$$\int e^{\sim} V e^{\sim} V e^{\sim} \psi_0 \qquad \underbrace{V \cdot V}_{\frac{V}{(\ell+1)^2 - e^2 + 1}}$$

$$\int_0^t \left(\frac{d}{ds} f_s\right) \cdot g_s \, ds = [f_s g_s]_0^t + \dots$$

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# Derivation of Hartree for Fermions

$\forall j = 1, \dots, N \quad p_j^\ell : |\varphi_j(x_\ell)\rangle\langle\varphi_j(x_\ell)|$

$\forall \ell = 1, \dots N$

$$p^\ell = \sum_j p_j^\ell \qquad q^\ell = 1 - p^\ell$$

The definitions of weight functions, "$\alpha$" carries over.

$$i \frac{d}{dt} p^\ell = [h^\rho, p^\ell]$$

$$i \frac{d}{dt} q^\ell = [h^\rho, p^\ell]$$

$$h^\rho := -\Delta + \lambda V * \underbrace{\sum_{j=1}^N |\varphi_j|^2}_{\rho}$$

We again arrive at terms I, II, III as for the Bosons.

II and III can be treated in a very similar manner as for Bosons

I is not zero any more!

## Term I, heuristics

$$I = N \langle \psi, p^1 p^2 V_{12} q^1 p^2 \psi \rangle . \qquad V_{12} = \lambda V(x_1 - x_2) - \lambda V * \sum_{j=1}^N |\varphi_j|^2 \cdot \frac{1}{N}$$

$$= N \sum_{j, \ell, e} \langle \psi, p_j^1 p_\ell^2 V_{12} q^1 p_e^2 \psi \rangle$$

Remark: There is no way of replacing $\langle \psi, p_j^1 p_\ell^2 \lambda V(x_1 - x_2) q^1 p_e^2 \psi \rangle$ for $j \neq \ell \neq e \neq j$ by a one particle operator!

$$\langle \psi, p_j^1 p_\ell^2 \, O(x_1) \, q^1 p_e^2 \psi \rangle = 0$$

$$\langle \psi, p_1^j p_\ell^2 \, O(x_2) \, q^1 p_e^2 \psi \rangle = 0$$

The other two options are: a) $\langle \psi, p_j^1 p_\ell^2 V_{12} q^1 p_\ell^2 \psi \rangle$ b) $\langle \psi, p_j^1 p_\ell^2 V_{12} q^1 p_j^2 \psi \rangle$

a) $$p_\ell^2 V(x_1 - x_2) p_\ell^2 = |\varphi_\ell(x_2)\rangle\langle\varphi_\ell(x_2)| V(x_1 - x_2) |\varphi_\ell(x_2)\rangle\langle\varphi_\ell(x_2)| = V * |\varphi_\ell|^2 p_\ell^2 =$$

$$= p_\ell^2 \, V * |\varphi_\ell|^2 \, p_\ell^2$$

b) This is subleading compared to a) (see below)

it can be cancelled by a one-body term we could add to $h^\rho$!

The so-called exchange term.

$$\left\langle \psi \begin{matrix} |\varphi_\ell(x_1)\rangle\langle\varphi_j(x_1)| \\ |\varphi_\ell(x_2)\rangle\langle\varphi_\ell(x_2)| \end{matrix} V(x_1 - x_2) \begin{matrix} q^1 \\ |\varphi_j(x_2)\rangle\langle\varphi_j(x_2)| \end{matrix} \psi \right\rangle$$

$$= -\left\langle \psi \begin{matrix} |\varphi_\ell(x_1)\rangle\langle\varphi_j(x_1)| \\ |\varphi_j(x_2)\rangle\langle\varphi_\ell(x_2)| \end{matrix} V(x_1 - x_2) \begin{matrix} q^1 \\ |\varphi_j(x_2)\rangle\langle\varphi_j(x_2)| \end{matrix} \psi \right\rangle$$

