development

Phonon operator definition:

$$O_\alpha = \sum_{p,h} \big( X^*_{ph,\alpha} a^\dagger_h a_p - Y^*_{ph,\alpha} a^\dagger_p a_h \big), \quad O^\dagger_\alpha = \sum_{p,h} \big( X_{ph,\alpha} a^\dagger_p a_h - Y_{ph,\alpha} a^\dagger_h a_p \big),$$

$p$ ($h$) label the unoccupied (occupied) orbitals in the mean field

$$a_p|\Phi\rangle = 0 \quad \text{and} \quad a^\dagger_h|\Phi\rangle = 0, \quad \Phi \text{ is non-degenerated}$$

Phonon amplitudes $X_{ph,\alpha}$ and $Y_{ph,\alpha}$:

$$\langle\Phi|\big[[O_\alpha, H], a^\dagger_p a_h\big]|\Phi\rangle = E_\alpha \langle\Phi|\big[O_\alpha, a^\dagger_p a_h\big]|\Phi\rangle,$$

$$\langle\Phi|\big[[O_\alpha, H], a^\dagger_h a_p\big]|\Phi\rangle = E_\alpha \langle\Phi|\big[O_\alpha, a^\dagger_h a_p\big]|\Phi\rangle.$$

Norm conditions: $\langle\Phi|\big[O_\alpha, O^\dagger_\beta\big]_-|\Phi\rangle = \mathrm{sign}(E_\alpha)\,\delta_{\alpha,\beta}\,;$

Positive $E_\alpha$ — excitation energies.

Transition amplitudes: $\langle\alpha|R|0\rangle_{\mathrm{RPA}} \equiv \langle\Phi|\big[O_\alpha, R\big]|\Phi\rangle\,.$

# Open Shell Nuclei. Pairing correlations.

Closed shell. Hartree-Fock conditions

$$\langle \Phi | a_h^\dagger a_p H | \Phi \rangle = 0.$$

Non-closed (open) shells:

$$\exists h : a_h | \Phi \rangle = 0,$$
$$\exists p : a_p^\dagger | \Phi \rangle = 0$$

Hartree-Fock conditions may be replaced by

$$\langle C | \alpha \alpha' H | C \rangle = 0,$$

where operators $\alpha$ and $\alpha'$ are the supperpositions of particle creation and destruction operators.

# Canonical transformations

$$H = \sum_{k,l} T(k,l) a_k^\dagger a_l + \frac{1}{2} \sum_{k,l,n,m} U(k,l;m,n) a_k^\dagger a_l^\dagger a_n a_m$$

$$H^\dagger = H \longrightarrow T^*(k,l) = T(l,k) \text{ and}$$

$$U^*(k,l;n,m) = U(m,n;l,k)$$

$$U(k,l;nm) = -U(k,l;m,n) = -U(l,k;n,m) = U(l,k;m,n)$$

$$\left[a_k,\, a_l^\dagger\right]_+ \equiv a_k a_l^\dagger + a_l^\dagger a_k = \delta_{k,l}; \quad [a_k,\, a_l]_+ = \left[a_k^\dagger,\, a_l^\dagger\right]_+ = 0.$$

$$T(k,l) = T_0(k,l) - \lambda\, \delta_{k,l}.$$

# General Bogoliubov-Valatin transformation I



$$a_k = \sum_\nu \left( u_{k,\nu}\alpha_\nu + v_{k,\nu}\alpha_\nu^\dagger \right),$$

$$a_l^\dagger = \sum_\nu \left( u_{l,\mu}^* \alpha_\mu^\dagger + v_{l,\mu}^* \alpha_\mu \right).$$

$$\left[\alpha_\nu,\, \alpha_\mu^\dagger\right]_+ = \delta_{\nu,\mu}; \quad [\alpha_\nu,\, \alpha_\mu]_+ = \left[\alpha_\nu^\dagger,\, \alpha_\mu^\dagger\right]_+ = 0$$

