WIGNER DYNAMICS CALCULATIONS OF ELECTRICAL CONDUCTIVITY OF STRONGLY COUPLED QUANTUM PLASMA

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QUANTUM DYNAMICS IN WIGNER REPRESENTATION

Quasi-distribution function in phase space for the quantum case

Density matrix: $\rho(q',q'') = \psi^*(q')\psi(q'')$ $\psi \in C$ $i\frac{\partial \rho}{\partial t} = [\hat{H}, \rho]$

↓

Wigner function: $W^L(q,p) = \frac{1}{(2\pi)^{Nd}} \int \rho\left(q + \frac{\xi}{2}, q - \frac{\xi}{2}\right) e^{-ip\xi} d\xi$

$$\rho(q',q'') = \int W^L\left(\frac{q'+q''}{2}, p\right) e^{i(q'-q'')p} dp \qquad W^L \in R$$

Evolution equation: $\frac{\partial W^L}{\partial t} + \left\langle \frac{p}{m} \middle| \frac{\partial W^L}{\partial q} \right\rangle = \int ds W^L(p-s,q,t)\,\omega(s,q)\,ds$

$$\omega(s,q) = \frac{2}{(2\pi)^{Nd}} \int dq' U(q-q') \sin\left[\frac{2sq'}{\hbar}\right]$$

Classical limit $\hbar \to 0$:

$$\frac{\partial W^L}{\partial t} + \left\langle \frac{p}{m} \middle| \frac{\partial W^L}{\partial q} \right\rangle - \left\langle \frac{\partial U}{\partial q} \middle| \frac{\partial W^L}{\partial p} \right\rangle = 0$$

Characteristics (Hamilton equations):

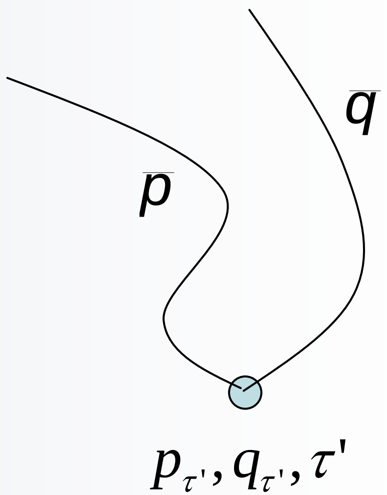
$$\langle \dot{q} | = \left\langle \frac{p}{m} \right| \qquad \langle \dot{p} | = -\left\langle \frac{\partial U}{\partial q} \right|$$

SOLUTION OF WIGNER EQUATION

$$W(p,q,t) = \int \Pi^W(p,q,t;p_0,q_0,0) \times W_0(p_0,q_0)\,dp_0\,dq_0 +$$

$$\int_0^t d\tau' \int\int dp_{\tau'}\,dq_{\tau'}\,\Pi^W(p,q,t;p_{\tau'},q_{\tau'},\tau') \times \int_{-\infty}^{\infty} ds\,W(p_{\tau'}-s,q_{\tau'},\tau')\,\omega(s,q_{\tau'})$$

Dynamical trajectories:



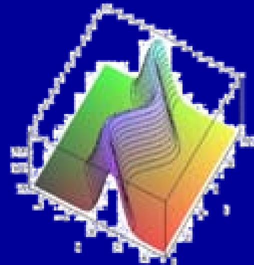
$$\frac{d\bar{p}}{dt} = F(\bar{q}(t)),\ \bar{q}_{\tau'}(\tau';p_{\tau'},q_{\tau'},\tau') = q_{\tau'}$$

