Sheet 3

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A1.1

a) for simplicity, Ψ_{ij} refers to a WF $\Psi(r_1 \dots r_i, r_j)$ without loss of gen.

$$P_{ij}\Psi_{ij} = \Psi_{ji}$$

$$\underbrace{P_{ij}^{-1}P_{ij}}_{\mathbb{1}}\Psi_{ij} = P_{ij}^{-1}\Psi_{ji}$$

$$\Psi_{ij} = P_{ij}^{-1}\Psi_{ji} = P_{ij}\Psi_{ji}$$

b) $\langle P_{ij}\Psi_{ij} | P_{ij}\Psi_{ij}\rangle = \langle P_{ij}^{\dagger}P_{ij}\Psi_{ij} | \Psi_{ij}\rangle \overset{!}{=} 1 \rightarrow P_{ij}^{\dagger} = P_{ij}^{-1} = P_{ij}$

$\quad\shortparallel$

$\langle \Psi_{ji} | \Psi_{ji}\rangle = 1$

c) unitary $\rightarrow$ EW has norm 1
hermitian $\rightarrow$ EW are real $\Big\}$ EW $= \pm 1$

d)

$$[P_{ij}, H] \Rightarrow (P_{ij}H)\Psi_{ij} - (H P_{ij})\Psi_{ij}$$

$$P_{kl}\sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m}\nabla_i^2 + V_{ext}(\vec{r}_i)\right) + \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{e^2}{|r_i - r_j|}$$

swapping $r_k \leftrightarrow r_l$ doesn't affect the first 2 terms because it sums over all contributions.

for the 3rd term: since its sym. in i and j, doesn't affect this term either.

$$\Rightarrow [P_{ij}, H] = 0$$

A1.2

a) $$\hat{A} = \frac{1}{\sqrt{N!}}\sum_{p\in S_N}(-1)^p\hat{P}^p$$

$$\hat{H} = \sum_{i=1}^{N} -\frac{\hbar^2}{2m}\nabla_i^2 + V_{ext}(\vec{r}_i) + \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{e^2}{|r_i - r_j|}$$

assuming that $[\hat{P}_{ij}, \hat{H}] = 0$:

$$[\hat{A}, \hat{H}] = \frac{1}{\sqrt{N!}}\sum_{p\in S_N}[\hat{P}^p, \hat{H}] \longrightarrow [\hat{P}^p, \hat{H}] = [\prod_{ij}\hat{P}^{ij}, \hat{H}] = 0$$

since $[\hat{P}_{ij}, \hat{H}] = 0$,

b) $$\frac{1}{\sqrt{N!}}\begin{vmatrix} \phi_a(r_1) & \dots & \phi_z(r_1) \\ \vdots & & \vdots \\ \phi_a(r_2) & \dots & \phi_z(r_N)\end{vmatrix} = \hat{A}\underbrace{\left[\phi_a(x_1)\dots\phi_z(r_N)\right]}_{\chi}$$

$$\hat{A} = \frac{1}{\sqrt{N!}}\sum_{p\in S_N}(-1)^p\,\hat{P}^p$$

Show: $P_{ij}\overbrace{\hat{A}\chi}^{\psi} = -A\chi$

$$\frac{1}{\sqrt{N!}}\sum_{p\in S_N}P_{ij}\,P^p(-1)^p\,\chi \overset{P_{ij}P^p=P^q}{=} \frac{1}{\sqrt{N!}}\sum_{p\in S_N}P^q(-1)^p\,\chi$$

$$\overset{p=q-1}{=} \frac{1}{\sqrt{N!}}\sum_{q\in S_N}(-1)^{q-1}\,P^q\,\chi$$

$$=(-1)\frac{1}{\sqrt{N}}\sum_{q\in S_N}\hat{P}^q\,\chi = -A\chi$$

c) $\Psi'(r_1\dots r_N)$ has one differing single particle state at N: $\varphi_z'(r_N)\neq\varphi_z(r_N)$

$$\int d^3r\,\Psi'(\vec{r}_1\dots\vec{r}_N)\,\Psi(r_1\dots r_N)$$

$$=\frac{1}{N!}\sum_{p,p'}(-1)^{p+p'}\left(\hat{P}^p+\hat{P}^{p'}\right)\underbrace{\int d^3r_1\,\varphi_a(r_1)\varphi_a(r_1)}_{1}\dots\underbrace{\int d^3r_N\,\varphi_z'(r_N)\,\varphi_z(r_N)}_{0} = 0$$

