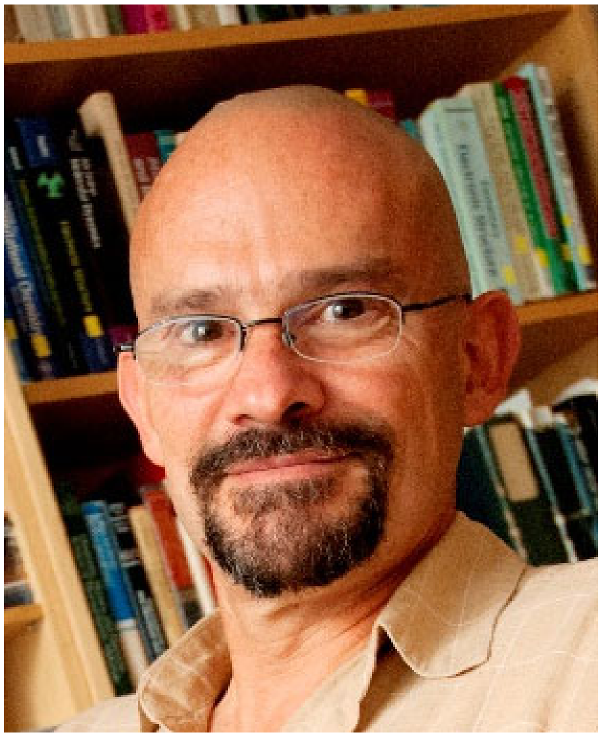
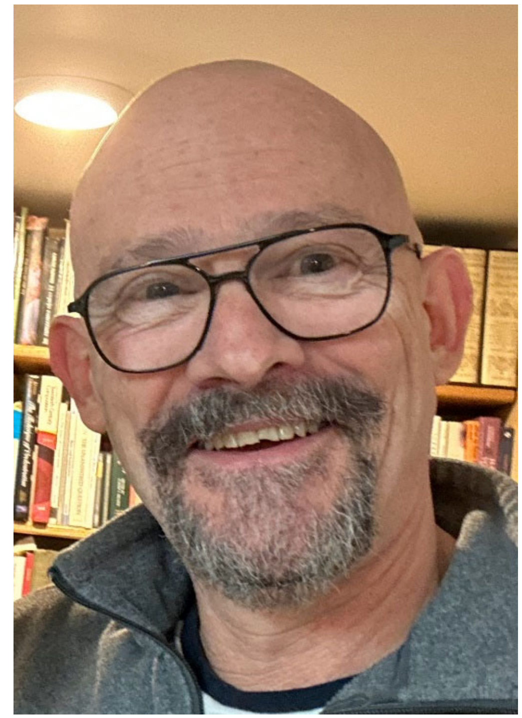
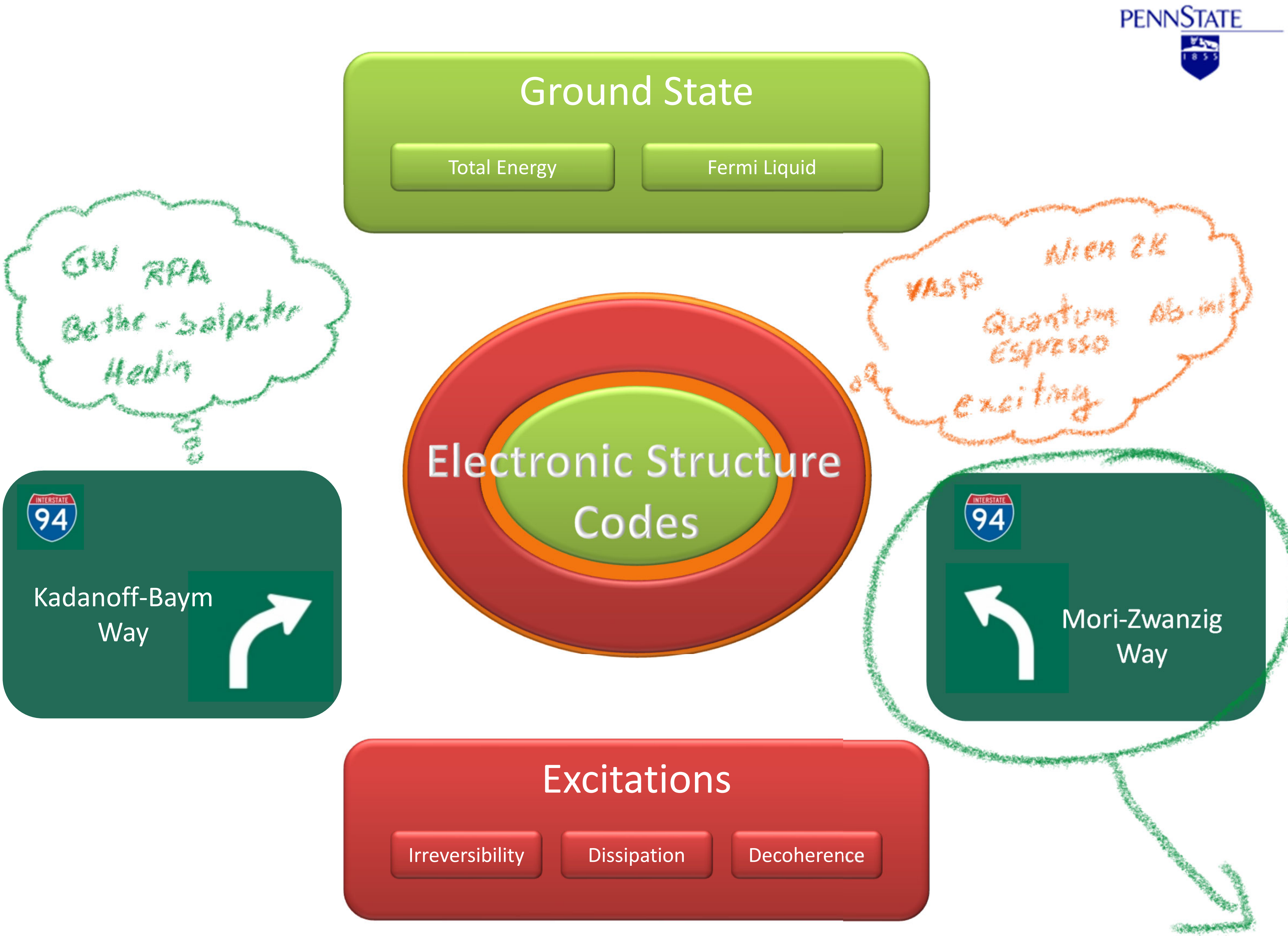
The Arrow of Time