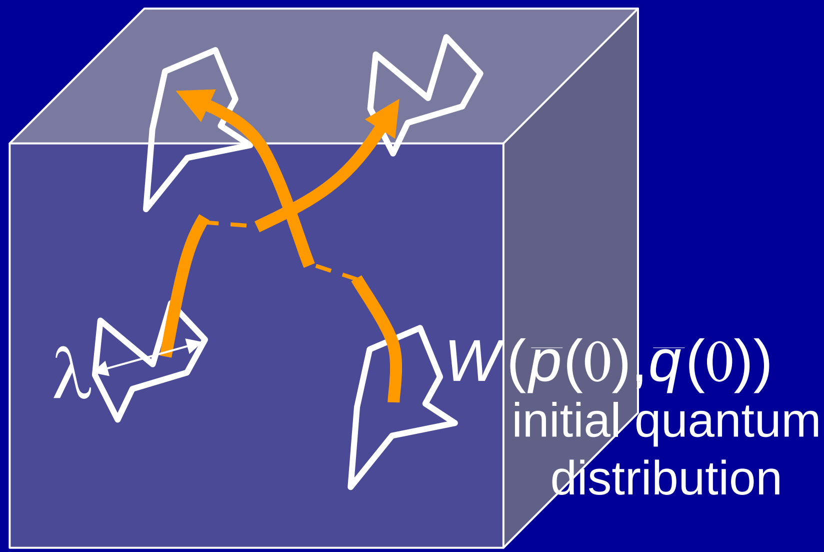
$$\frac{d\bar{q}}{dt} = \bar{p}(t)/m,\ \bar{p}_{\tau'}(\tau';p_{\tau'},q_{\tau'},\tau') = p_{\tau'}$$

Propagator:

$$\Pi^W(p,q,t;p_{\tau'},q_{\tau'},\tau') = \delta(p-\bar{p}_t(t;p_{\tau'},q_{\tau'},\tau'))\,\delta(q-\bar{q}_t(t;p_{\tau'},q_{\tau'},\tau'))$$