# General Bogoliubov-Valatin transformation II



To keep the anticommutation relations:

$$\left[a_k,\, a_l^\dagger\right]_+ = \sum_{\nu,\mu}\left(u_{k,\nu}u_{l,\mu}^*\left[\alpha_\nu,\, \alpha_\mu^\dagger\right]_+ + v_{k,\nu}v_{l,\mu}^*\left[\alpha_\nu^\dagger,\, \alpha_\mu\right]_+\right)$$

$$= \sum_{\nu,\mu}\left(u_{k,\nu}u_{l,\mu}^*\delta_{\nu,\mu} + v_{k,\nu}v_{l,\mu}^*\delta_{\nu,\mu}\right)$$

$$= \sum_{\nu}\left(u_{k,\nu}u_{l,\nu}^* + v_{k,\nu}v_{l,\nu}^*\right) = \delta_{k,l}$$

$$[a_k,\, a_l]_+ = 0 \longrightarrow \sum_\nu \left(u_{k,\nu}v_{l,\nu} + v_{k,\nu}u_{l,\nu}\right) = 0$$

$$\left[a_k^\dagger,\, a_l^\dagger\right]_+ = 0 \longrightarrow \sum_\nu \left(u_{k,\nu}^*v_{l,\nu}^* + v_{k,\nu}^*u_{l,\nu}^*\right) = 0.$$

# Matrices of the coefficients



Collect the coefficients of B-V transformation

$$\|\mathcal{U}\|_{k,\nu} = u_{k,\nu} \quad \text{and} \quad \|\mathcal{V}\|_{k,\nu} = v_{k,\nu}$$

$$\sum_{\nu} \left( u_{k,\nu} u^*_{l,\nu} + v_{k,\nu} v^*_{l,\nu} \right) = \|\mathcal{U}\mathcal{U}^\dagger + \mathcal{V}\mathcal{V}^\dagger\|_{k,l} = \delta_{k,l}$$

$$\|U^\dagger\|_{\nu,k} = \|U\|^*_{k,\nu} = u^*_{k,\nu} \quad \text{and} \quad \|V^\dagger\|_{\nu,k} = v^*_{k,\nu}$$

$$\mathcal{U}\mathcal{U}^\dagger + \mathcal{V}\mathcal{V}^\dagger = \mathcal{I},$$

$$\mathcal{U}\tilde{\mathcal{V}} + \mathcal{V}\tilde{\mathcal{U}} = 0,$$

$$\mathcal{U}^*\mathcal{V}^\dagger + \mathcal{V}^*\mathcal{U}^\dagger = 0.$$

# Unitary matrix



$$\mathbb{U} = \begin{Vmatrix} \mathcal{U} & \mathcal{V} \\ \mathcal{V}^* & \mathcal{U}^* \end{Vmatrix},$$

$$\begin{aligned} \mathbb{U}\mathbb{U}^\dagger &= \begin{Vmatrix} \mathcal{U} & \mathcal{V} \\ \mathcal{V}^* & \mathcal{U}^* \end{Vmatrix} \begin{Vmatrix} \mathcal{U}^\dagger & \tilde{\mathcal{V}} \\ \mathcal{V}^\dagger & \tilde{\mathcal{U}} \end{Vmatrix} \\ &= \begin{Vmatrix} \mathcal{U}\mathcal{U}^\dagger + \mathcal{V}\mathcal{V}^\dagger & \mathcal{U}\tilde{\mathcal{V}} + \mathcal{V}\tilde{\mathcal{U}} \\ \mathcal{V}^*\mathcal{U}^\dagger + \mathcal{U}^*\mathcal{V}^\dagger & \mathcal{V}^*\tilde{\mathcal{V}} + \mathcal{U}^*\tilde{\mathcal{U}} \end{Vmatrix} \\ &= \begin{Vmatrix} \mathcal{I} & 0 \\ 0 & \mathcal{I} \end{Vmatrix}, \end{aligned}$$

and

$$\mathbb{U}^\dagger\mathbb{U} = \begin{Vmatrix} \mathcal{U}^\dagger & \tilde{\mathcal{V}} \\ \mathcal{V}^\dagger & \tilde{\mathcal{U}} \end{Vmatrix} \begin{Vmatrix} \mathcal{U} & \mathcal{V} \\ \mathcal{V}^* & \mathcal{U}^* \end{Vmatrix} = \begin{Vmatrix} \mathcal{I} & 0 \\ 0 & \mathcal{I} \end{Vmatrix}.$$

