TECHNISCHE UNIVERSITÄT DRESDEN

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$$\frac{1}{|\vec{r}-\vec{r}'|} = \frac{4\pi}{2l+1} \frac{r_<^{l}}{r_>^{l+1}} Y_{lm}(\hat{r}) Y^*_{lm}(\hat{r}')$$

$$U_{m_1 m_2 m_3 m_4} = \int d^3r\, d^3r' \left(\frac{u_e(r)}{r}\right)^2 \left(\frac{u_e(r')}{r'}\right)^2 Y^*_{lm_1}(\hat{r}) Y_{lm_4}(\hat{r}) Y^*_{lm_2}(\hat{r}') Y_{lm_3}(\hat{r}') \times \frac{1}{|\vec{r}-\vec{r}'|}$$

$$\cancel{\frac{1}{|\vec{r}-\vec{r}'|}}$$

$$\tilde{U}_{m_1 m_2 m_3 m_4} = \int d\Omega \int d\Omega' \int_0^\infty dr \int_0^\infty dr'\, u_e^2(r)\, u_e^2(r')\, Y^*_{lm_1}(\hat{r}) Y_{lm_4}(\hat{r}) Y^*_{lm_2}(\hat{r}') Y_{lm_3}(\hat{r}') \times \frac{e^{-\lambda|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}$$

$$\lambda\vec{r} = \tilde{r}$$

$$\tilde{U} = \int d\Omega \int d\Omega' \int_0^\infty \frac{d\tilde{r}}{\lambda} \int_0^\infty \frac{d\tilde{r}'}{\lambda}\, u_e^2\left(\frac{\tilde{r}}{\lambda}\right) u_e^2\left(\frac{\tilde{r}'}{\lambda}\right) Y^*_{lm_1}(\hat{r}) Y_{lm_4}(\hat{r}) Y^*_{lm_2}(\hat{r}') Y_{lm_3}(\hat{r}') \times \frac{\lambda e^{-|\tilde{r}-\tilde{r}'|}}{|\tilde{r}-\tilde{r}'|}$$

$$\tilde{U} = \frac{1}{\lambda} \int d\Omega \int d\Omega' \int_0^\infty d\tilde{r} \int_0^\infty d\tilde{r}'\, u_e^2\left(\frac{\tilde{r}}{\lambda}\right) u_e^2\left(\frac{\tilde{r}'}{\lambda}\right) Y^*_{lm_1}(\hat{r}) Y_{lm_4}(\hat{r}) Y^*_{lm_2}(\hat{r}') Y_{lm_3}(\hat{r}') \frac{e^{-|\tilde{r}-\tilde{r}'|}}{|\tilde{r}-\tilde{r}'|}$$

$$4\pi \frac{I_{l+\frac{1}{2}}(r_<) K_{l+\frac{1}{2}}(r_>)}{\sqrt{r_< r_>}} \times \sum_m Y_L Y_L^*$$

$$\tilde{U} = \underbrace{\langle Y_{lm_1} | Y_{lm} | Y_{lm_4}\rangle \langle Y_{lm_2} | Y^*_{lm} | Y_{lm_3}\rangle \times \frac{4\pi}{2l+1}}_{\text{"gaunts"}} \times$$

$$\times \frac{(2l+1)}{\lambda} \times \int_0^\infty d\tilde{r} \int_0^\infty d\tilde{r}'\, u_e^2\left(\frac{\tilde{r}}{\lambda}\right) u_e^2\left(\frac{\tilde{r}'}{\lambda}\right) \frac{I_{l+\frac{1}{2}}(\tilde{r}_<) K_{l+\frac{1}{2}}(\tilde{r}_>)}{\sqrt{\tilde{r}_< \tilde{r}_>}}$$

$$\tilde{U} = \text{gaunts} \times \frac{2l+1}{\lambda} \int_0^\infty \lambda\, dr \int_0^\infty \lambda\, dr'\, u_e^2(r)\, u_e^2(r') \frac{I_{l+\frac{1}{2}}(\lambda r_<) K_{l+\frac{1}{2}}(\lambda r_>)}{\lambda \sqrt{r_< r_>}}$$

$$\boxed{\tilde{U} = \text{gaunts} \times (2l+1) \int_0^\infty dr \int_0^\infty dr'\, u_e^2(r)\, u_e^2(r')\, I_{l+\frac{1}{2}}(\lambda r_<) K_{l+\frac{1}{2}}(\lambda r_>)}$$

$$1)\quad \underbrace{\mathrm{Tr}(H_0 G)}_{\text{SUM}} + \underbrace{\tfrac{1}{2}\mathrm{Tr}((\Sigma - V_{dc})G) + \tfrac{1}{2}\mathrm{Tr}(V_{dc}\cdot M) - \Phi^{DC}(M)}_{\text{EORB}} + \cdots$$

$$2)\quad \underbrace{\mathrm{Tr}(H_0 G)}_{\text{lattice}} + \underbrace{\tfrac{1}{2}\mathrm{Tr}(\Sigma_{imp} G_{imp}) - \Phi^{DC}[M_{imp}]}_{\text{impurity}} + \cdots \quad \checkmark$$