Quantum dynamics in Wigner and tomography representations





$$\frac{d\bar{p}}{dt} = \bar{F}(\bar{q}(t))$$

$$\frac{d\bar{q}}{dt} = \frac{\bar{p}(t)}{m}$$

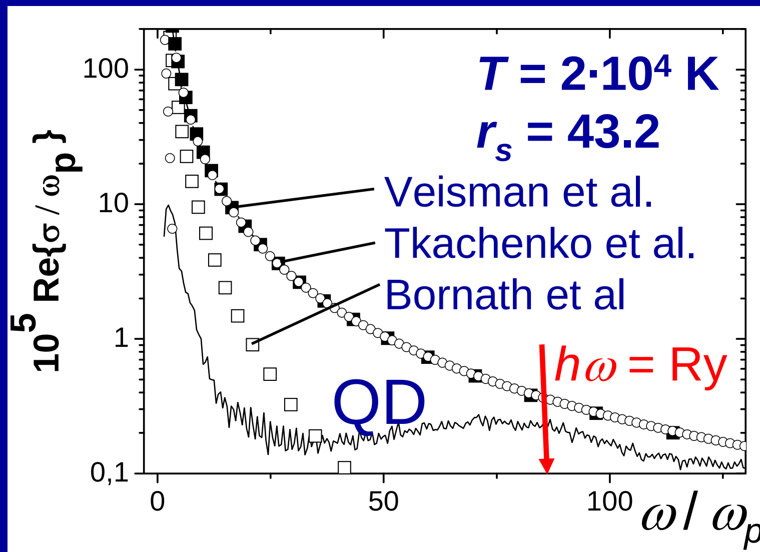
5000-20000 configurations

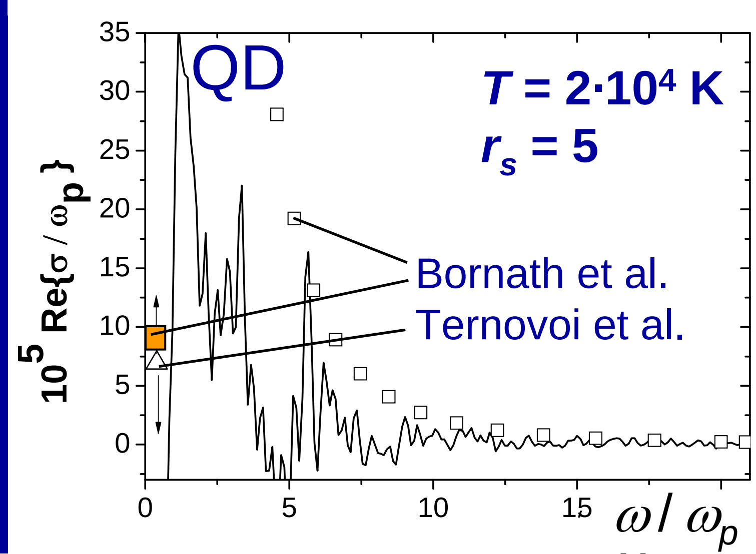
\+ random momentum jumps

$$\sigma \sim FT(<\bar{p}(t)\bar{p}(0)>)$$

$$\sigma_{\alpha\gamma}(\omega)=\int_0^\infty dt\, e^{i\omega t-\epsilon t}\int_0^\beta d\lambda \langle \hat{J}_\gamma \hat{J}_\alpha(t+i\hbar\lambda)\rangle$$