# Compensation of dangerous diagrams I



$$\langle \alpha_\nu \alpha_\mu H \rangle_0 \equiv (C_0^*, \alpha_\nu \alpha_\mu H C_0) = 0,$$

$$\text{where} \quad \alpha_\nu C_0 = 0 \quad \text{and} \quad C_0^* \alpha_\nu^\dagger = 0.$$

$$\text{Quasiparticle vacuum state} \;\; C_0 = \prod_\nu \alpha_\nu |0\rangle$$

$$\text{with} \;\; a_k|0\rangle = 0$$

$$(\textit{compare to} \;\; \langle \Phi | a_h^\dagger a_p H | \Phi \rangle = 0).$$

$$\mathfrak{A}(k,l) \equiv \langle [a_k a_l, \, H] \rangle_0 \, ,$$

$$\mathfrak{B}(k,l) \equiv \left\langle \left[ a_k^\dagger a_l, \, H \right] \right\rangle_0 .$$

# Compensation of dangerous diagrams II

$$\mathfrak{A}(k,l) = \sum_{\nu,\mu} \left\langle \left[ \left( u_{k,\nu}\alpha_\nu + v_{k,\nu}\alpha_\nu^\dagger \right) \left( u_{l,\mu}\alpha_\mu + v_{l,\mu}\alpha_\mu^\dagger \right),\ H \right] \right\rangle_0$$

$$= \sum_{\nu,\mu} \Bigg( u_{k,\nu}u_{l,\mu} \left\langle \alpha_\nu\alpha_\mu H - H\alpha_\nu\alpha_\mu \right\rangle_0 + u_{k,\nu}v_{l,\mu} \left\langle \alpha_\nu\alpha_\mu^\dagger H - H\alpha_\nu\alpha_\mu^\dagger \right\rangle_0$$

$$+ v_{k,\nu}u_{l,\mu} \left\langle \alpha_\nu^\dagger\alpha_\mu H - H\alpha_\nu^\dagger\alpha_\mu \right\rangle_0 + v_{k,\nu}v_{l,\mu} \left\langle \alpha_\nu^\dagger\alpha_\mu^\dagger H - H\alpha_\nu^\dagger\alpha_\mu^\dagger \right\rangle_0 \Bigg)$$

$$= \sum_{\nu,\mu} \Bigg( u_{k,\nu}u_{l,\mu} \left\langle \alpha_\nu\alpha_\mu H \right\rangle + u_{k,\nu}v_{l,\mu} \left\langle \alpha_\nu\alpha_\mu^\dagger H - H\alpha_\nu\alpha_\mu^\dagger \right\rangle_0$$

$$- v_{k,\nu}v_{l,\mu} \left\langle H\alpha_\nu^\dagger\alpha_\mu^\dagger \right\rangle_0 \Bigg),$$

# Compensation of dangerous diagrams III

but

$$\left\langle \alpha_\nu \alpha_\mu^\dagger H - H \alpha_\nu \alpha_\mu^\dagger \right\rangle_0 = \left\langle \left( \delta_{\nu,\mu} - \alpha_\mu^\dagger \alpha_\nu \right) H - H \left( \delta_{\nu,\mu} - \alpha_\mu^\dagger \alpha_\nu \right) \right\rangle_0$$
$$= \delta_{\nu,\mu} \left\langle H - H \right\rangle_0 = 0.$$

$$\mathfrak{A}(k,l) = \sum_{\nu,\mu} \left( u_{k,\nu} u_{l,\mu} \left\langle \alpha_\nu \alpha_\mu H \right\rangle + v_{k,\nu} v_{l,\mu} \left\langle \alpha_\nu \alpha_\mu H \right\rangle_0^* \right) = 0,$$

$$\text{if} \quad \left\langle \alpha_\nu \alpha_\mu H \right\rangle_0 = 0;$$

$$\mathfrak{B}(k,l) \equiv \left\langle \left[ a_k^\dagger a_l ,\, H \right] \right\rangle_0$$
$$= \sum_{\nu,\mu} \left( -u_{k,\nu}^* v_{l,\mu} \left\langle H \alpha_\nu^\dagger \alpha_\mu^\dagger \right\rangle_0 + v_{k,\nu}^* u_{l,\mu} \left\langle \alpha_\nu \alpha_\mu H \right\rangle_0 \right) = 0$$

# Compensation of dangerous diagrams IV



Therefore,

$$\langle \alpha_\nu \alpha_\mu H \rangle_0 = 0 \longrightarrow \begin{cases} \mathfrak{A}(k,l) = 0, \\ \mathfrak{B}(k,l) = 0. \end{cases}$$

One can show that

$$\left. \begin{aligned} \mathfrak{A}(k,l) = 0 \\ \mathfrak{B}(k,l) = 0 \end{aligned} \right\} \longrightarrow \langle \alpha_\nu \alpha_\mu H \rangle_0 = 0.$$

