

An Average-Atom Model

$$\left[h_0 - \frac{Z}{r} + V(r) \right] \phi_a(\mathbf{r}) = \epsilon_a \phi_a(\mathbf{r})$$

potential:

$$V(r) = \begin{cases} \int \rho(r')/R d\tau' - (3\rho(r)/\pi)^{1/3} & r \leq R_0 \\ 0 & r > R_0 \end{cases}$$

density:

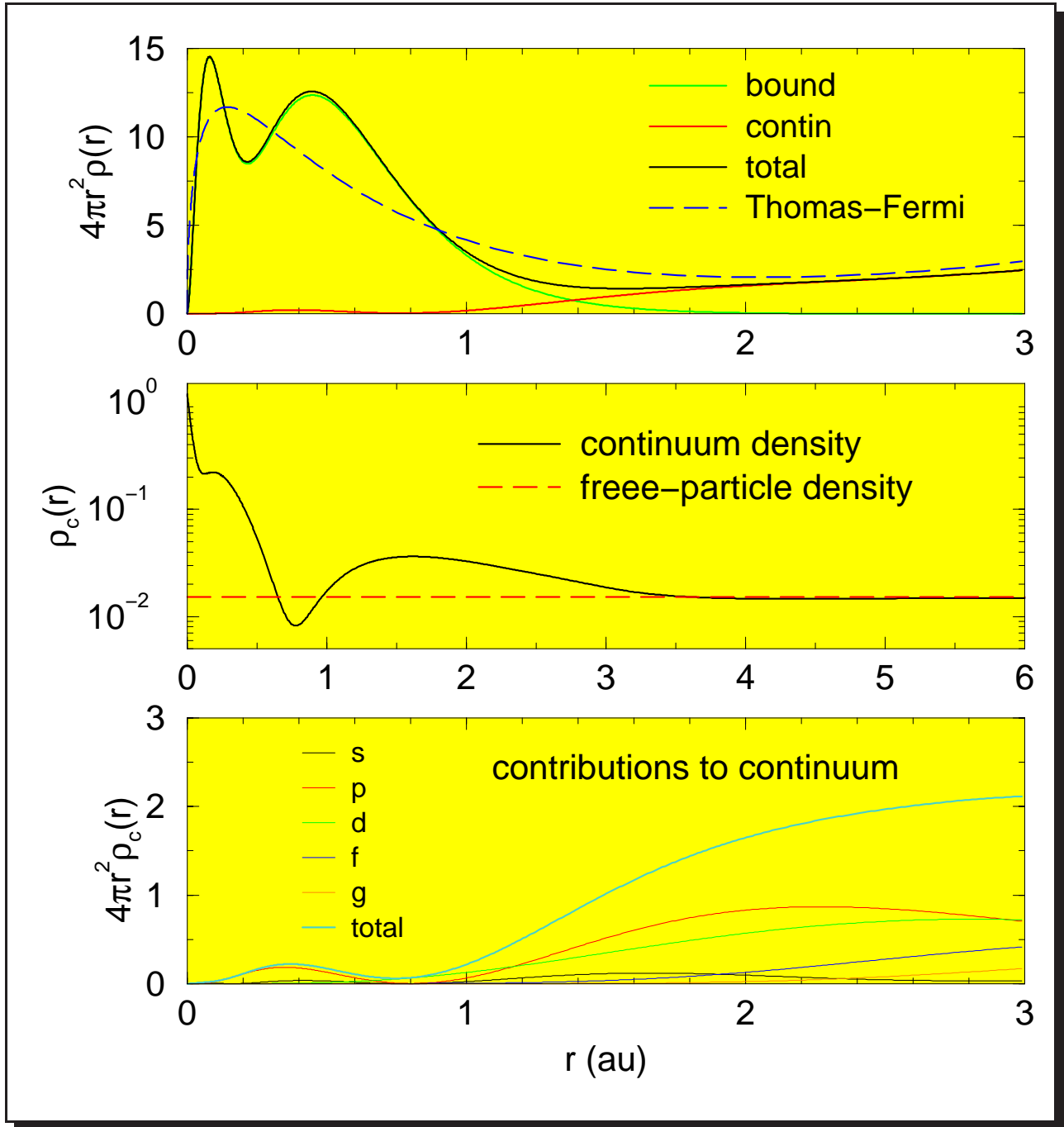
$$\rho_b(r) = \sum_a \frac{2j_a + 1}{1 + \exp[(\epsilon_a - \mu)/kT]} P_a^2(r)$$

$$\rho_c(r) = \sum_{\kappa} \int_0^{\infty} \frac{(2j_{\kappa} + 1) d\epsilon}{1 + \exp[(\epsilon - \mu)/kT]} P_{\epsilon\kappa}^2(r)$$