Dynamic conductivity

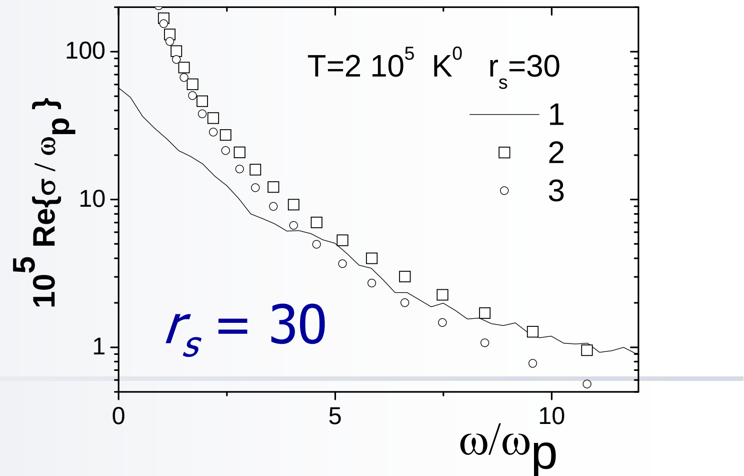


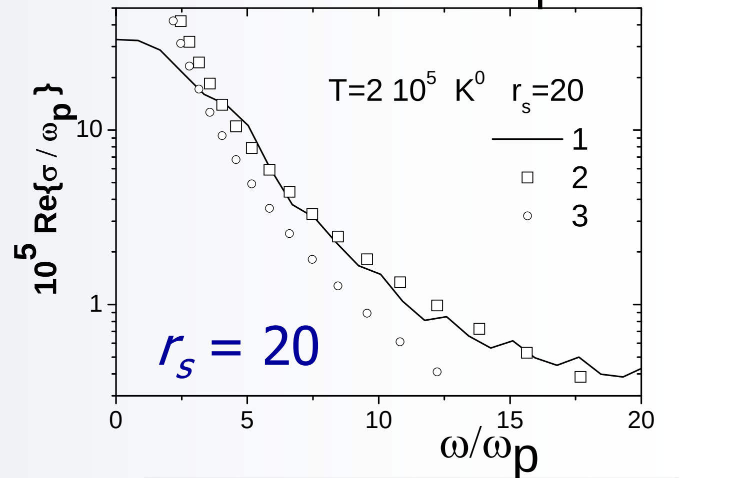


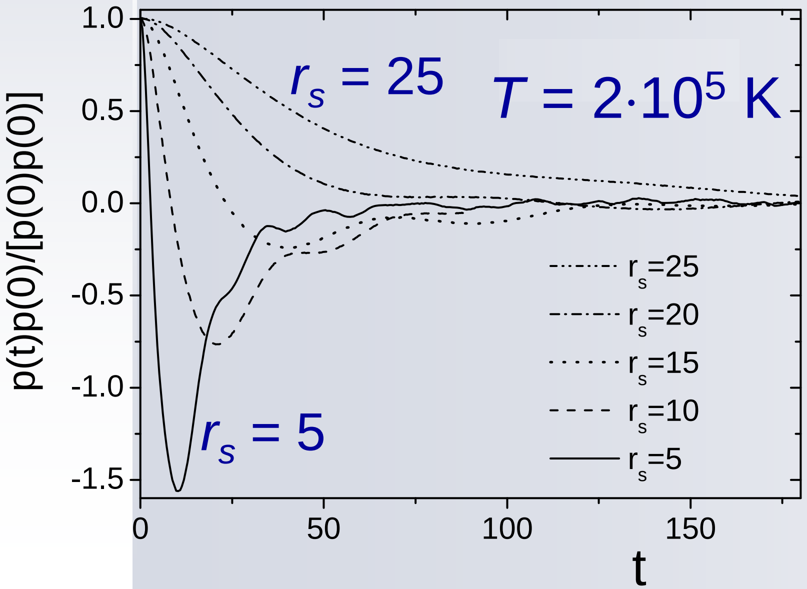
Temporal momentum-momentum correlation functions and electroconductivity

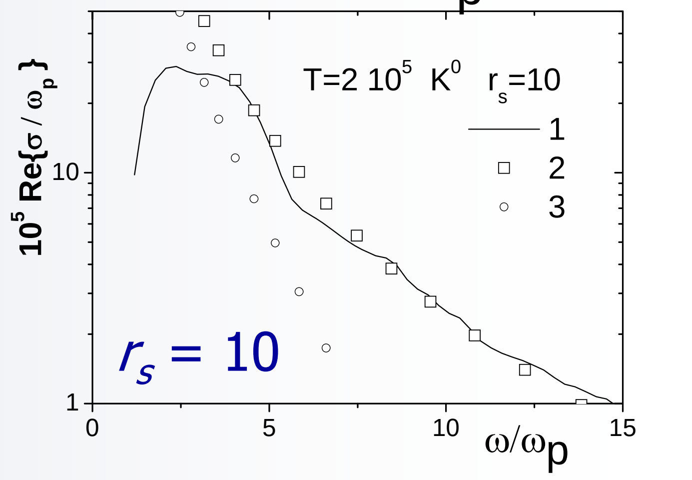
T = 200 000 K

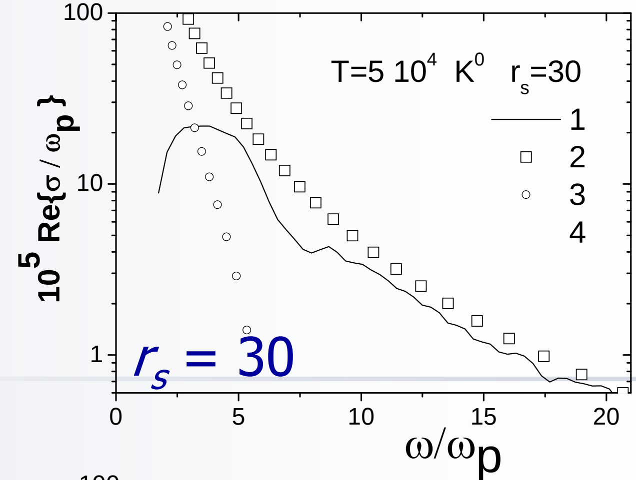
1 – Quantum Dynamics
2 – Bornath T. et al., LPB, 18, 535 (2000)
3 – Silin V.P., ZhETF 47 2254 (1964)