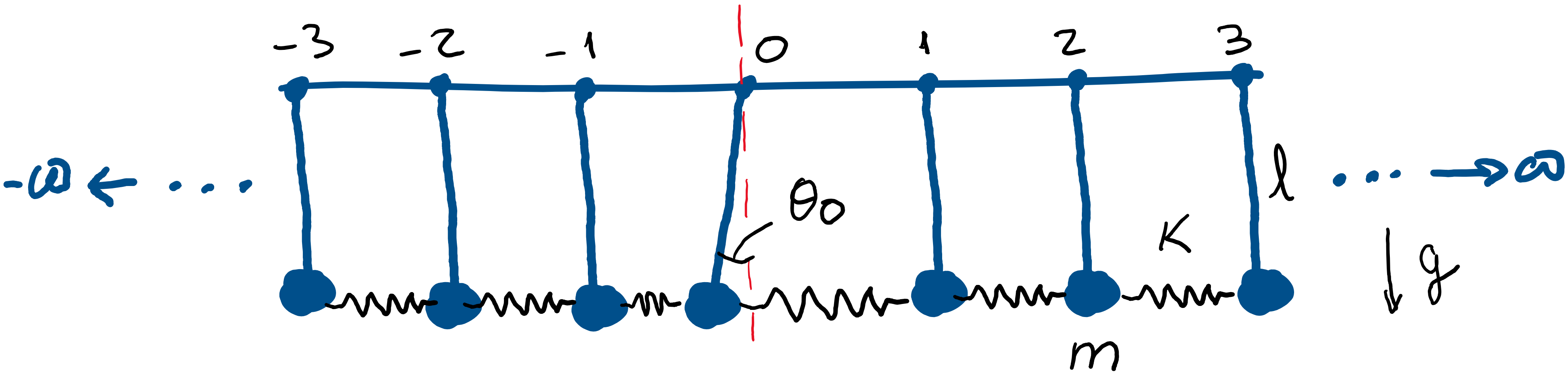


We can distinguish past from present…

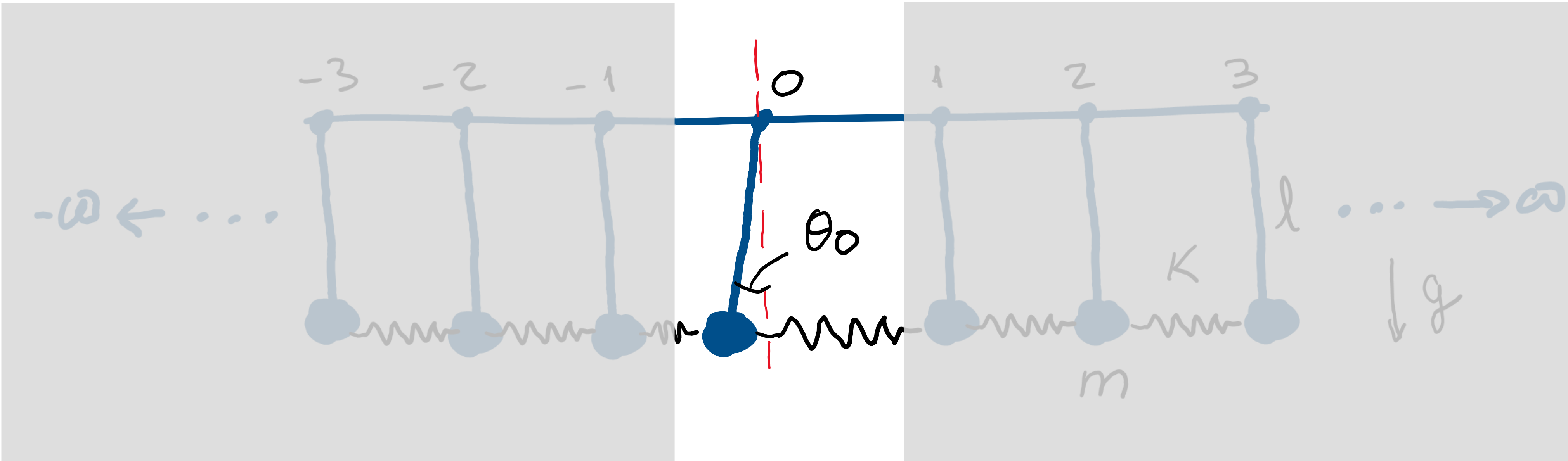


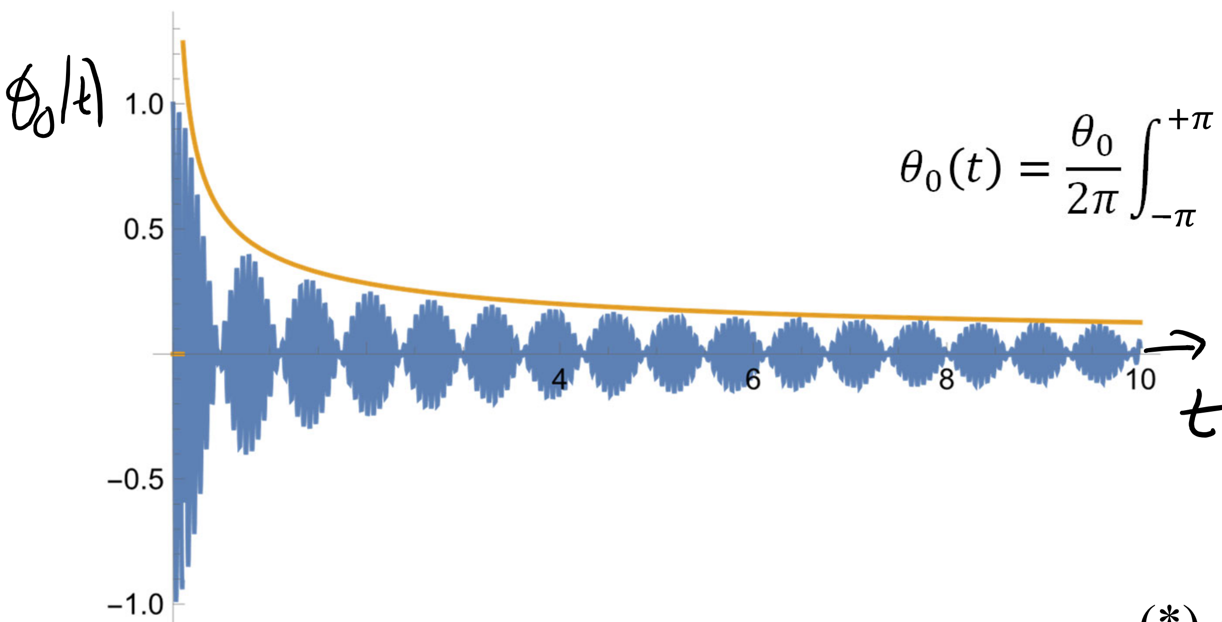
PENNSTATE
Ground State
Total Energy
Fermi Liquid
GW RPA
Bethe-Salpeter
Hedin
VASP
Wien 2K
Quantum Espresso
Ab-init
exciting
Electronic Structure Codes
94
Kadanoff-Baym Way
94
Mori-Zwanzig Way
Excitations
Irreversibility
Dissipation
Decoherence

The Illusion of Irreversibility (Classical)



The Illusion of Irreversibility (Classical)

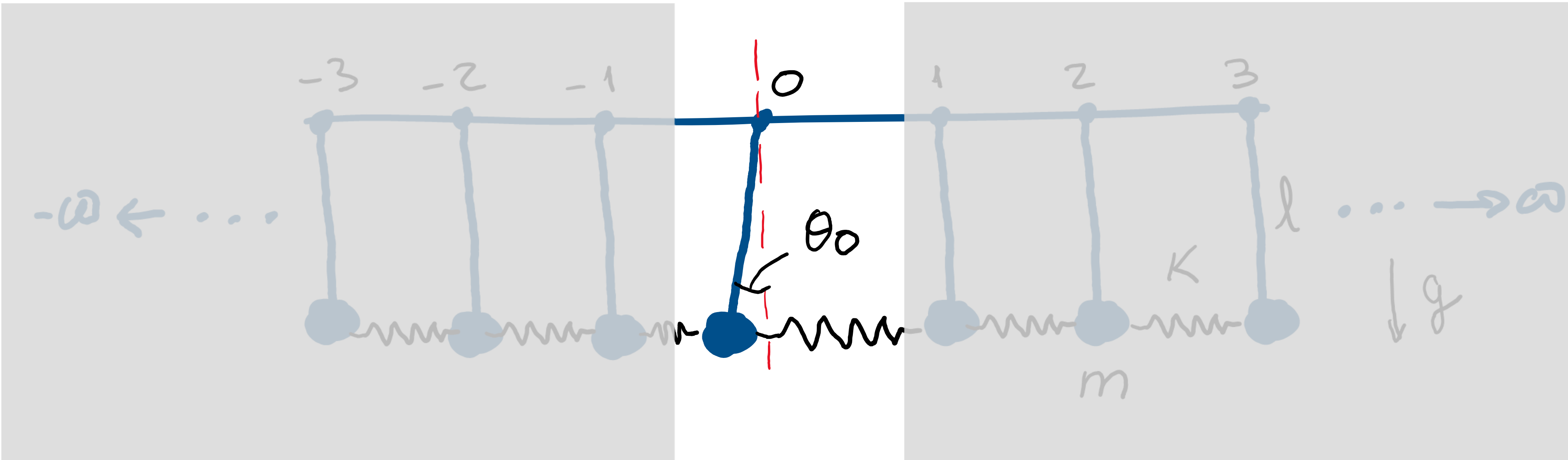


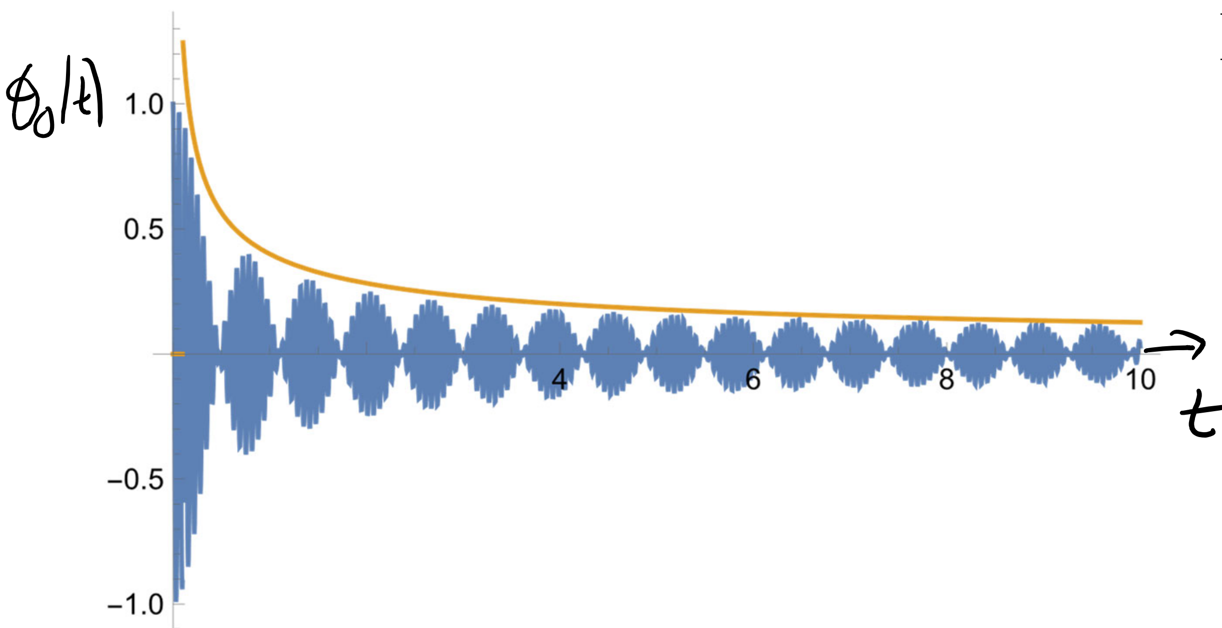


$$\theta_0(t) = \frac{\theta_0}{2\pi}\int_{-\pi}^{+\pi} dk \cos\left[t\sqrt{\omega_0^2 + 4\omega_K^2 \sin\left(\frac{k}{2}\right)}\right]^{(*)}$$

(*) Alberto Rojo, private communication.

