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PHY 981

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Exercise 3

The Slater determinant

$$\Phi_\lambda^{AS}(x_1 \ldots x_N ; \alpha_1 \ldots \alpha_N) = \frac{1}{\sqrt{N!}} \sum_p (-)^p P \prod_{i=1}^{N} \psi_{\alpha_i}(x_i)$$

assume $N_{ptcls} = N_\alpha$

a) for $N=3$

$\psi_{\alpha_1}(x_1)$	$\psi_{\alpha_2}(x_2)$	$\psi_{\alpha_3}(x_3)$,	$p=0$
1	3	2,	$p=1$
2	1	3,	$p=1$
2	3	1,	$p=2$
3	1	2,	$p=2$
3	2	1,	$p=2$

$$\Phi_\lambda^{AS} = \frac{1}{\sqrt{6}} \Big[\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\psi_{\alpha_3}(x_3) - \psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_3)\psi_{\alpha_3}(x_2)$$

$$- \psi_{\alpha_1}(x_2)\psi_{\alpha_2}(x_1)\psi_{\alpha_3}(x_3) + \psi_{\alpha_1}(x_2)\psi_{\alpha_2}(x_3)\psi_{\alpha_3}(x_1)$$

$$+ \psi_{\alpha_1}(x_3)\psi_{\alpha_2}(x_1)\psi_{\alpha_3}(x_2) + \psi_{\alpha_1}(x_3)\psi_{\alpha_2}(x_2)\psi_{\alpha_3}(x_1) \Big]$$

b) $\int dx_1 \dots dx_N \left| \varphi_\lambda^{AS}(x_1 \dots x_N ; \alpha_1 \dots \alpha_N) \right|^2$

$$= \frac{1}{N!} \int dx_1 \dots dx_N \left(\sum_P (-)^P P \prod_{i=1}^{N} \psi^*_{\alpha_i}(x_i) \right) \left(\sum_P (-)^P P \prod_{i=1}^{N} \psi_{\alpha_i}(x_i) \right) \quad (\times)$$

take normal ordering from first sum (no permutation)

$$\int dx_1 \dots dx_N \left(\prod_{i=1}^{N} \psi^*_{\alpha_i}(x_i) \right) \underbrace{\left(\sum_P (-)^P P \prod_{i=1}^{N} \psi_{\alpha_i}(x_i) \right)}$$

↳ from this sum, only the term with the same ordering makes the integral non zero

$$\int dx_1 \dots dx_N \left(\prod_{i=1}^{N} \psi_{\alpha_i}(x_i) \right) \left(\prod_{i=1}^{N} \psi_{\alpha_i}(x_i) \right) = 1$$

In this way, each term from the first sum in $(\times)$ picks out the term in the second sum with its same ordering so that

$$\int dx_1 \dots dx_N \left(\sum_P (-)^P P \prod_{i=1}^{N} \psi^*_{\alpha_i}(x_i) \right) \left(\sum_P (-)^P P \prod_{i=1}^{N} \psi_{\alpha_i}(x_i) \right) = N!$$

$$\therefore \int dx_1 \dots dx_N \left| \varphi_\lambda^{AS} \right|^2 = 1$$

e.g. for $N = 3$

$$|\varphi_3^{AS}|^2 = \frac{1}{N!} \Big(\langle \alpha_1 \alpha_2 \alpha_3 | - \langle \alpha_1 \alpha_3 \alpha_2 | - \langle \alpha_2 \alpha_1 \alpha_3 | + \langle \alpha_3 \alpha_1 \alpha_2 | + \langle \alpha_2 \alpha_3 \alpha_1 | + \langle \alpha_3 \alpha_2 \alpha_1 | \Big)$$

$$\Big(|\alpha_1 \alpha_2 \alpha_3\rangle - |\alpha_1 \alpha_3 \alpha_2\rangle - |\alpha_2 \alpha_1 \alpha_3\rangle + |\alpha_3 \alpha_1 \alpha_2\rangle + |\alpha_2 \alpha_3 \alpha_1\rangle + |\alpha_3 \alpha_2 \alpha_1\rangle \Big)$$