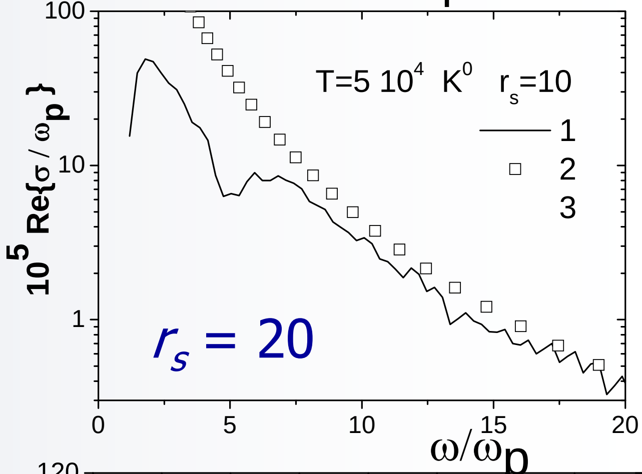






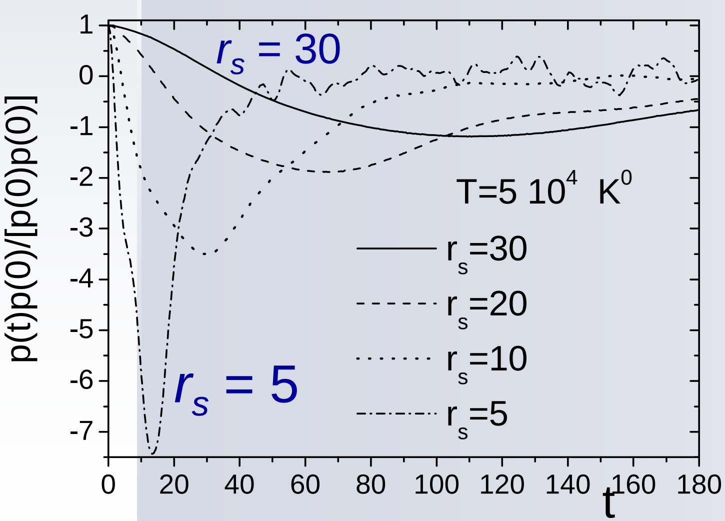


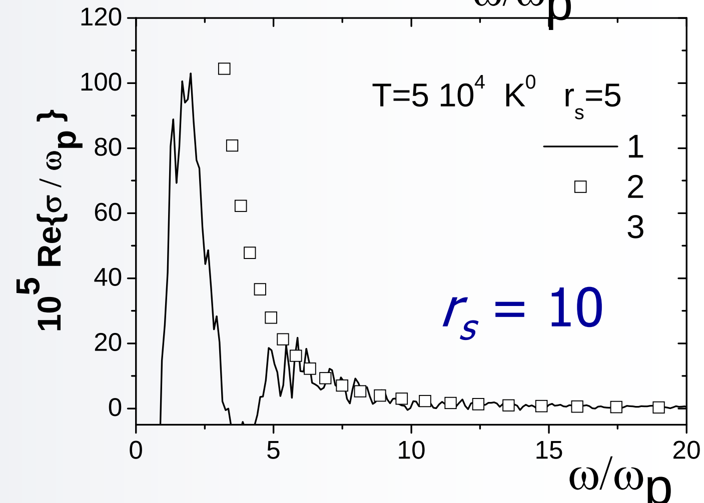
Temporal momentum-momentum correlation functions and electroconductivity