The Illusion of Irreversibility (Classical)





Ingredients:

- Initial condition
- Projection
- Limiting process (∞)

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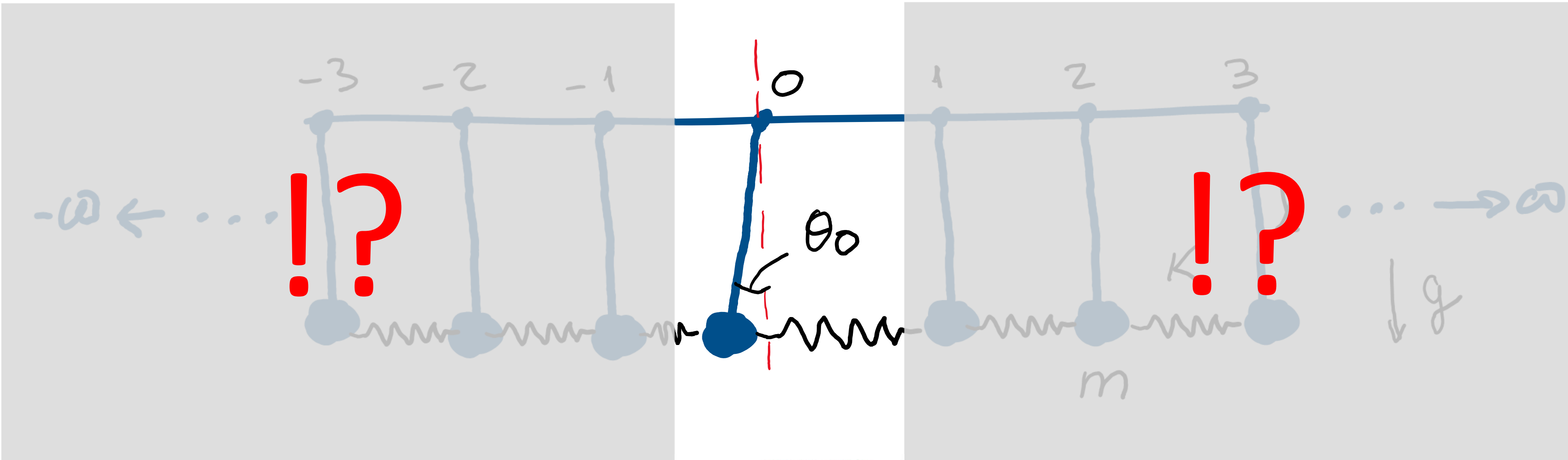
The Illusion of Irreversibility (Quantum)



Global

Local (in some representation)

$$\langle x_0 \rangle_t = Tr\left(\rho e^{iLt} \hat{x}_0\right)$$

One possible avenue:

Projection on “local” observables

to disentangle the dynamics

$L\blacksquare = [H, \blacksquare]$

$\hbar = 1$

Generalized Quantum Langevin Equation for Transport:

The case for Interband Coherence

Jorge O. Sofo
Department of Physics
Department of Materials Science and Engineering
Materials Research Institute
Penn State

In collaboration with:

Brett R. Green and Cristobal I. Vallejos Benavides
Physics, Penn State

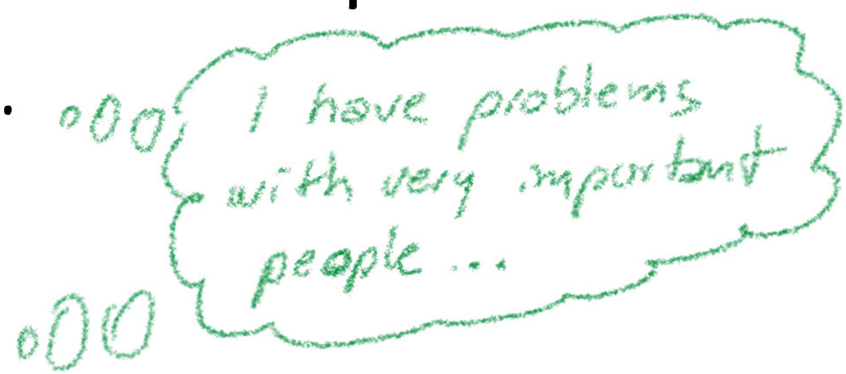
Maria Troppenz, Santiago Rigamonti, and Claudia Draxl
Humboldt Universität zu Berlin (exciting)

Anooja Jayaraj and Marco Buongiorno Nardelli
University of North Texas (PAOFlow)

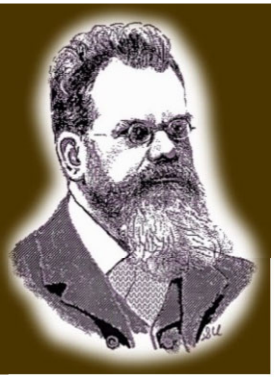
During the rest of the talk…

Concentrate on electrical transport

- Review the Quantum Boltzmann Equation
  – Problems with Boltzmann…



- Review the Kubo formula
  – Problems with Kubo…
- Discuss the Generalized Langevin Equation
  – Show that in the hydrodynamic regime provides a quantum correction to Boltzmann



Semiclassical Dynamics "a la" Boltzmann

$$\langle x_0 \rangle_t = Tr\left(\rho e^{iLt} \hat{x}_0\right)$$

Quantum coherence is lost

$$\rho(t) \rightarrow \rho_1(t) \rightarrow f(\vec{r}, \vec{p}, t)$$

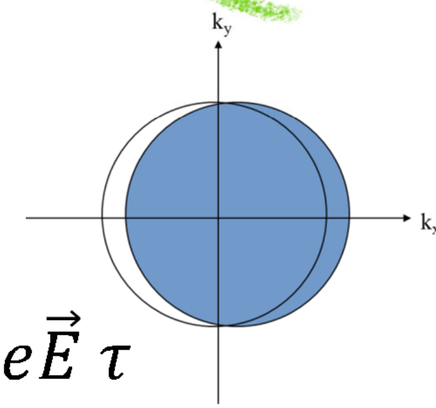
$$\partial_t f - \{H, f\} = C[f]$$

Relaxation time approx

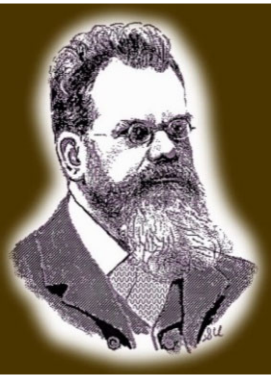
$$C_{RT}[f] = \frac{f(\vec{p}) - f_{eq}(\vec{p})}{\tau}$$

Valid for weak scattering

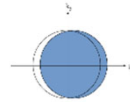
$$f(\vec{p}) = f_{eq}(\vec{p}) + \partial_{\vec{p}} f(\vec{p})\, \vec{F}\, \tau$$



$$f_{n\vec{k}} = f_0(\varepsilon_{n\vec{k}}) - f_0'(\varepsilon_{n\vec{k}}) \vec{v}_{n\vec{k}}\, e\vec{E}\, \tau$$



$$f_{n\vec{k}} = f_0(\varepsilon_{n\vec{k}}) - f_0'(\varepsilon_{n\vec{k}})\vec{v}_{n\vec{k}} \cdot e\vec{E}\,\tau$$



Conductivity “a la” Boltzmann

$$\vec{j} = \sum_{n\vec{k}} f_{n\vec{k}}\,\vec{v}_{n\vec{k}}$$

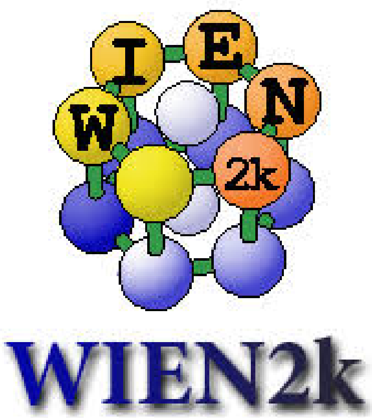
$$\vec{j}_{RT} = e\sum_{n\vec{k}} [-f_0'(\varepsilon_{n\vec{k}})]\,\tau\,\vec{v}_{n\vec{k}}\vec{v}_{n\vec{k}} \cdot \vec{E}$$