$$= \frac{1}{N!} (1 + 5\times 0 + 1 + 5\times 0 + 1 + 5\times 0 + 1 + 5\times 0 + 1 + 5\times 0 + 1 + 5\times 0)$$

$$= \frac{6}{3!} = 1$$

c) One-body operator $\hat{F} = \sum_{i}^{N} \hat{f}(x_i)$

Two-body operator $\hat{G} = \sum_{i>j}^{N} \hat{g}(x_i\ x_j)$

For a two ptcl Slater determinant

$$|\Phi^{AS}_{\alpha_1\alpha_2}\rangle = \frac{1}{\sqrt{2}}\left(|\alpha_1\alpha_2\rangle - |\alpha_2\alpha_1\rangle\right)$$

$$\langle \Phi^{AS}_{\alpha_1\alpha_2}|\hat{F}|\Phi^{AS}_{\alpha_1\alpha_2}\rangle = \frac{1}{2}\Big[\langle\alpha_1\alpha_2|\hat{f}_1+\hat{f}_2|\alpha_1\alpha_2\rangle - \langle\alpha_1\alpha_2|\hat{f}_1+\hat{f}_2|\alpha_2\alpha_1\rangle$$
$$- \langle\alpha_2\alpha_1|\hat{f}_1+\hat{f}_2|\alpha_1\alpha_2\rangle + \langle\alpha_2\alpha_1|\hat{f}_1+\hat{f}_2|\alpha_2\alpha_1\rangle\Big]$$

$\hat{f}_i$ is single ptcl op for i^{th} ptcl

$$= \frac{1}{2}\Big[\langle\alpha_1|\hat{f}_1|\alpha_1\rangle\langle\alpha_2|\alpha_2\rangle + \langle\alpha_1|\alpha_1\rangle\langle\alpha_2|\hat{f}_2|\alpha_2\rangle$$
$$-\langle\alpha_1|\hat{f}_1|\alpha_2\rangle\underbrace{\cancel{\langle\alpha_2|\alpha_1\rangle}}_{\to 0} - \underbrace{\cancel{\langle\alpha_1|\alpha_2\rangle}}_{\to 0}\langle\alpha_2^*|\hat{f}_2|\alpha_1\rangle$$
$$-\ 0 \qquad \text{b/c similar to}$$
$$+\ \langle\alpha_2|f_1|\alpha_2\rangle\langle\alpha_1|\alpha_1\rangle + \langle\alpha_1|f_2|\alpha_1\rangle\langle\alpha_2|\alpha_2\rangle\Big]$$

$$\doteq \frac{1}{2}\begin{pmatrix} \langle\alpha_1|\hat{f}_1|\alpha_1\rangle + \langle\alpha_2|\hat{f}_2|\alpha_2\rangle & 0 \\ 0 & \langle\alpha_2|f|\alpha_2\rangle + \langle\alpha_1|f|\alpha_1\rangle \end{pmatrix}$$

$$\langle\Phi^{AS}_{\alpha_1\alpha_2}|\hat{G}|\Phi^{AS}_{\alpha_1\alpha_2}\rangle \doteq \frac{1}{2}\begin{pmatrix} \langle\alpha_1\alpha_2|g(x_1x_2)|\alpha_1\alpha_2\rangle & \langle\alpha_1\alpha_2|g(x_1x_2)|\alpha_2\alpha_1\rangle \\ \langle\alpha_2\alpha_1|g(x_1x_2)|\alpha_1\alpha_2\rangle & \langle\alpha_2\alpha_1|g(x_1x_2)|\alpha_2\alpha_1\rangle \end{pmatrix}$$

Slater determinant short-hand notation

$|\varphi^{AS}_{\lambda}\rangle$ represents a properly anti-symmetrized N-ptcl wavefunction

permutation operator changes indices of 2 ptcls

$$\frac{1}{\sqrt{N!}} \sum_{P} (-)^{p} P \prod_{i=1}^{N} \psi_{\alpha_i}(x_i)$$

product of N single ptcl states

normalization

sum over all possible permutations

\# of permutations needed to restore normal ordering of ptcl indices

The one and two body operators will be Hermitian

The one body operator will have non zero elements only on the main diagonal (MD)

The two body operator will have non zero elements on either side of the MD.