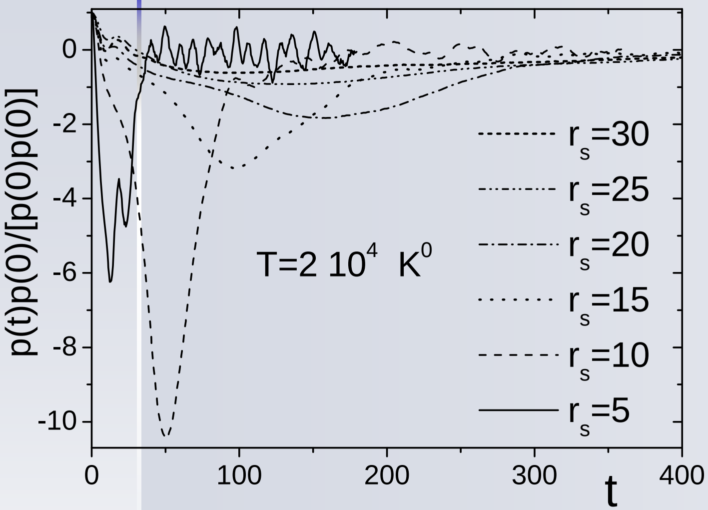
$T = 50\ 000$ K

1 – Quantum Dynamics
2 – Bornath T. et al., LPB, 18, 535 (2000)
3 – Silin V.P., ZhETF 47 2254 (1964)

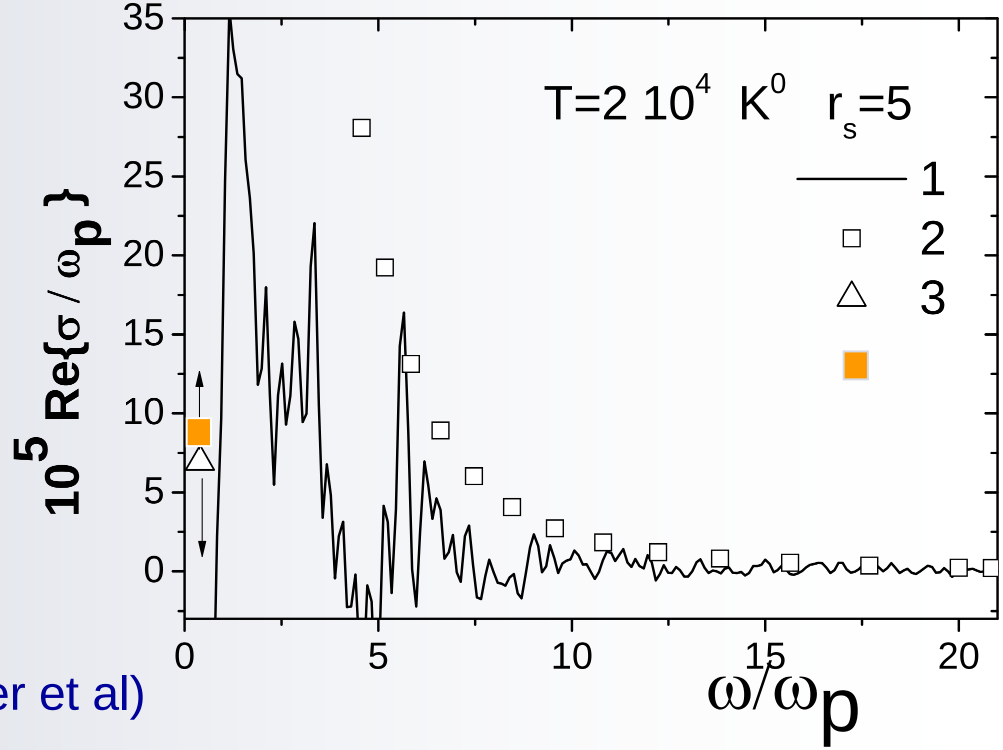




Temporal momentum-momentum correlation functions and electrical conductivity



$r_s = 5, \quad T = 20\ 000$



1 – QMD
2 – LPB, 18, 535 (2000) (Bornath et al.)
3 - Experimental points for hydrogen plasma– Nellis et al. and Ternovoi et al.
4 - Phys.Rev.B, 63, 233104(2001)(Redmer et al)