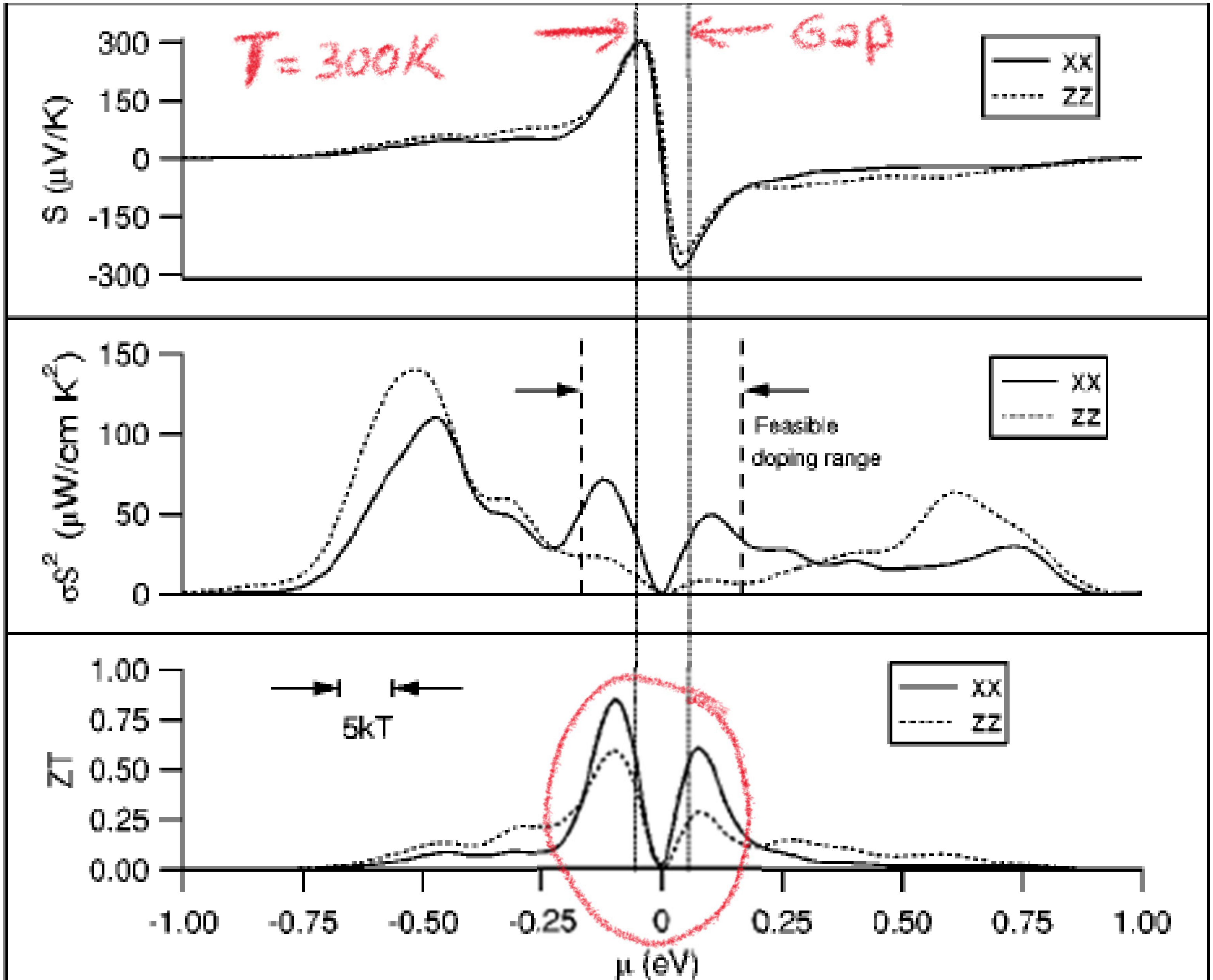
$$\overleftrightarrow{\sigma}_{RT} = e\tau \sum_{n,\vec{k}} [-f_0'(\varepsilon_{n\vec{k}})]\;\vec{v}_{n\vec{k}}\vec{v}_{n\vec{k}}$$

τ typically taken from 1st Born approximation

An example of Boltzmann: Optimal Doping Range

Bi_2Te_3

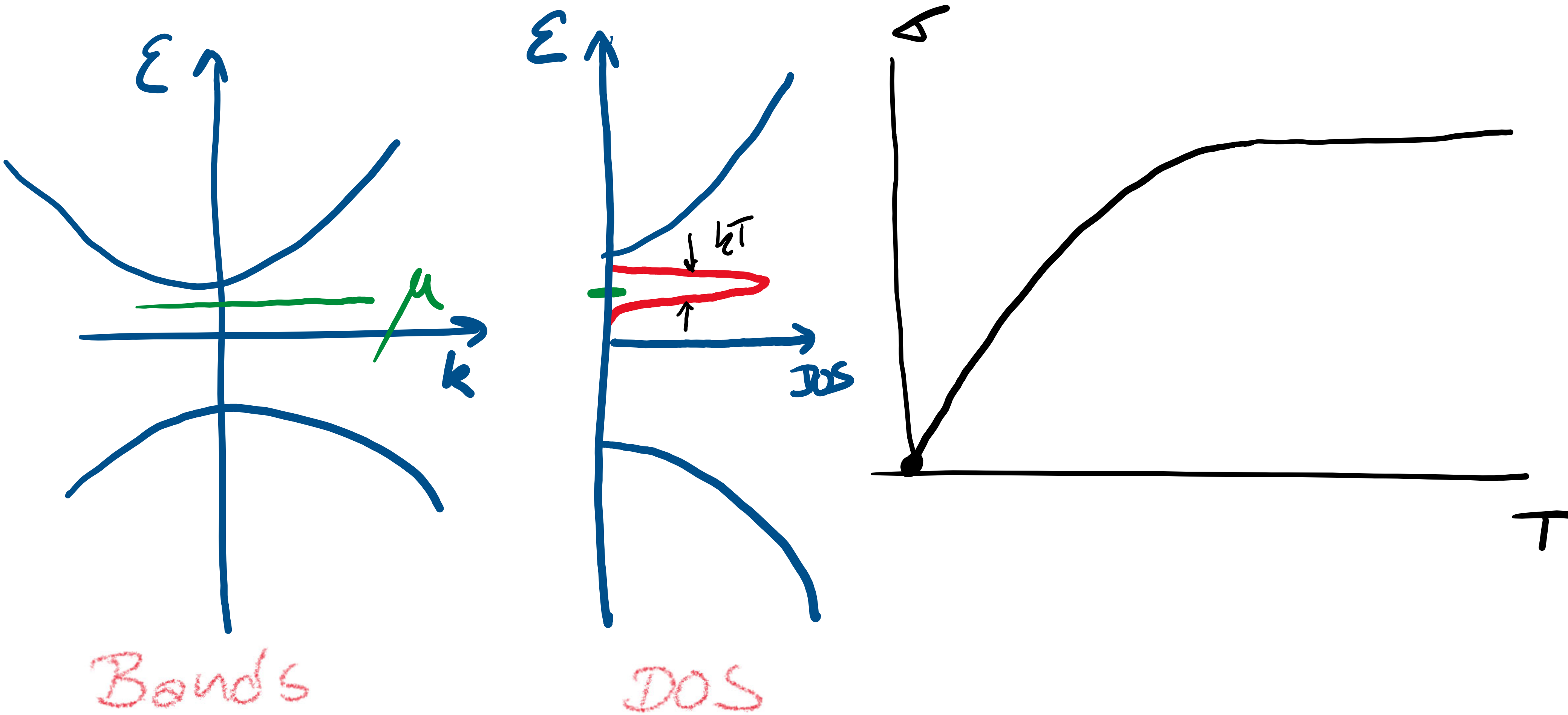




T. J. Scheidemantel, C. Ambrosch-Draxl, T. Thonhauser, J. V. Badding, and J. O. Sofo. "Transport Coefficients from First-principles Calculations." *Phys. Rev. B* **68**, 125210 (2003)