The forms $\mathfrak{A}(k,l)$ and $\mathfrak{B}(k,l)$ are not independent:

$$\left\langle \alpha_\nu^\dagger \alpha_\mu H - H \alpha_\nu^\dagger \alpha_\mu \right\rangle_0 = \left\langle \left[ \alpha_\nu^\dagger \alpha_\mu,\, H \right] \right\rangle_0 = 0.$$

# Compensation of dangerous diagrams V



From the unitarity of matrix $\mathbb{U}$

$$\mathbb{U}^\dagger \cdot \mathbb{U} = \begin{Vmatrix} \mathcal{U}^\dagger & \tilde{\mathcal{V}} \\ \mathcal{V}^\dagger & \tilde{\mathcal{U}} \end{Vmatrix} \cdot \begin{Vmatrix} \mathcal{U} & \mathcal{V} \\ \mathcal{V}^* & \mathcal{U}^* \end{Vmatrix} = \begin{Vmatrix} \mathcal{I} & 0 \\ 0 & \mathcal{I} \end{Vmatrix}$$

$$\sum_l \left(u^*_{l,\nu} u_{l,\mu} + v_{l,\nu} v^*_{l,\mu}\right) = \delta_{\nu,\mu},$$

$$\sum_l \left(v^*_{l,\nu} u_{l,\mu} + u_{l,\nu} v^*_{l,\mu}\right) = 0.$$

$$\begin{array}{c|l} u^*_{k,\nu} & a_k = \sum_\mu \left(u_{k,\mu}\alpha_\mu + v_{k,\mu}\alpha^\dagger_\mu\right) \\ v_{k,\nu} & a^\dagger_k = \sum_\mu \left(u^*_{k,\mu}\alpha^\dagger_\mu + v^*_{k,\mu}\alpha_\mu\right) \end{array}$$

# Compensation of dangerous diagrams VI



$$\sum_k \left(u_{k,\nu}^* a_k + v_{k,\nu} a_k^\dagger\right) = \sum_\mu \sum_k \Big[\left(u_{k,\nu}^* u_{k,\mu} + v_{k,\nu} v_{k,\mu}^*\right)\alpha_\mu$$
$$+ \left(u_{k,\nu}^* v_{k,\mu} + v_{k,\nu} u_{k,\mu}^*\right)\alpha_\mu^\dagger\Big]$$
$$= \alpha_\nu;$$
$$\alpha_\nu = \sum_k \left(u_{k,\nu}^* a_k + v_{k,\nu} a_k^\dagger\right),$$
$$\alpha_\nu^\dagger = \sum_k \left(u_{k,\nu} a_k^\dagger + v_{k,\nu}^* a_k\right).$$

The identity $\left\langle \left[\alpha_\nu^\dagger \alpha_\mu,\, H\right]\right\rangle_0 = 0$ shows that the forms $\mathfrak{A}(k,l)$ and $\mathfrak{B}(k,l)$ are not independent.

# Evaluation of the forms

$$\begin{aligned}
\mathfrak{A}(k,l) &= \langle \left[ a_k a_l, \sum_{m,n} T(m,n)\, a_m^\dagger a_n + \frac{1}{2} \sum_{m,n,n',m'} U(m,n;n',m')\, a_m^\dagger a_n^\dagger a_{n'} a_{m'} \right]_- \rangle_0 \\
&= \sum_m \{ T(k,m) \langle a_m a_l \rangle_0 + T(l,m) \langle a_k a_m \rangle_0 \} + \sum_{m,n} U(k,l;n,m) \langle a_m a_n \rangle_0 \\
&+ \sum_{m,n',m'} \left\{ U(k,m;n',m') \langle a_m^\dagger a_l a_{n'} a_{m'} \rangle_0 + U(m,l;n',m') \langle a_m^\dagger a_k a_{n'} a_{m'} \rangle_0 \right\}, \\
\mathfrak{B}(k,l) &= \langle \left[ a_k^\dagger a_l,\ H \right]_- \rangle_0 \\
&= \sum_m \left\{ T(l,m) \langle a_k^\dagger a_m \rangle_0 - T(m,k) \langle a_m^\dagger a_l \rangle_0 \right\} \\
&+ \sum_{m,n',m'} \left\{ U(l,m;n',m') \langle a_k^\dagger a_m^\dagger a_{n'} a_{m'} \rangle_0 - U(m',n';m,k) \langle a_{m'}^\dagger a_{n'}^\dagger a_m a_l \rangle_0 \right\}.
\end{aligned}$$