For n-body operators ($n \leq N_{ptcl}$) there will be n diagonals on either side of the MD since n-body operators have n permutations (including the normal ~~permut~~ ordering) for which the integrals may not be 0 due to the orthogonality of the single ptcl states.

Exercise 4

Three-level system, each level 2-fold degenerate, level spacing d

a) Two-ptcl Slater determinates:

ways to order 2 indistinguishable across 6 bins

$$\binom{6}{2} = 15 \quad \text{Slater dets}$$

b) Two lowest orbits, two ptcls

One-body part of $\hat{H}$: $\hat{h}_0 \psi_{p\sigma} = p d \psi_{p\sigma}$

Only consider 2 ptcl states where ptcls have same p: $\{|1\,1\rangle, |2\,2\rangle\}$

One-body Hamiltonian:

$$\hat{H}_0 |1\,1\rangle = \hat{h}_0^{(1)} |\psi_{1\uparrow}(x_1) \psi_{1\downarrow}(x_2)\rangle + \hat{h}_0^{(2)} |\psi_{1\uparrow}(x_1) \psi_{1\downarrow}(x_2)\rangle$$

$$= (d + d)|1\,1\rangle$$

$$\hat{H}_0 |2\,2\rangle = \hat{h}_0^{(1)} |\psi_{2\uparrow}(x_1) \psi_{2\downarrow}(x_2)\rangle + \hat{h}_0^{(2)} |\psi_{2\uparrow}(x_1) \psi_{2\downarrow}(x_2)\rangle$$

$$= (2d + 2d)|2\,2\rangle$$

$$\therefore \quad \hat{H}_0 \doteq \begin{pmatrix} 2d & 0 \\ 0 & 4d \end{pmatrix}$$

since $\langle 1\,1 | \hat{H}_0 | 2\,2\rangle = 4d \langle 1|2\rangle \langle 1|2\rangle = 0 = \langle 2\,2 | \hat{H}_0 | 1\,1\rangle$

$$\hat{H}_1 \doteq \begin{pmatrix} -g & -g \\ -g & -g \end{pmatrix}$$

and

$$\hat{H} \doteq \begin{pmatrix} 2d - g & -g \\ -g & 4d - g \end{pmatrix} = \hat{H}_0 + \hat{H}_1$$

$$\hat{H} \doteq g \begin{pmatrix} \alpha - 1 & -1 \\ -1 & 2\alpha - 1 \end{pmatrix} \qquad \alpha \equiv \frac{2d}{g}$$

$$\begin{vmatrix} \alpha - 1 - \lambda & -1 \\ -1 & 2\alpha - 1 - \lambda \end{vmatrix} = 0 \Rightarrow (\alpha - 1 - \lambda)(2\alpha - 1 - \lambda) - 1 = 0$$

$$\Rightarrow 2\alpha^2 - \alpha - \alpha\lambda - 2\alpha + \cancel{1} + \lambda - 2\alpha\lambda + \lambda + \lambda^2 - \cancel{1} = 0$$

$$\lambda^2 + \lambda(2 - 3\alpha) - 3\alpha + 2\alpha^2 = 0$$

$$\lambda_\pm = \frac{3\alpha - 2 \pm \sqrt{(2-3\alpha)^2 - 4(-3\alpha + 2\alpha^2)}}{2}$$

$4 + 9\alpha^2 - \cancel{12\alpha} + \cancel{12\alpha} - 8\alpha^2 \Rightarrow \alpha^2 + 4$

$$= \frac{3}{2}\alpha - 1 \pm \sqrt{\frac{\alpha^2}{4} + 1} \qquad \text{eigenvalues}$$

$$\begin{pmatrix} \alpha - 1 - \lambda_\pm & -1 \\ -1 & 2\alpha - 1 - \lambda_\pm \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 0 \Rightarrow c_1 = \frac{c_2}{\alpha - 1 - \lambda_\pm}$$

$$\Rightarrow \frac{c_1}{c_2} = \frac{1}{\alpha - \cancel{1} - \frac{3}{2}\alpha + \cancel{1} \mp \sqrt{\frac{\alpha^2}{4} + 1}} = \frac{1}{-\frac{\alpha}{2} \mp \sqrt{\frac{\alpha^2}{4} + 1}}$$

$$= \frac{-2}{\alpha \pm \sqrt{\alpha^2 + 4}}$$

~~ratio of~~ ~~mixing~~ ratio of "ptcls in $p=1$" admixture to "ptcls in $p=2$"