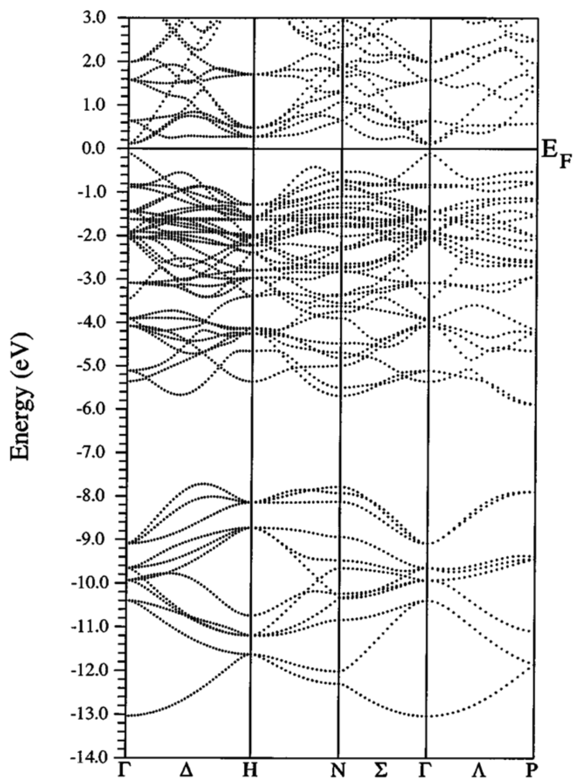
Problems with Boltzmann…

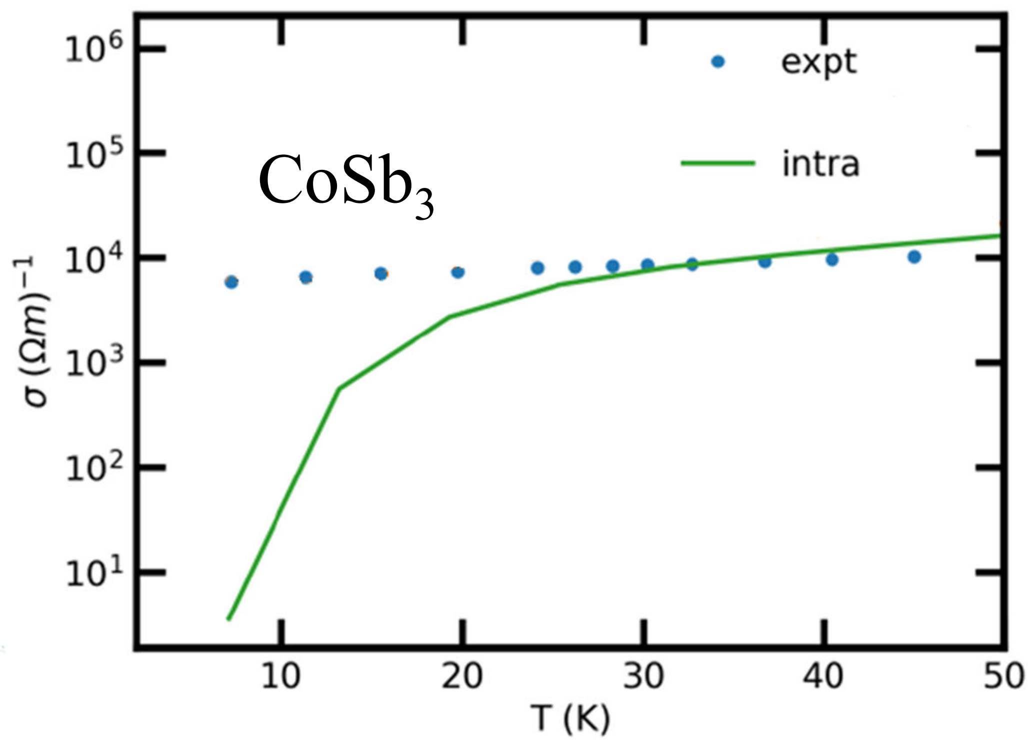
$$\overleftrightarrow{\sigma} = e\tau \sum_{n,\vec{k}} [-f_0'(\varepsilon_{n\vec{k}})]\ \vec{v}_{n\vec{k}}\vec{v}_{n\vec{k}}$$



Problems with Boltzmann…

$$\overleftrightarrow{\sigma} = e\tau \sum_{n,\vec{k}} [-f_0'(\varepsilon_{n\vec{k}})] \; \vec{v}_{n\vec{k}} \vec{v}_{n\vec{k}}$$





E. Arushanov, et al., *Transport Properties of Lightly Doped $CoSb_3$ Single Crystals*, Phys. Rev. B **56**, 1911 (1997). (Experiment)
A. Jayaraj, et al., *Relaxation Time Approximations in PAOFLOW 2.0*, ArXiv:2111.09274 [Cond-Mat] (2021). (High T Fit)

With the memory function approach…

Coherence

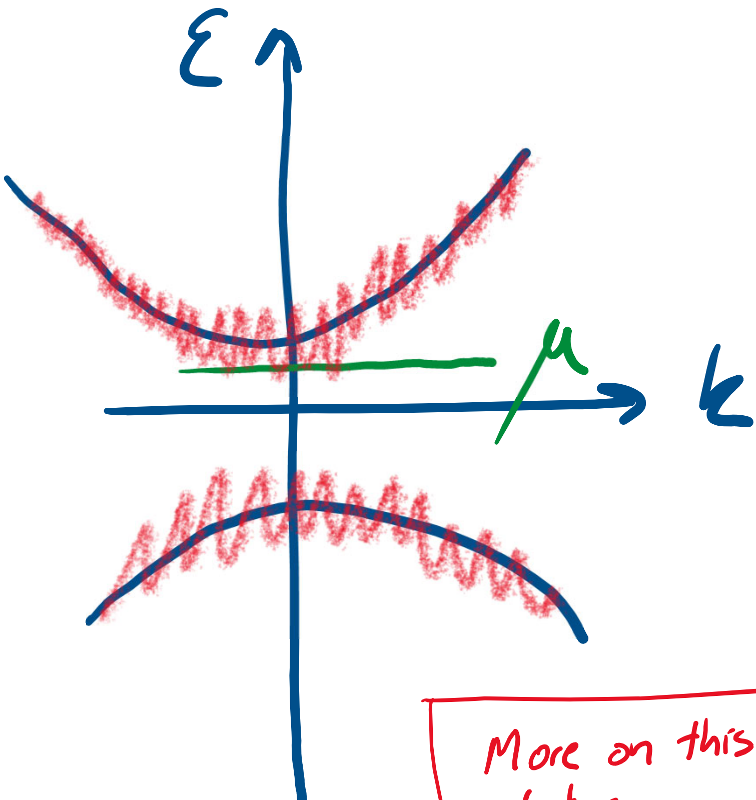
Only at low T

$$\overleftrightarrow{\sigma} = \tau \sum_{n,\vec{k}} [-f_0'(\varepsilon_{n\vec{k}})]\ \vec{v}_{n\vec{k}}\vec{v}_{n\vec{k}} + \frac{1}{\tau} \sum_{n,n',\vec{k}} \frac{\vec{v}_{n,n',\vec{k}}\ \vec{v}_{n',n,\vec{k}}}{\varepsilon_{n,\vec{k}} - \varepsilon_{n',\vec{k}}} \frac{f_0\left(\varepsilon_{n,\vec{k}}\right) - f_0\left(\varepsilon_{n',\vec{k}}\right)}{\left(\frac{1}{\tau}\right)^2 + \left(\varepsilon_{n,\vec{k}} - \varepsilon_{n',\vec{k}}\right)^2}$$