$$F(k,l) \equiv \langle a_k^\dagger a_l \rangle_0 = \sum_{\nu,\mu} \langle (u_{k,\nu}^* \alpha_\nu^\dagger + v_{k,\nu}^* \alpha_\nu)(u_{l,\mu}\alpha_\mu + v_{l,\mu}\alpha_\mu^\dagger)\rangle_0$$

$$= \sum_{\nu,\mu} v_{k,\nu}^* v_{l,\mu} \langle \alpha_\nu \alpha_\mu^\dagger \rangle_0$$

$$= \sum_{\nu} v_{k,\nu}^* v_{l,\nu}$$

$$\Phi(k,l) \equiv \langle a_k a_l \rangle_0 = \sum_{\nu,\mu} \langle (u_{k,\nu} \alpha_\nu + v_{k,\nu} \alpha_\nu^\dagger)(u_{l,\mu}\alpha_\mu + v_{l,\mu}\alpha_\mu^\dagger)\rangle_0$$

$$= \sum_{\nu,\mu} u_{k,\nu} v_{l,\mu} \langle \alpha_\nu \alpha_\mu^\dagger \rangle_0$$

$$= \sum_{\nu} u_{k,\nu} v_{l,\nu}$$

# Two-body densities I

$$
\begin{aligned}
F_2(k,l;n,m) &\equiv \langle a_k^\dagger a_l^\dagger a_n a_m \rangle_0 \\
&= \sum_{\nu,\nu'} \langle (u_{k,\nu}^* \alpha_\nu^\dagger + v_{k,\nu}^* \alpha_\nu) a_l^\dagger a_n (u_{m,\nu'} \alpha_{\nu'} + v_{m,\nu'} \alpha_{\nu'}^\dagger) \rangle_0 \\
&= \sum_{\nu,\mu,\mu'\nu'} v_{k,\nu}^* v_{m,\nu'} \langle \alpha_\nu (u_{l,\mu}^* \alpha_\mu^\dagger + v_{l,\mu}^* \alpha_\mu)(u_{n,\mu'} \alpha_{\mu'} + v_{n,\mu'} \alpha_{\mu'}^\dagger) \alpha_{\nu'}^\dagger \rangle_0 \\
&= \sum_{\nu,\mu,\mu'\nu'} v_{k,\nu}^* v_{m,\nu'} \langle \alpha_\nu \left\{ u_{l,\mu}^* u_{n,\mu'} \alpha_\mu^\dagger \alpha_{\mu'} + v_{l,\mu}^* v_{n,\mu'} \alpha_\mu \alpha_{\mu'}^\dagger \right\} \alpha_{\nu'}^\dagger \rangle_0 \\
&= \sum_{\nu,\mu,\mu'\nu'} \left\{ v_{k,\nu}^* v_{m,\nu'} u_{l,\mu}^* u_{n,\mu'} \langle \alpha_\nu \alpha_\mu^\dagger \alpha_{\mu'} \alpha_{\nu'}^\dagger \rangle_0 \right. \\
&\qquad \left. + v_{k,\nu}^* v_{m,\nu'} v_{l,\mu}^* v_{n,\mu'} \langle \alpha_\nu \alpha_\mu \alpha_{\mu'}^\dagger \alpha_{\nu'}^\dagger \rangle_0 \right\}
\end{aligned}
$$

# Two-body densities II

$$\langle \alpha_\nu \alpha^\dagger_\mu \alpha_{\mu'} \alpha^\dagger_{\nu'} \rangle_0 = \delta_{\nu,\mu}\delta_{\mu',\nu'}, \quad \langle \alpha_\nu \alpha_\mu \alpha^\dagger_{\mu'} \alpha^\dagger_{\nu'} \rangle_0 = \delta_{\nu,\nu'}\delta_{\mu,\mu'} - \delta_{\nu,\mu'}\delta_{\nu,\mu'}$$