$|+\rangle = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$

$\lim \alpha \ll 1 \Rightarrow g \gg d$ (strong interaction): even mixing $|-\rangle = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$\lim \alpha \gg 1 \Rightarrow g \ll d$ (weak interaction): recovers original e.vectors

$|+\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$|-\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

c) Two ptcl states, both ptcls in same level, can be in $p=3$

$$\hat{H} \doteq \begin{pmatrix} 2d-3g & -3g & -3g \\ -3g & 4d-3g & -3g \\ -3g & -3g & 6d-3g \end{pmatrix} = 3g \begin{pmatrix} \beta-1 & -1 & -1 \\ -1 & 2\beta-1 & -1 \\ -1 & -1 & 3\beta-1 \end{pmatrix}$$

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In[1]:= Eigenvectors[{{x - 1, -1, -1}, {-1, 2 x - 1, -1}, {-1, -1, 3 x - 1}}]
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$$\text{Out[1]=}\ \left\{\left\{-1 + 3\,x - \text{Root}\left[11\,x^2 - 6\,x^3 + \left(-12\,x + 11\,x^2\right)\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,1\right] + \frac{-3\,x + \text{Root}[11\,x^2 - 6\,x^3 + (-12\,x + 11\,x^2)\,\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,1]}{2\,x - \text{Root}[11\,x^2 - 6\,x^3 + (-12\,x + 11\,x^2)\,\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,1]},\ -\frac{-3\,x + \text{Root}[11\,x^2 - 6\,x^3 + (-12\,x + 11\,x^2)\,\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,1]}{2\,x - \text{Root}[11\,x^2 - 6\,x^3 + (-12\,x + 11\,x^2)\,\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,1]},\ 1\right\},\right.$$

$$\left\{-1 + 3\,x - \text{Root}\left[11\,x^2 - 6\,x^3 + \left(-12\,x + 11\,x^2\right)\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,2\right] + \frac{-3\,x + \text{Root}[11\,x^2 - 6\,x^3 + (-12\,x + 11\,x^2)\,\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,2]}{2\,x - \text{Root}[11\,x^2 - 6\,x^3 + (-12\,x + 11\,x^2)\,\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,2]},\ -\frac{-3\,x + \text{Root}[11\,x^2 - 6\,x^3 + (-12\,x + 11\,x^2)\,\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,2]}{2\,x - \text{Root}[11\,x^2 - 6\,x^3 + (-12\,x + 11\,x^2)\,\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,2]},\ 1\right\},$$

$$\left.\left\{-1 + 3\,x - \text{Root}\left[11\,x^2 - 6\,x^3 + \left(-12\,x + 11\,x^2\right)\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,3\right] + \frac{-3\,x + \text{Root}[11\,x^2 - 6\,x^3 + (-12\,x + 11\,x^2)\,\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,3]}{2\,x - \text{Root}[11\,x^2 - 6\,x^3 + (-12\,x + 11\,x^2)\,\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,3]},\ -\frac{-3\,x + \text{Root}[11\,x^2 - 6\,x^3 + (-12\,x + 11\,x^2)\,\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,3]}{2\,x - \text{Root}[11\,x^2 - 6\,x^3 + (-12\,x + 11\,x^2)\,\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,3]},\ 1\right\}\right\}$$

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In[2]:= Eigenvalues[{{x - 1, -1, -1}, {-1, 2 x - 1, -1}, {-1, -1, 3 x - 1}}]
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$$\text{Out[2]=}\ \left\{\text{Root}\left[11\,x^2 - 6\,x^3 + \left(-12\,x + 11\,x^2\right)\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,1\right],\ \text{Root}\left[11\,x^2 - 6\,x^3 + \left(-12\,x + 11\,x^2\right)\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,2\right],\ \text{Root}\left[11\,x^2 - 6\,x^3 + \left(-12\,x + 11\,x^2\right)\#1 + (3 - 6\,x)\,\#1^2 + \#1^3\,\&,\,3\right]\right\}$$