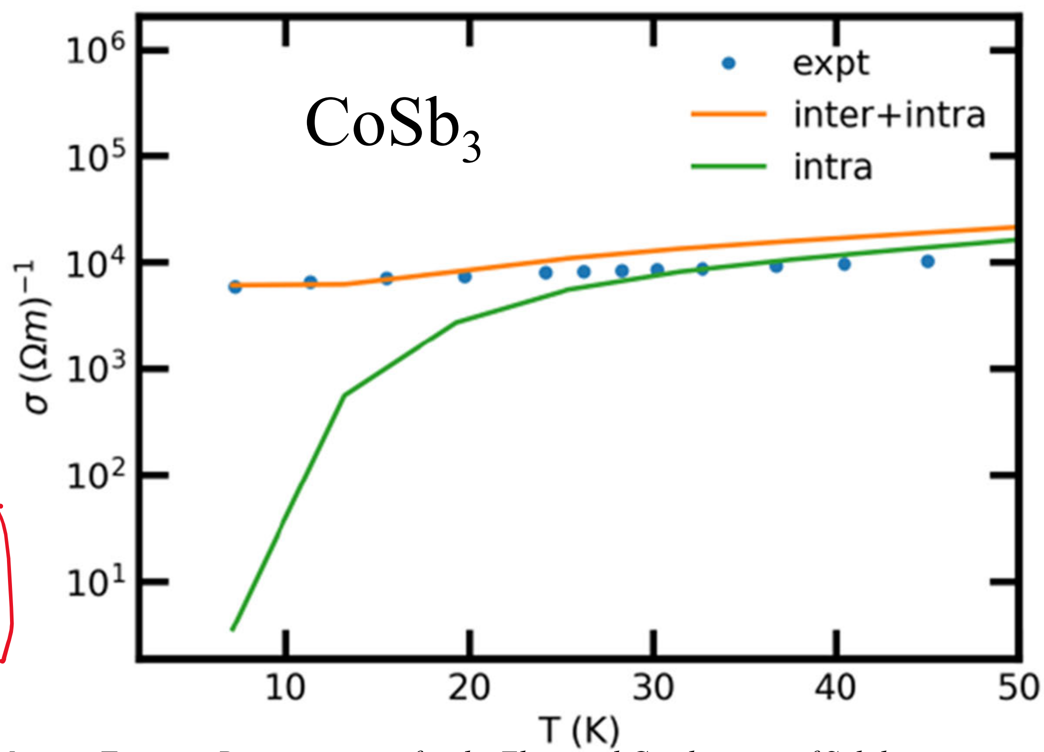
$\frac{1}{\tau}$ = 1meV

Broadening

Optical transition



More on this later…



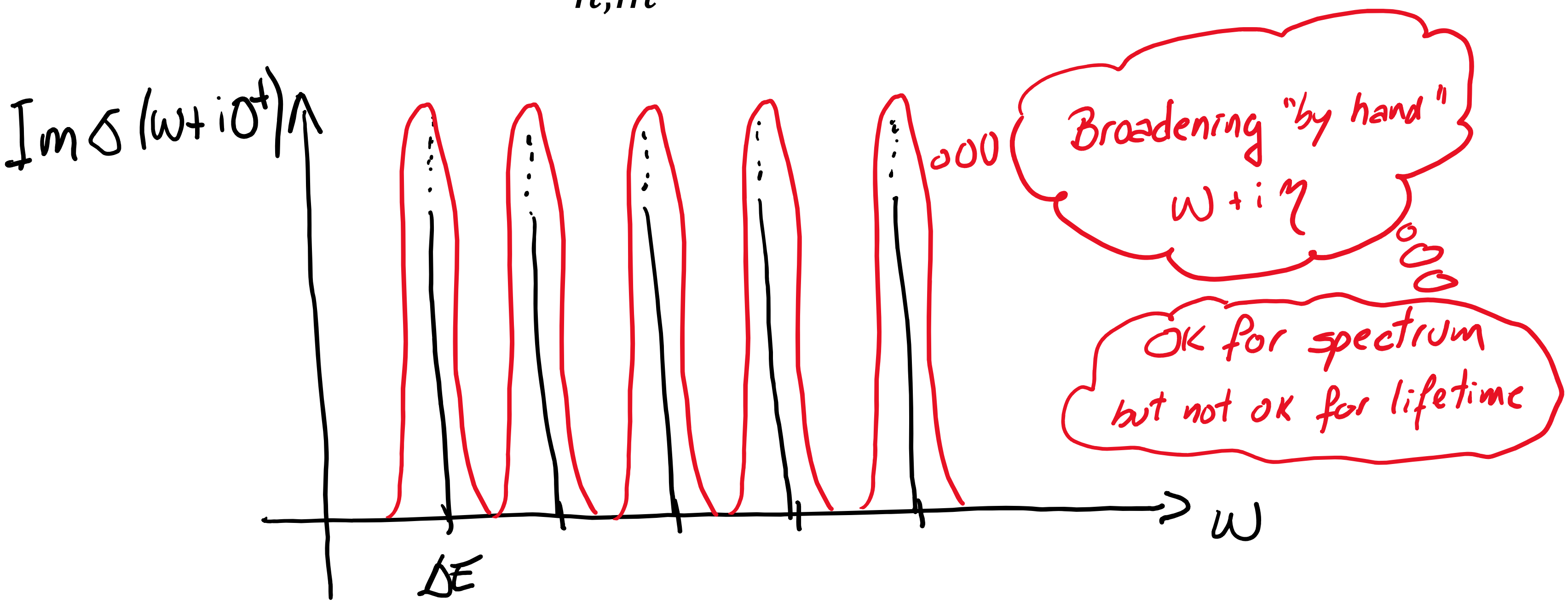
B. R. Green, M. Troppenz, S. Rigamonti, C. Draxl, and J. O. Sofo, *Memory Function Representation for the Electrical Conductivity of Solids*, ArXiv:2110.02859 [Cond-Mat] (2021).

Linear Response (Kubo)

$$J(t) = \int_{-\infty}^{t} i\langle[J(t-t'),P]\rangle\, E(t')\, dt' \quad \Longrightarrow \quad \sigma(t) = i\langle[J(t),P]\rangle$$

Lehmann representation $\quad H|n\rangle = E_n|n\rangle$

$$\sigma(z) = \int_0^{\infty} dt\, e^{izt}\sigma(t) = \frac{1}{Z}\sum_{n,m} \frac{e^{-\beta E_m} - e^{-\beta E_n}}{z - E_n + E_m} \langle n|J|m\rangle\langle m|P|n\rangle$$



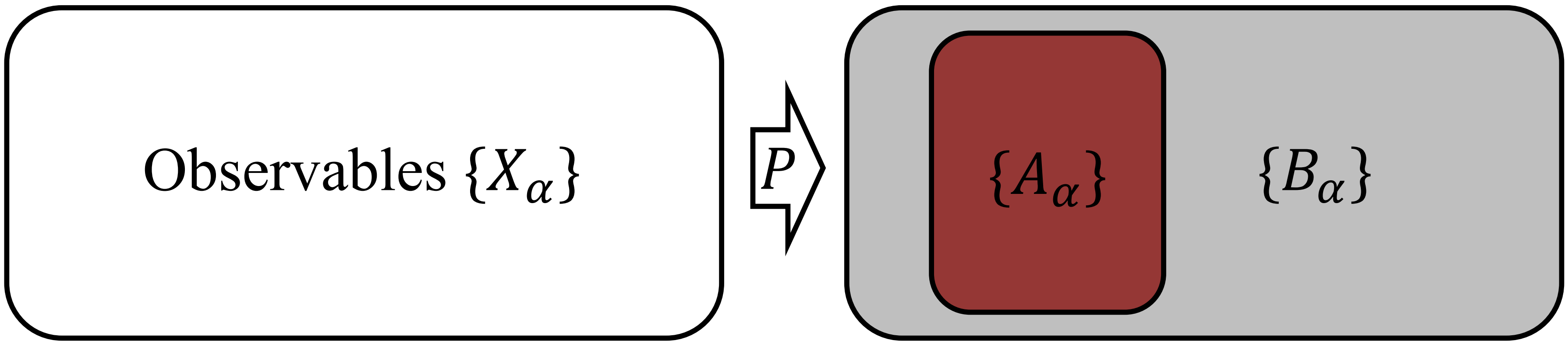
During the rest of the talk…

Concentrate on electrical transport

- Review the Quantum Boltzmann Equation
  – Problems with Boltzmann…
- Review the Kubo formula
  – Problems with Kubo…

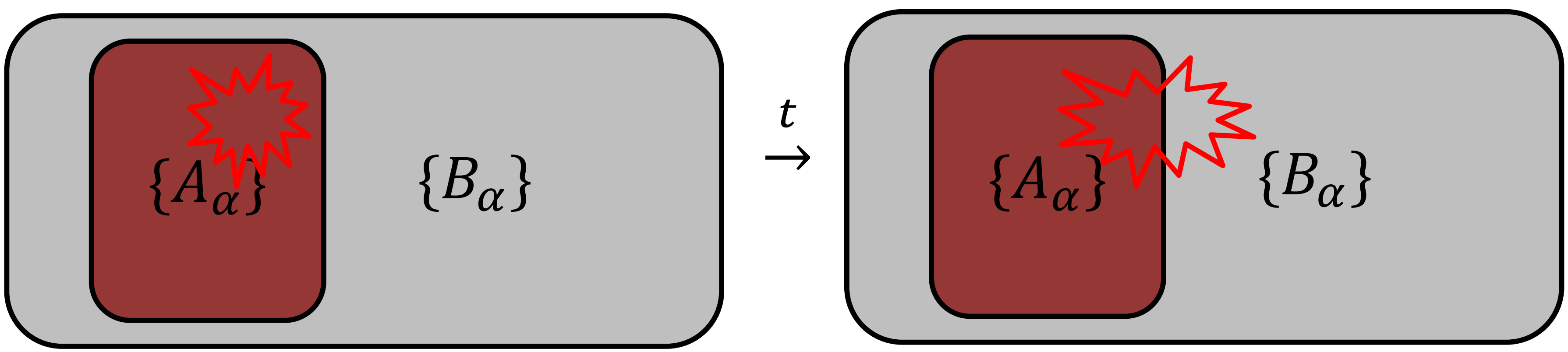
- Discuss the Generalized Langevin Equation
  – Show that in the hydrodynamic regime provides a quantum correction to Boltzmann

Mori Projection



$$PX_\alpha = \sum_\beta A_\beta \left(A_\beta | X_\alpha \right) \qquad Q = 1 - P$$

$$\partial_t A_\alpha(t) = \partial_t e^{iLt} A_\alpha = iLA_\alpha(t) = iPLA_\alpha(t) + QLA_\alpha(t)$$