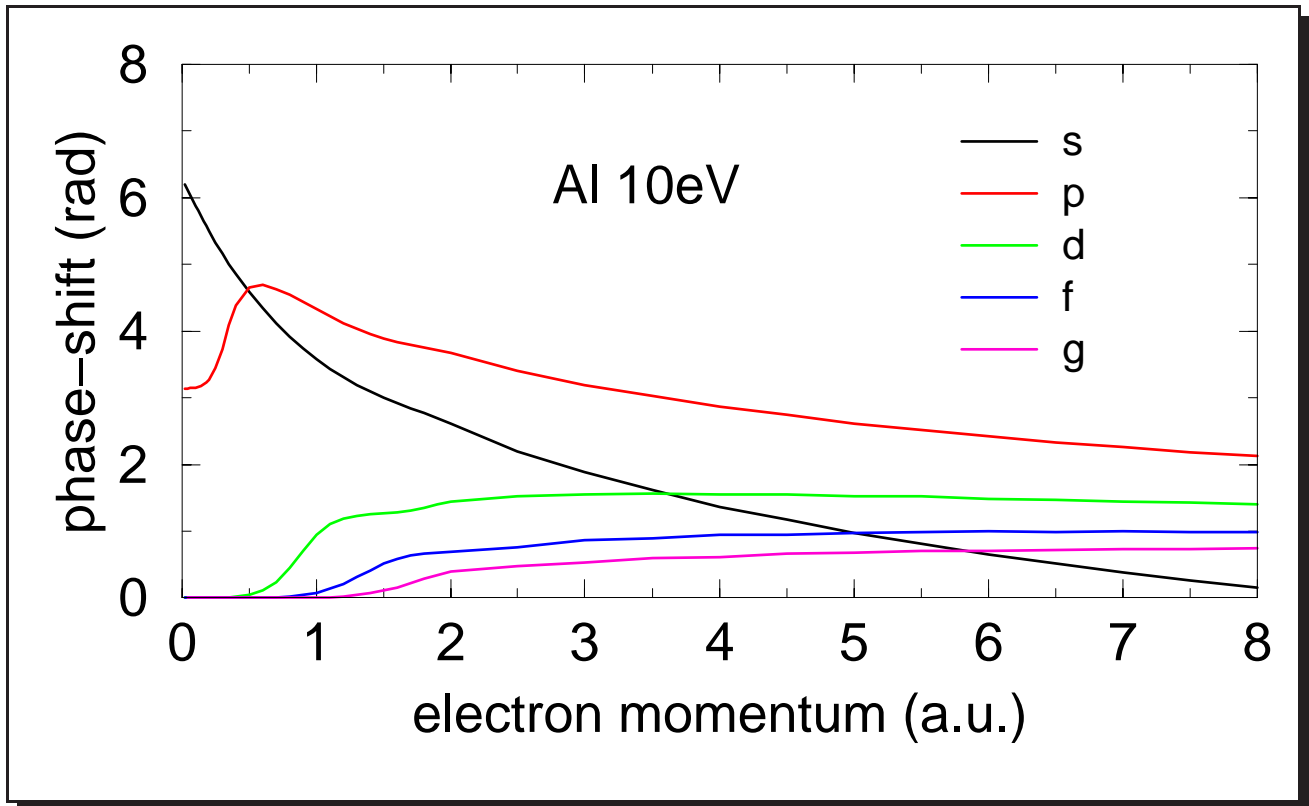
norm:

$$Z = \int_0^R 4\pi r^2 \rho(r) dr$$

Electron density: Al - T=10eV



Phase shifts: Al - T=10eV



Resistivity:

Drude picture: 1900

$$\rho = \rho_0 / (n_e \tau)$$

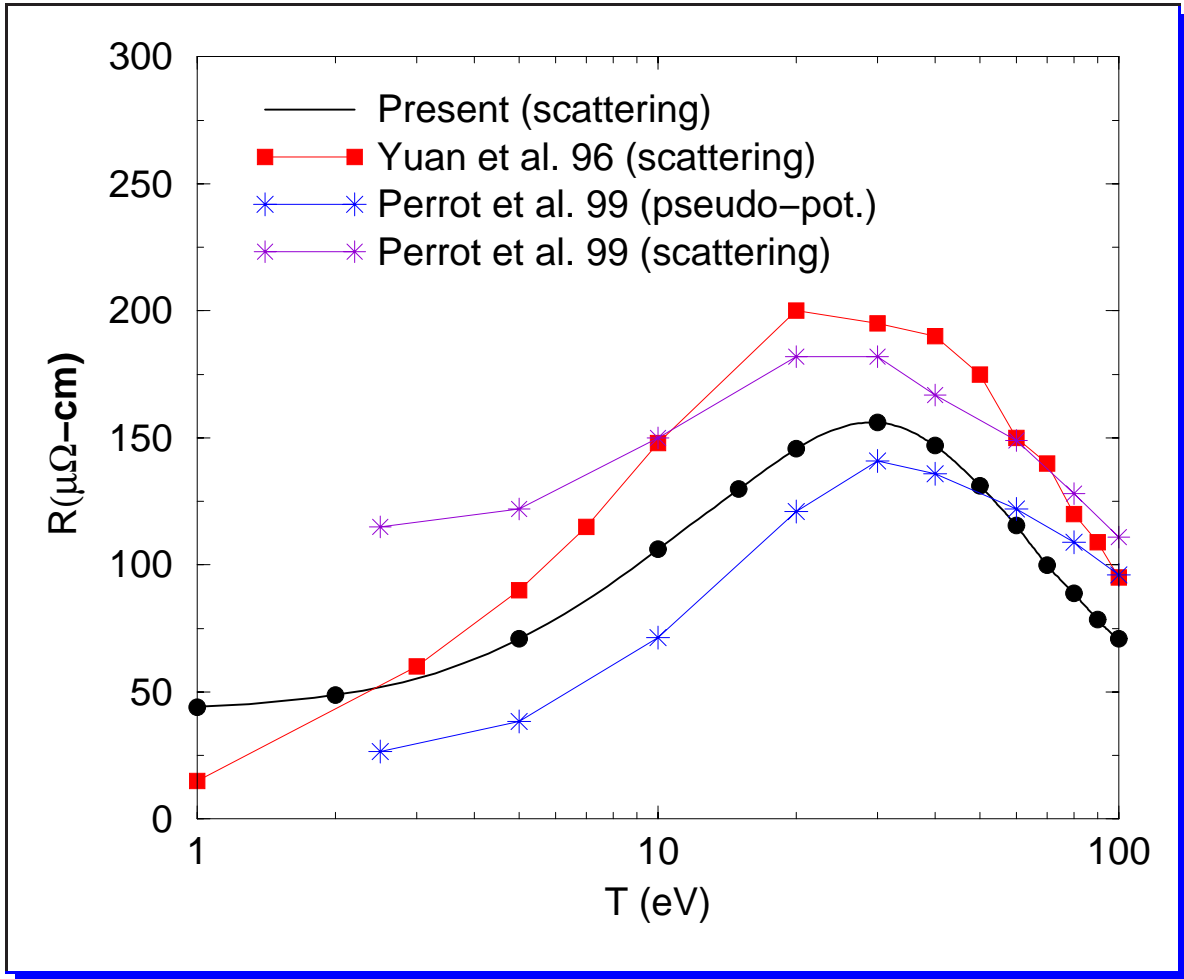
$$\rho_0 = m a_0^3 / (e^2 \tau_0) = 21.74 \mu \Omega\text{-cm}$$

Ziman: 1972 - 1988

$$\frac{1}{\tau} = \frac{1}{3\pi Z^*} \left\langle \int_0^{2p} dq q^3 \sigma(q) S(q) \right\rangle$$

$$\langle F(\epsilon) \rangle = - \int_0^\infty d\epsilon \frac{d}{d\epsilon} \left(\frac{1}{1 + \exp(\epsilon - \mu)/kT} \right) F(\epsilon)$$

Resistivity: Al - T=10eV



Present calculation of resistivity of aluminum compared with other calculations. ^{1 2}

¹J. K. Yuan, Y. S. Sun, and S. T. Zheng, Phys. Rev. E **53**, 1059 (1996).

²F. Perrot and M. W. C. Dharma-wardana, Int. Jour. of Thermophys. **20**, 1299 (1999).