$$\begin{aligned}
F_2(k,l;n,m) &= \Big(\sum_\nu v^*_{k,\nu} u^*_{l,\nu}\Big)\Big(\sum_\mu v_{n,\mu} u_{m,\mu}\Big) \\
&\quad + \Big(\sum_\nu v^*_{l,\nu} v_{n,\nu}\Big)\Big(\sum_\mu v^*_{k,\mu} v_{m,\mu}\Big) - \Big(\sum_\nu v^*_{k,\nu} v_{n,\nu}\Big)\Big(\sum_\mu v^*_{l,\mu} v_{m,\mu}\Big) \\
&= F(k,m)F(l,n) - F(k,n)F(l,m) + \Phi^*(k,l)\,\Phi(m,n), \\
\Phi_2(k;l,m,n) &\equiv \langle a^\dagger_k a_l a_m a_n \rangle_0 \\
&= F(k,l)\,\Phi(m,n) - F(k,m)\,\Phi(l,n) + F(k,n)\,\Phi(l,m).
\end{aligned}$$

$$\mathfrak{A}(k,l|F\Phi) = \sum_m \{E(k,m)\Phi(m,l) + E(l,m)\Phi(k,m)\}$$
$$+ S(k,l) - \sum_m \{F(m,k)S(m,l) + S(k,m)F(m,l)\},$$

where

$$E(k,l) \equiv T(k,l) + \sum_{m,n} \{U(k,m;n,l) - U(k,m;l,n)\} F(m,n),$$
$$S(k,l) \equiv \sum_{n,m} U(k,l;n,m)\,\Phi(m,n).$$

Number of particles in the system

$$(C_0^*, \sum_k a_k^\dagger a_k C_0) = \sum_k F(k,k) = N.$$

Finally:

$$\langle \alpha_k \alpha_l H \rangle_0 = 0 \longrightarrow \begin{cases} \mathfrak{A}(k,l|F,\Phi) = 0 \\ \mathfrak{B}(k,l|F,\Phi) = 0 \end{cases}$$

with subsidiary conditions

$$F(k,l) = \sum_\nu v^*_{k,\nu} v_{l,\nu} \,,$$

$$\Phi(k,l) = \sum_\nu u_{k,\nu} v_{l,\nu} \,,$$

where $u_{k,\nu}$ and $v_{k,\nu}$ are the coefficients of B-V transformation. The problem: to express the subsidiary conditions for densities $F(k,l)$ and $\Phi(k,l)$ in terms of the densities.

# Properties of coefficients



The coefficients of B-V transformations form a unitary matrix

$$\mathbb{U} = \begin{Vmatrix} \mathcal{U} & \mathcal{V} \\ \mathcal{V}^* & \mathcal{U}^* \end{Vmatrix}, \quad \|\mathcal{U}\|_{k,\nu} = u_{k,\nu} \quad \text{and} \quad \|\mathcal{V}\|_{k,\nu} = v_{k,\nu}.$$

Unitarity — rows of $\mathbb{U}$ are orthonormal:

$$\mathbb{U} \cdot \mathbb{U}^\dagger = \mathbb{I} \quad \text{or} \quad \begin{cases} \sum\limits_\nu (u_{k,\nu} u^*_{l,\nu} + v_{k,\nu} v^*_{l,\nu}) & = \delta_{k,l} \\ \sum\limits_\nu (u_{k,\nu} v_{l,\nu} + v_{k,\nu} u_{l,\nu}) & = 0 \\ \text{and h.c.} \end{cases}$$

$$\mathbb{K}_1 \equiv \sum_\nu \begin{Vmatrix} u_{k,\nu} \\ v^*_{k,\nu} \end{Vmatrix} \begin{Vmatrix} u^*_{l,\nu} & v_{l,\nu} \end{Vmatrix}, \quad \mathbb{K}_1^\dagger = \mathbb{K}_1, \quad \mathbb{K}_1 \cdot \mathbb{K}_1 = \mathbb{K}_1$$

$\mathbb{K}_1$ — projection matrix

# Projection matrices I



$$\mathbb{K}_1 = \left\| \begin{array}{cc} \sum\limits_\nu u_{k,\nu} u^*_{l,\nu} & \sum\limits_\nu u_{k,\nu} v_{l,\nu} \\ \sum\limits_\nu v^*_{k,\nu} u^*_{l,\nu} & \sum\limits_\nu v^*_{k,\nu} v_{l,\nu} \end{array} \right\| = \left\| \begin{array}{cc} \delta_{k,l} - F^*(k,l) & \Phi(k,l) \\ -\Phi^*(k,l) & F(k,l) \end{array} \right\|$$