H. Mori, *Transport, Collective Motion, and Brownian Motion*, Prog Theor Phys **33**, 423 (1965).

Mori's Projected Dynamics aka Generalized Langevin Equation

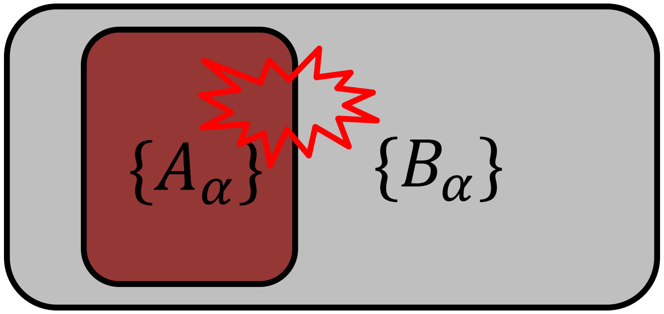
$$\partial_t e^{iLt} = ie^{iLt}PL + ie^{iQLt}QL - \int_0^t dt' e^{iL(t-t')}PLe^{iQLt'}QL$$

$$\phi_{\alpha,\beta}(t) = (e^{iLt}A_\alpha|A_\beta)$$

$$\partial_t \phi_{\alpha,\beta}(t) = -\sum_\mu \left[i\phi_{\alpha,\mu}(t)\Omega_{\mu,\beta} + \int_0^t dt'\, \phi_{\alpha,\mu}(t') m_{\mu,\beta}(t-t') \right]$$

$$\Omega_{\mu,\beta} = (A_\mu|LA_\beta)$$

$$m_{\mu,\beta}(t) = (e^{iQLt}QLA_\mu|QLA_\beta)$$



H. Mori, *Transport, Collective Motion, and Brownian Motion*, Prog Theor Phys **33**, 423 (1965).

Memory Function:Brief and Incomplete History

- Götze, W., and P. Wölfle. 1971. "Dynamical Impurity Spin Susceptibility in Metals." *J. Low Temp. Phys.* 5 (5): 575–89.
- ———. 1972. "Homogeneous Dynamical Conductivity of Simple Metals." *Phys. Rev. B* 6 (4): 1226–38.
- Götze, W. 1978. "An Elementary Approach towards the Anderson Transition." *Solid State Comm.* 27 (12): 1393–95.
- ———. 1979. "A Theory for the Conductivity of a Fermion Gas Moving in a Strong Three-Dimensional Random Potential." *J. Phys. C: Solid State Phys.* 12 (7): 1279.
- ———. 1981. "The Mobility of a Quantum Particle in a Three-Dimensional Random Potential." *Phil. Mag. B* 43 (2): 219–50.
- Zheng, Lian, and A. H. MacDonald. 1993. "Coulomb Drag between Disordered Two-Dimensional Electron-Gas Layers." *Physical Review B* 48 (11): 8203–9.
- Jackeli, G., and N. M. Plakida. 1999. "Charge Dynamics and Optical Conductivity of the t-J Model." *Phys. Rev. B* 60 (8): 5266–75.
- Rojo, A. G. 1999. "Electron-Drag Effects in Coupled Electron Systems." *J. Phys.: Condens. Matter* 11 (5): R31.
- Ullrich, C. A., and G. Vignale. 2002. "Time-Dependent Current-Density-Functional Theory for the Linear Response of Weakly Disordered Systems." *Physical Review B* 65 (24): 24510.
- Kyrychenko, F. V., and C. A. Ullrich. 2007. "Enhanced Carrier Scattering Rates in Dilute Magnetic Semiconductors with Correlated Impurities." *Physical Review B* 75 (4): 045205.
- ———. 2009a. "Transport and Optical Conductivity in Dilute Magnetic Semiconductors." *Journal of Physics: Condensed Matter* 21 (8): 084202.
- ———. 2009b. "Temperature-Dependent Resistivity of Ferromagnetic $Ga_{1-x}Mn_{x,}As$: Interplay between Impurity Scattering and Many-Body Effects." *Physical Review B* 80 (20): 205202.
- Kupčić, Ivan. 2004. "Memory-Function Approach to the Normal-State Optical Properties of the Bechgaard Salt (TMTSF)2PF6." *Physica B: Condensed Matter* 344 (1): 27–40.
- Kupčić, I. 2017. "Intraband Memory Function and Memory-Function Conductivity Formula in Doped Graphene." *Physical Review B* 95 (3): 035403.

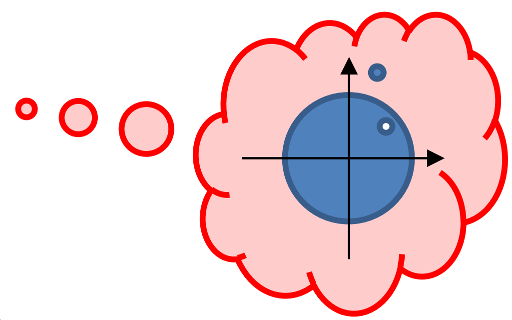
The details…

Skip details

Memory function for solids with impurities: Hamiltonian and degrees of freedom

$$H_0 = \sum_{n,\mathbf{k}} \varepsilon_{n,\mathbf{k}}\, c^{+}_{n,\mathbf{k}} c_{n,\mathbf{k}} \qquad H_i = \sum_{\mathbf{q}} U(\mathbf{q})\rho(-\mathbf{q})$$

$$\xi_{n',n,\mathbf{k}}(\mathbf{q}) = c^{+}_{n',\mathbf{k}-\mathbf{q}} c_{n,\mathbf{k}}$$



$$[H_0, \xi_{m,n,\mathbf{k}}(\mathbf{q})] = \left(\varepsilon_{m,\mathbf{k}-\mathbf{q}} - \varepsilon_{n,\mathbf{k}}\right) \xi_{m,n,\mathbf{k}}(\mathbf{q})$$

$$\left[H_i, \xi_{m,n,\mathbf{k}}(\mathbf{q})\right] = \frac{1}{V}\sum_{\mathbf{q}'} U(\mathbf{q}') \sum_{l} \left[M_{l,m,\mathbf{k}-\mathbf{q}}(-\mathbf{q}')\xi_{l,n,\mathbf{k}}(\mathbf{q}-\mathbf{q}') - M_{n,l,\mathbf{k}-\mathbf{q}'}(-\mathbf{q}')\xi_{m,l,\mathbf{k}-\mathbf{q}'}(\mathbf{q}-\mathbf{q}')\right]$$

$$M_{n',n,\mathbf{k}}(\mathbf{q}) = \int_{\Omega} d\mathbf{s}\, u^{*}_{n,\mathbf{k}}(\mathbf{s}) u_{n,\mathbf{k}}(\mathbf{s})$$

Memory function for solids: Projectors

$$A_0(\boldsymbol{q}) = \frac{\rho(\boldsymbol{q})}{N_0(\boldsymbol{q})} = \frac{1}{N_1(\boldsymbol{q})} \sum_{n',n,\boldsymbol{k}} M_{n',n,\boldsymbol{k}}(\boldsymbol{q})\, \xi_{n',n,\boldsymbol{k}}(\boldsymbol{q})$$

$$A_1(\boldsymbol{q}) = \frac{\boldsymbol{q}\cdot \boldsymbol{j}(\boldsymbol{q})}{N_1(\boldsymbol{q})} = \frac{1}{mN_1(\boldsymbol{q})} \sum_{n',n,\boldsymbol{k}} \boldsymbol{q}\cdot\left[\left(\boldsymbol{k}-\frac{\boldsymbol{q}}{2}\right) M_{n',n,\boldsymbol{k}}(\boldsymbol{q}) + \boldsymbol{P}_{n',n,\boldsymbol{k}}(\boldsymbol{q})\right] \xi_{n',n,\boldsymbol{k}}(\boldsymbol{q})$$

$$\vdots$$

$$A_\alpha(\boldsymbol{q}) = \sum_{n',n,\boldsymbol{k}} a^{(\alpha)}_{n',n,\boldsymbol{k}}(\boldsymbol{q})\,\xi_{n',n,\boldsymbol{k}}(\boldsymbol{q})$$

$$M_{n',n,\boldsymbol{k}}(\boldsymbol{q}) = \int_\Omega d\boldsymbol{s}\; u^*_{n',\boldsymbol{k}-\boldsymbol{q}}(\boldsymbol{s})\, u_{n,\boldsymbol{k}}(\boldsymbol{s})$$

$$\boldsymbol{P}_{n',n,\boldsymbol{k}}(\boldsymbol{q}) = \int_\Omega d\boldsymbol{s}\; u^*_{n',\boldsymbol{k}-\boldsymbol{q}}(\boldsymbol{s})\, \boldsymbol{p}\, u_{n,\boldsymbol{k}}(\boldsymbol{s})$$

$$P(\boldsymbol{q}) \blacksquare = \sum_\alpha A_\alpha(\boldsymbol{q}) (A_\alpha(\boldsymbol{q}) | \blacksquare)$$

$$\partial_t \phi_{\alpha,\beta}(t) = -\sum_{\mu} \left[i\phi_{\alpha,\mu}(t)\Omega_{\mu,\beta} + \int_0^t dt'\, \phi_{\alpha,\mu}(t') m_{\mu,\beta}(t-t') \right]$$

PENNSTATE 1855

Memory function for solids: GLE

$$\sum_{\mu} \Phi_{\alpha,\mu}(\boldsymbol{q},z)\left[z\delta_{\mu,\beta} - \Omega_{\mu,\beta}(\boldsymbol{q}) + M_{\mu,\beta}(\boldsymbol{q},z)\right] = i\delta_{\alpha,\beta}$$

$$\Phi_{\alpha,\beta}(\boldsymbol{q},z) \equiv \left(A_\alpha(\boldsymbol{q})\middle| R(z) A_\beta(\boldsymbol{q})\right)$$

$$\Omega_{\mu,\beta}(\boldsymbol{q}) \equiv \left(A_\mu(\boldsymbol{q})\middle| L A_\beta(\boldsymbol{q})\right)$$

$$M_{\mu,\beta}(\boldsymbol{q},z) \equiv i\left(\mathcal{Q}(\boldsymbol{q}) L A_\mu(\boldsymbol{q})\middle| R_{\mathcal{Q}(\boldsymbol{q})}(z) \mathcal{Q}(\boldsymbol{q}) L A_\beta(\boldsymbol{q})\right)$$

$$R(z) = i[z - L]^{-1}$$

$$R_{\mathcal{Q}(\boldsymbol{q})}(z) = i[z - \mathcal{Q}(\boldsymbol{q})L]^{-1}$$