DFT-MD CONDUCTIVITY CALCULATION

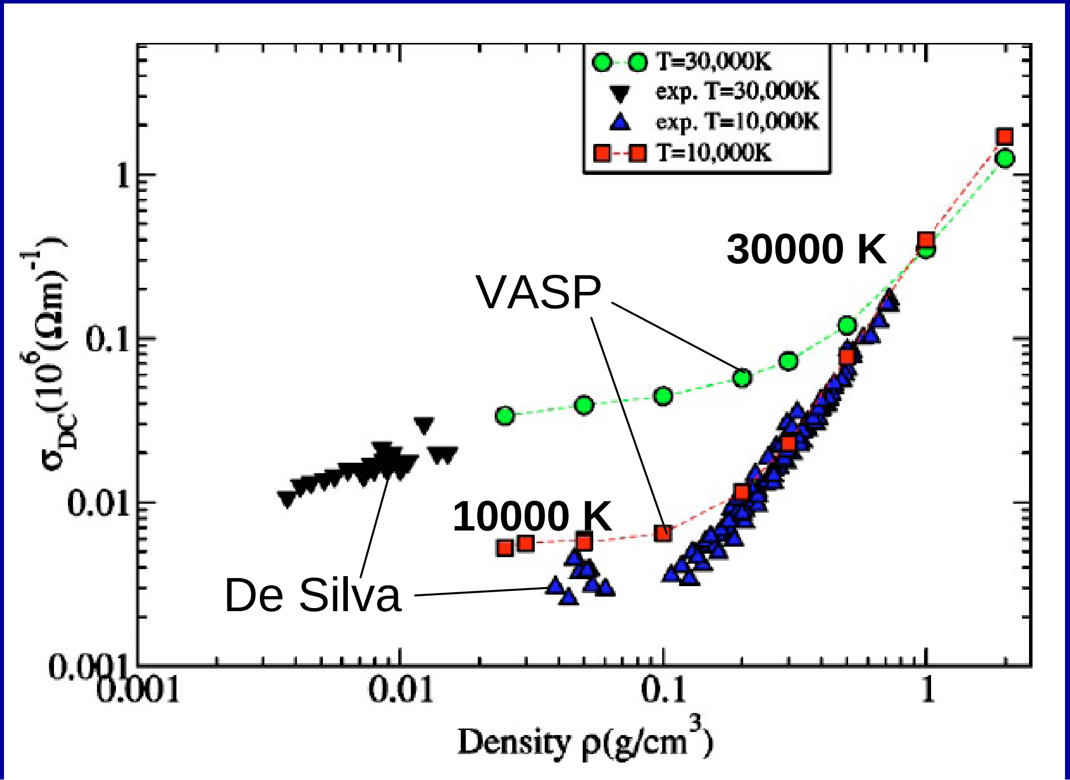
Kubo-Greenwood formula:

$$\sigma_{\mathbf{k}}(\omega)=\frac{2\pi e^2\hbar^2}{3m^2\omega\Omega}\sum_{j=1}^{N}\sum_{i=1}^{N}\sum_{\alpha=1}^{3}[F(\epsilon_{i,\mathbf{k}})-F(\epsilon_{j,\mathbf{k}})]\times|\langle\Psi_{j,\mathbf{k}}|\nabla_\alpha|\Psi_{i,\mathbf{k}}\rangle|^2\delta(\epsilon_{j,\mathbf{k}}-\epsilon_{i,\mathbf{k}}-\hbar\omega),$$

Fermi function

Static electrical conductivity of aluminum

8-108 atoms
10-30 QMD steps



Mazevet *et al.*
PRE **71**, 016409 (2005)

CONCLUSIONS

- Kubo formula leads to two computational approaches
- One-electron approach requires less temporal steps and gives better results especially at low frequencies
- Momentum-momentum approach is more general, but requires more temporal steps
- Wigner quantum dynamics calculations for electrical conductivity give good agreement with other theories for ideal plasma; for non-ideal plasma distinctions can be significant
- Comparison with QMD and DFT-MD data is planned