H2.1

$$\hat{H} = \hat{T}_e+\hat{V}_{ex} = -\frac{\nabla^2}{2}-\sum_{\nu=\uparrow\downarrow}\sum_{j=1}^{\tilde{N}}\int d^3r'\frac{1}{|r'-r|}\,\frac{\phi_{j,\nu}^*(\vec{r}')\;\phi_{i,\sigma}(\vec{r}')\,\phi_{j,\nu}(\vec{r})}{\phi_{i,\sigma}(\vec{r})}$$

a) Ansatz: $e^{i\vec{k}\cdot\vec{r}}$, $\vec{k}\in\mathbb{R}^3\to$ continous

until E_F: $\frac{1}{(2\pi)^3}\int_{\Omega k_F}d^3k$

$$H = -\frac{\nabla^2}{2}-\sum_{\nu=\uparrow\downarrow}\frac{1}{(2\pi)^3}\int_{\Omega k_F}d^3k\int d^3r'\frac{1}{|r-r'|}\,\frac{\phi_{j,\nu}^*(\vec{r}')\;\phi_{i,\sigma}(\vec{r}')\,\phi_{j,\nu}(\vec{r})}{\phi_{i,\sigma}(\vec{r})}$$

$\to$ apply $e^{i\vec{k}\vec{r}}$: $-\frac{\nabla^2}{2}e^{i\vec{k}\vec{r}} = \frac{k^2}{2}e^{i\vec{k}\vec{r}}$, σ is either $\uparrow$ or $\downarrow$

$$\to He^{i\vec{k}\vec{r}} = \frac{k^2}{2}e^{i\vec{k}\vec{r}} - \frac{1}{(2\pi)^3}\int d^3k'\int d^3r'\,\frac{\overbrace{e^{-ik'r'}\cdot e^{ikr'}}^{e^{i(k-k')r'}}\,e^{ik'r}}{|r-r'|}$$

$e^{ik'r}\to e^{ik'r} = e^{i(k'-k)r}e^{ikr}$

$$=\frac{k^2}{2}e^{ikr}-\frac{1}{(2\pi)^3}\int d^3k'\int d^3r'\,\frac{e^{i(k-k')r'}\,e^{i(k'-k)r}}{|r-r'|}\,e^{ikr}$$

$dk = dq$

$\Rightarrow k' - k = q$: looking only at the last term, we get:

$$\frac{1}{(2\pi)^3} \int d^3q \int d^3r' \frac{e^{-iqr} e^{iqr'}}{|r-r'|} e^{ikr}$$

$$= \frac{1}{(2\pi)^3} \int d^3q \int d^3r' \frac{e^{iq(r'-r)}}{|r-r'|} e^{ikr} \rightarrow \begin{array}{l} r'-r = \rho \\ dr' = d\rho \end{array}$$

$$= \frac{1}{(2\pi)^3} \int d^3q \underbrace{\int d^3\rho \frac{e^{i\vec{q}\vec{\rho}}}{|\rho|}}$$

Fourier-transform of Potential $\frac{1}{|\rho|}$, you get: $\frac{4\pi}{|q|^2}$

$$= 8\pi \cdot \frac{1}{(2\pi)^3} \int d^3q \frac{4\pi}{|q|^2} \overset{\text{Hinweis}}{=} \frac{k_F}{\pi} \left(1 + \frac{1}{2} \left(\frac{k_F}{k} - \frac{k}{k_F} \right) \ln \left(\frac{k_F + k}{k_F - k} \right) \right)$$

$$\rightarrow E = \frac{k^2}{2} - k_F \left(1 + \frac{1}{2} \left(\frac{k_F}{k} - \frac{k}{k_F} \right) \ln \left(\frac{k_F + k}{k_F - k} \right) \right)$$

2.2

a) $$n_\uparrow = \frac{1}{(2\pi)^3} \int_{\Omega_{k_F}(\uparrow)} d^3k_\uparrow = \frac{1}{(2\pi)^3} \int d\Omega \int_0^{k_{F(\uparrow)}} k_r^2 \, dk_r = \frac{4\pi}{3(2\pi)^3} k_{F(\uparrow)}^3 = \frac{k_{F(\uparrow)}^3}{6\pi^2}$$

$$\Rightarrow n_\downarrow = \frac{k_{F\downarrow}^3}{6\pi^2} \rightarrow k_{F\downarrow} = (6\pi^2 n_\downarrow)^{1/3}$$

$$\Lambda = \frac{n_\uparrow - n_\downarrow}{n_B} = \frac{n_\uparrow + n_\downarrow}{n_B} - \frac{n_\uparrow - n_\downarrow}{n_B} = \frac{2n_\downarrow}{n_B}$$

$$\Rightarrow n_\downarrow = \frac{n_B(1-\varsigma)}{2}$$

$$n_\uparrow = \frac{n_B(1+\varsigma)}{2}$$

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