$$\mathbb{K}_2 \equiv \sum_\nu \left\| \begin{array}{c} v_{k,\nu} \\ u^*_{k,\nu} \end{array} \right\| \left\| \begin{array}{cc} v^*_{l,\nu} & u_{l,\nu} \end{array} \right\|, \quad \mathbb{K}_2^\dagger = \mathbb{K}_2, \quad \mathbb{K}_2 \cdot \mathbb{K}_2 = \mathbb{K}_2$$

$$\mathbb{K}_2 = \left\| \begin{array}{cc} F^*(k,l) & -\Phi(k,l) \\ \Phi^*(k,l) & \delta_{k,l} - F(k,l) \end{array} \right\|$$

$$\mathbb{K}_1 + \mathbb{K}_2 = \mathbb{I} \longrightarrow \mathbb{K}_1 \cdot \mathbb{K}_2 = 0$$

# Projection matrices II



$$\left\| \begin{array}{cc} \delta_{k,m} - F^*(k,m) & \Phi(k,m) \\ -\Phi^*(k,m) & F(k,m) \end{array} \right\| \cdot \left\| \begin{array}{cc} F^*(m,l) & -\Phi(m,l) \\ \Phi^*(m,l) & \delta_{m,l} - F(m,l) \end{array} \right\| = 0$$

Matrix element $(2,2)$:

$$\sum_m \Phi^*(k,m)\,\Phi(m,l) + F(k,l) - \sum_m F(k,m)F(m,l) = 0$$

$$F(k,l) = \sum_m \{F(k,m)F(m,l) + \Phi^*(m,k)\,\Phi(m,l)\}$$

Matrix element $(1,2)$:

$$-\Phi(k,l) + \sum_m F^*(k,m)\,\Phi(m,l) + \Phi(k,l) - \sum_m \Phi(k,m)F(m,l) = 0$$

$$\sum_m \{\Phi(l,m)F(m,k) + \Phi(k,m)F(m,l)\} = 0$$

Also valid: any $F(k,l)$ and $\Phi(k,l)$ such as

$$F^*(k,l) = F(l,m),$$
$$\Phi(k,l) = -\Phi(l,k),$$
$$F(k,l) = \sum_m \left\{F(k,m)F(m,l) + \Phi^*(m,k)\,\Phi(m,l)\right\},$$
$$\sum_m \left\{\Phi(l,m)F(m,k) + \Phi(k,m)F(m,l)\right\} = 0$$

can be expressed as

$$F(k,l) = \sum_\nu v^*_{k,\nu} v_{l,\nu}, \quad \Phi(k,l) = \sum_\nu u_{k,\nu} v_{l,\nu}$$

where $u_{k,\nu}$ and $v_{k,\nu}$ are coefficients of a B-V transformation.

The set of equation.

$$\mathfrak{A}(k, l|F, \Phi) = 0,$$

$$\mathfrak{B}(k, l|F, \Phi) = 0,$$

$$\sum_k F(k, k) = N,$$

$$F^\dagger = F,$$

$$\tilde{\Phi} = -\Phi,$$

$$F = F^2 + \Phi^\dagger \Phi,$$

$$-\tilde{F}\,\Phi + \Phi F = 0.$$

Eigenvalue problem:

$$\mathbb{K}_1 x = \lambda x, \quad \mathbb{K}_1^2 x = \lambda^2 x,$$
$$\mathbb{K}_1^2 = \mathbb{K}_1, \quad ,\lambda^2 = \lambda, \quad \lambda = 0,\, 1$$

Vectors (columns of matrix $\mathbb{U}$) $\left\| \begin{matrix} u_{k,\nu} \\ v_{k,\nu} \end{matrix} \right\|$ belong to $\lambda = 1$. Any unitary transformation among them conserve the matrix $\mathbb{K}_1$, and the forms $F(k,l|F\Phi)$ and $\Phi(k,l|F\Phi)$. This freedom allows one to simplify B-V transformation.