cancel out

$$3)\quad \underbrace{\mathrm{Tr}\ln G - \mathrm{Tr}\ln G_{loc} + \mathrm{Tr}\left(\left(\Delta - \omega_n \frac{\partial \Delta}{\partial \omega_n}\right) G_{loc}\right) + \mathrm{Tr}((\varepsilon_{imp} + V_{dc}) G)}_{\text{lattice}} - \tfrac{1}{2}\mathrm{Tr}(V_{dc} G) + \cdots$$

$$+\tfrac{1}{2}\mathrm{Tr}(V_{dc} M_{imp}) + \underbrace{\tfrac{1}{2}\mathrm{Tr}(\Sigma_{imp} G_{imp}) - \Phi_{DC}[M_{imp}]}_{\text{impurity}} \quad \checkmark$$

$$4)\quad \underbrace{\mathrm{Tr}\ln G - \mathrm{Tr}\ln G_{loc} + \mathrm{Tr}\left(\left(\Delta - \omega_n \frac{\partial \Delta}{\partial \omega_n}\right) G_{loc}\right) + \mathrm{Tr}((\varepsilon_{imp} + V_{dc}) G) + \tfrac{1}{2}\mathrm{Tr}((\Sigma - V_{dc}) G) - \tfrac{1}{2}\mathrm{Tr}(V_{dc} G)}_{\text{lattice}} + \cdots$$

$$+\mathrm{Tr}(V_{dc} G) - \Phi_{DC}[M]$$

$$\boxed{\begin{aligned} E &= \mathrm{Tr}(H^{LDA} G) + \tfrac{1}{2}\mathrm{Tr}(\Sigma G) - \Phi_{DC} + \cdots \\ F + T S_{imp} &= \mathrm{Tr}\ln G - \mathrm{Tr}\ln G_{loc} + \mathrm{Tr}\left(\left(\varepsilon_{imp} + \Delta - \omega_n \frac{\partial \Delta}{\partial \omega_n}\right) G\right) + \tfrac{1}{2}\mathrm{Tr}(\Sigma G_{imp}) \end{aligned}}$$

1) SUM: $\mathrm{Tr}(H^{LDA} G)$ EORB: $\tfrac{1}{2}\mathrm{Tr}(\Sigma \cdot G) - \Phi^{DC}[M]$

2) SUM: $\mathrm{Tr}(H^{LDA} G)$ IEORB: $\tfrac{1}{2}\mathrm{Tr}(\Sigma_{imp} G_{imp}) - \Phi^{DC}[M_{imp}]$

3) XSUM: $\mathrm{Tr}\ln G - \mathrm{Tr}\ln G_{loc} + \mathrm{Tr}\left(\left(\Delta - \omega_n \frac{\partial \Delta}{\partial \omega_n}\right) G_{loc}\right) + \mathrm{Tr}((\varepsilon_{imp} + V_{dc}) G)$

XEORB: $\tfrac{1}{2}\mathrm{Tr}(\Sigma_{imp} G_{imp}) - \Phi_{DC}[M_{imp}] + \tfrac{1}{2} V_{dc} M_{imp}$; $-\tfrac{1}{2}\mathrm{Tr}(V_{dc} G)$

4) YSUM: $\mathrm{Tr}\ln G - \mathrm{Tr}\ln G_{loc} + \mathrm{Tr}\left(\left(\Delta - \omega_n \frac{\partial \Delta}{\partial \omega_n}\right) G_{loc}\right) + \mathrm{Tr}((\varepsilon_{imp} + V_{dc}) G) + \tfrac{1}{2}\mathrm{Tr}((\Sigma - V_{dc}) G)$

; $-\tfrac{1}{2}\mathrm{Tr}(V_{dc} G)$

$$X = F_{imp}[\Delta] - \mathrm{Tr}\left(\left(\varepsilon_{imp} + V_{dc} + \Delta - \omega_n \frac{\partial \Delta}{\partial \omega_n}\right) G\right) =$$

$$X = F_{imp}[\Delta] - \mathrm{Tr}\left(\left(\varepsilon_{imp} + \Delta - \omega_n \frac{\partial \Delta}{\partial \omega_n}\right) G\right) - \Phi_{DC}(M_{imp}]$$

$$\delta X = -\mathrm{Tr}\left(\left(\varepsilon_{imp} + \Delta - \omega_n \frac{\partial \Delta}{\partial \omega_n}\right)\delta G\right) + \mathrm{Tr}\left(\omega_n \left(\frac{\partial}{\partial \omega_n}\delta\Delta\right) G\right) - \mathrm{Tr}(V_{dc}\,\delta G)$$

Should try: $G = G_0(G^{-1} + \Sigma) G$

$$5)\quad F = \mathrm{Tr}\ln(-G_0) + \mathrm{Tr}\ln(1 + \Sigma G_{loc}) - \mathrm{Tr}\ln G_{loc} + \mathrm{Tr}\left(\left(\Delta - \omega_n \frac{\partial \Delta}{\partial \omega_n}\right) G_{loc}\right) + \mathrm{Tr}((\varepsilon_{imp} + V_{dc}) G) + \tfrac{1}{2}\mathrm{Tr}(\Sigma_{imp} G_{imp}) - \Phi_{DC}[M_{imp}]$$