To cancel this term, we have to modify the effective equation of orbital $j$ in the following way:

$$i \frac{d}{dt} \varphi_j = h^g \varphi_j - \lambda \sum_{g=1}^{N} V*(\varphi_g^* \varphi_j)\, \varphi_g \qquad (*)$$

This change in the effective description gives:

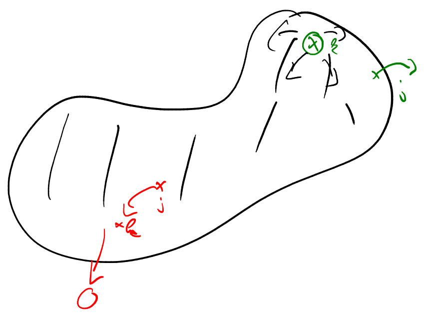
$$q^1 = 1 - \sum p_j^1$$

Considering the time derivative we get in addition for each $j$

$$i \dot{p}_j^1 = [h^\varphi, p_j^1] - \sum_g \left( \lambda \boxed{V*(\varphi_g^* \varphi_j)\, |\varphi_g\rangle\langle\varphi_j|} - \dots \right)$$

$$\langle\varphi_g| \; V \; |\varphi_g\rangle\langle\varphi_j| \quad |\varphi_j\rangle$$

Why is the exchange term subleading?



For the direct term, $j$ has to be close to the surface

For the exchange term, $g$ has to be close to the surface, and $j$ close to $g$.

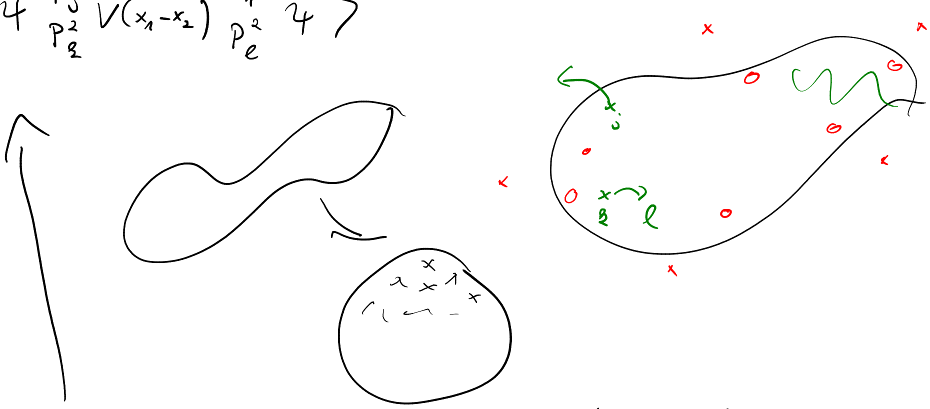
That limits the # of options in choosing $g$ and $j$.

Remark: The equations considering the exchange term $(*)$ are called "Hartree-Fock" equations

$$i \frac{d}{dt} \varphi_j = -\Delta \varphi_j + \sum_{g=1}^{N} \lambda V * |\varphi_g|^2 \varphi_j - \sum_{g=1}^{N} \lambda V * \varphi_j \varphi_g^* \, \varphi_g$$

Let us come back to the $j \neq g \neq \ell \neq j$ - term. Why is it small?

$$\sum_{j \neq g \neq \ell \neq j} N \lambda \left\langle \psi \; \begin{matrix} p_j^1 \\ p_g^2 \end{matrix} V(x_1 - x_2) \begin{matrix} q_1 \\ p_\ell^2 \end{matrix} \; \psi \right\rangle$$



Let us compare this to the direct term $(\ell = g)$

For the direct term, $j$ must be close to the surface, $g$ can be anything

For the $g \neq \ell$ - term $j$ must be close to the surface, $\ell$ must be among the few unoccupied orbitals $g$ must be close to $\ell$.

it is small