Spherical symmetry:

$$a_{kj,m} = u_{kj}\alpha_{kj,m} + (-1)^{j-m} v_{kj}\alpha^\dagger_{kj,-m}\,, \quad m = -j, -j+1, \ldots j.$$

Axial symmetry:

$$a_{r,\sigma} = u_r \alpha_{r,\sigma} + \sigma v_r \alpha^\dagger_{r,-\sigma}, \quad \sigma = \pm 1.$$

# Variational description



$$H_0 = \sum_{s,\sigma} E_0(s) a^\dagger_{s\sigma} a_{s\sigma} - G \sum_{s,s'} a^\dagger_{s,+} a^\dagger_{s,-} a_{s',-} a_{a',+},$$

$$E_0(s) \neq E_0(s') \text{ if } s \neq s', \ \sigma = \pm 1,$$

Number of particles, $N$, is even.

$$a_{s,\sigma} = u_s \alpha_{s,-\sigma} + \sigma v_s \alpha^\dagger_{s,\sigma} \quad \text{and} \quad a^\dagger_{s,\sigma} = u_s \alpha^\dagger_{s,-\sigma} + \sigma v_s \alpha_{s,\sigma},$$

$$\eta_s \equiv u_s^2 + v_s^2 - 1 = 0$$

$$\delta \left\{ \langle H \rangle_0 - \lambda \left( \langle \sum_{s,\sigma} a^\dagger_{s,\sigma} a_{s,\sigma} \rangle_0 - N \right) - \sum_s \mu_s \eta_s \right\} = 0$$

$$\text{where } \langle \ldots \rangle_0 = (C_0^*, \ldots C_0), \text{ with } \alpha_{s,\sigma} C_0 = 0$$

$$2 \left[ E_0(s) - \frac{G}{2} v_s^2 - \lambda \right] u_s v_s - \left( u_s^2 - v_s^2 \right) G \sum_{s'} u_{s'} v_{s'} = 0$$

# Trivial solution



$$E_0(s) - \frac{G}{2}v_s^2 \text{ is replaced by } E(s)$$

$$\langle \sum_{s,\sigma} a^\dagger_{s,\sigma} a_{s,\sigma} \rangle_0 = \sum_{s,\sigma} v_s^2 = N$$

Trivial solution $u_s v_s = 0$:

$$u_s = 1 - \Theta_{\rm F}(s)$$

$$v_s = \Theta_{\rm F}(s),$$

$$\Theta_{\rm F}(s) \equiv \begin{cases} 1, & \text{if} \quad E(s) \leq \lambda, \\ 0, & \text{if} \quad E(s) > \lambda. \end{cases}$$

# Non-trivial solution



Correlation function:

$$\Delta = G \sum_s u_s v_s,$$

assuming:

$$u_s^2 = \frac{1}{2}\left[1 + \frac{E(s)-\lambda}{\Omega(s)}\right], \quad v_s^2 = \frac{1}{2}\left[1 - \frac{E(s)-\lambda}{\Omega(s)}\right],$$

from the equation:

$$\Omega_s = \sqrt{(E_s-\lambda)^2 + \Delta^2}.$$

$$1 = \frac{G}{2}\sum_s \frac{1}{\sqrt{\Delta^2 + [E(s)-\lambda]^2}},$$

$$N = \sum_s \left\{1 - \frac{E(s)-\lambda}{\sqrt{\Delta^2 + [E(s)-\lambda]^2}}\right\}.$$

## Quasiparticle Random Phase Approximation

Phonon operator definition:

$$O_k = \sum_{\nu,\mu} \big( X^*_{\nu\mu,k} \alpha_\mu \alpha_\nu - Y^*_{\nu\mu,k} \alpha^\dagger_\nu \alpha^\dagger_\mu \big), \quad O^\dagger_k = \sum_{\nu,\mu} \big( X_{\nu\mu,k} \alpha^\dagger_\nu \alpha^\dagger_\mu - Y_{\nu\mu,k} \alpha_\mu \alpha_\nu \big),$$

$\nu$, $\mu$ run over all orbitals in the mean field

$$\alpha_\nu |C_0\rangle = 0$$

Phonon amplitudes:

$$\langle \big[ [O_k, H]_-, \alpha^\dagger_\nu \alpha^\dagger_\mu \big]_- \rangle_0 = E_k \langle \big[ O_k, \alpha^\dagger_\nu \alpha^\dagger_\mu \big]_- \rangle_0,$$

$$\langle \big[ [O_k, H]_-, \alpha_\mu \alpha_\nu \big]_- \rangle_0 = E_k \langle \big[ O_k, \alpha_\mu \alpha_\nu \big]_- \rangle_0.$$

Norm conditions: $\langle \big[ O_k, O^\dagger_l \big]_- \rangle_0 = \mathrm{sign}(E_k)\, \delta_{k,l}\,;$

Positive $E_k$ — excitation energies.

Transition amplitudes: $\langle k|R|0\rangle_{\mathrm{QRPA}} \equiv \langle \big[ O_k, R \big]_- \rangle_0\,.$