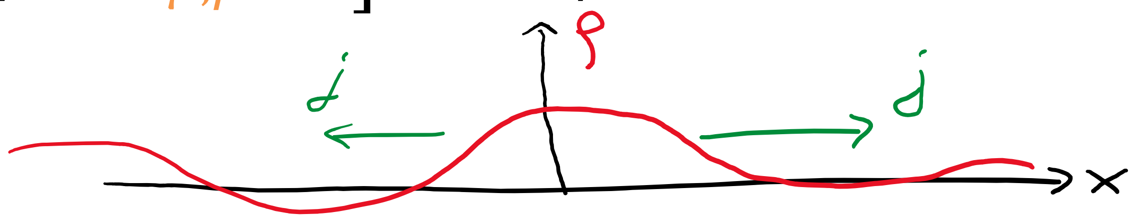
Approximations for hydrodynamics

$$\sum_{\mu} \Phi_{\alpha,\mu}(\boldsymbol{q}, z)\left[z\delta_{\mu,\beta} - \Omega_{\mu,\beta}(\boldsymbol{q}) + M_{\mu,\beta}(\boldsymbol{q}, z)\right] = i\delta_{\alpha,\beta}$$

$$\Omega_{\mu,\beta}(\boldsymbol{q}) \equiv \left(A_\mu(\boldsymbol{q})\middle|LA_\beta(\boldsymbol{q})\right) \approx \left(A_\mu(\boldsymbol{q})\middle|L_0A_\beta(\boldsymbol{q})\right) = \Omega^{(0)}_{\mu,\beta}(\boldsymbol{q})$$ (1)

$$\sum_{\mu} \Phi^{(0)}_{\alpha,\mu}(\boldsymbol{q}, z)\left[z\delta_{\mu,\beta} - \Omega^{(0)}_{\mu,\beta}(\boldsymbol{q})\right] = i\delta_{\alpha,\beta}$$

$$M_{\alpha,\beta} = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ 0 & M & 0 & 0 & \cdots \\ 0 & 0 & M & 0 & \cdots \\ 0 & 0 & 0 & M & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$



$$M(\boldsymbol{q}, z) = M_{1,1}(\boldsymbol{q}, z) \equiv i\left(Q(\boldsymbol{q})j_l(\boldsymbol{q})\middle|R(z)Q(\boldsymbol{q})j_l(\boldsymbol{q})\right)$$ (2)

(1) W. Götze, *The Mobility of a Quantum Particle in a Three-Dimensional Random Potential*, Phil. Mag. B **43**, 219 (1981). (Homogeneous Electron Gas)
(2) G. F. Mazenko, *Nonequilibrium Statistical Mechanics* (Wiley-VCH, 2006). Sec. 5.3.7

Back to details

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Götze hydrodynamic equations

$$\Phi(\boldsymbol{q},z) = \frac{\Phi_{0,0}(\boldsymbol{q},z)}{g(\boldsymbol{q})} \qquad g(\boldsymbol{q}) = (\rho(\boldsymbol{q})|\rho(\boldsymbol{q}))$$

Charge relaxation of the ordered system from DFT code

$$\Phi(\boldsymbol{q},z) = \frac{\Phi^{(0)}(\boldsymbol{q},z + M(\boldsymbol{q},z))}{1 + i\,M(\boldsymbol{q},z)\,\Phi^{(0)}\big(\boldsymbol{q},z + M(\boldsymbol{q},z)\big)/g(\boldsymbol{q})}$$

$$M(\boldsymbol{q},z) = \frac{1}{N_e m}\sum_{\boldsymbol{q}}\left(\frac{\boldsymbol{q}\cdot\boldsymbol{q}'}{q}\right)^2 |U(\boldsymbol{q}')|^2\Phi(\boldsymbol{q}-\boldsymbol{q}',z)$$

Model of disorder: alloy, solvent, …

$L\rho(\boldsymbol{q}) = -\boldsymbol{q}\cdot j(\boldsymbol{q})$

$$\sigma(\boldsymbol{q},z) = \frac{z}{q^2}[z\Phi(\boldsymbol{q},z) - ig(\boldsymbol{q})]$$

General

Optical Conductivity: The $q \to 0$ limit

$$\sigma(\boldsymbol{q},z) = \frac{\boldsymbol{q}}{q}\cdot\overleftrightarrow{\sigma}(\boldsymbol{q},z)\cdot\frac{\boldsymbol{q}}{q} = \frac{z}{q^2}\chi(\boldsymbol{q},z) \xrightarrow[q\to 0]{} \frac{\boldsymbol{q}}{q}\cdot z\,\overleftrightarrow{\alpha}(z)\cdot\frac{\boldsymbol{q}}{q}$$

$$\chi(\boldsymbol{q},z) = \langle[\rho^+(\vec{q},z),\rho(\vec{q})]\rangle$$

$$\Longrightarrow \lim_{q\to 0}\overleftrightarrow{\sigma}(\boldsymbol{q},z) = \overleftrightarrow{\sigma}(z) = z\,\overleftrightarrow{\alpha}(z) \quad \text{and} \quad \overleftrightarrow{\sigma}^{(0)}(z) = z\overleftrightarrow{\alpha}^{(0)}$$

$$\Phi(\boldsymbol{q},z) = \frac{\Phi_0\big(\boldsymbol{q},z+M(\boldsymbol{q},z)\big)}{1+i\,M(\boldsymbol{q},z)\,\Phi_0(\boldsymbol{q},z+M(\boldsymbol{q},z))\,/g(\boldsymbol{q})}$$

$$\sigma(\boldsymbol{q},z) = \frac{z}{q^2}[z\Phi(\boldsymbol{q},z) - ig(\boldsymbol{q})]$$

$q \to 0$

$$\overleftrightarrow{\sigma}(z) = [z+M(z)]\overleftrightarrow{\alpha}^{(0)}\big(z+M(z)\big) = \overleftrightarrow{\sigma}^{(0)}\big(z+M(z)\big)$$

Optical Conductivity: The dc limit

$$\overleftrightarrow{\sigma}(z) = \overleftrightarrow{\sigma}^{(0)}\big(z + M(z)\big)$$

$$\overleftrightarrow{\sigma}^{(0)}(z) = \frac{i}{z}\sum_{n,\vec{k}}[-f_0'(\varepsilon_{n\vec{k}})]\ \vec{v}_{n\vec{k}}\vec{v}_{n\vec{k}} + i\sum_{n,n',\vec{k}} \frac{\vec{v}_{n,n',\vec{k}}\ \vec{v}_{n',n,\vec{k}}}{\varepsilon_{n,\vec{k}} - \varepsilon_{n',\vec{k}}}\ \frac{f_0\left(\varepsilon_{n,\vec{k}}\right) - f_0\left(\varepsilon_{n',\vec{k}}\right)}{z + \varepsilon_{n,\vec{k}} - \varepsilon_{n',\vec{k}}}$$

$$\overleftrightarrow{\sigma}(z) = \frac{i}{z + M(z)}\sum_{n,\vec{k}}[-f_0'(\varepsilon_{n\vec{k}})]\ \vec{v}_{n\vec{k}}\vec{v}_{n\vec{k}} + i\sum_{n,n',\vec{k}} \frac{\vec{v}_{n,n',\vec{k}}\ \vec{v}_{n',n,\vec{k}}}{\varepsilon_{n,\vec{k}} - \varepsilon_{n',\vec{k}}}\ \frac{f_0\left(\varepsilon_{n,\vec{k}}\right) - f_0\left(\varepsilon_{n',\vec{k}}\right)}{z + M(z) + \varepsilon_{n,\vec{k}} - \varepsilon_{n',\vec{k}}}$$

$$\lim_{\omega\to 0}\lim_{\eta\to 0} M\,(\omega + i\eta) = i\,\frac{1}{\tau} \qquad\qquad \lim_{\omega\to 0} Re[\overleftrightarrow{\sigma}\,(\omega + i0^{+})] = \overleftrightarrow{\sigma}$$

$$\overleftrightarrow{\sigma} = \tau\sum_{n,\vec{k}}[-f_0'(\varepsilon_{n\vec{k}})]\ \vec{v}_{n\vec{k}}\vec{v}_{n\vec{k}} + \frac{1}{\tau}\sum_{n,n',\vec{k}} \frac{\vec{v}_{n,n',\vec{k}}\ \vec{v}_{n',n,\vec{k}}}{\varepsilon_{n,\vec{k}} - \varepsilon_{n',\vec{k}}}\ \frac{f_0\left(\varepsilon_{n,\vec{k}}\right) - f_0\left(\varepsilon_{n',\vec{k}}\right)}{\left(\frac{1}{\tau}\right)^2 + \left(\varepsilon_{n,\vec{k}} - \varepsilon_{n',\vec{k}}\right)^2}$$

Optical Conductivity: The dc limit

$$\overleftrightarrow{\sigma}(z) = \overleftrightarrow{\sigma}^{(0)}\big(z + M(z)\big)$$

$$\overleftrightarrow{\sigma}^{(0)}(z) = \frac{i}{z}\sum_{n,\vec{k}}[-f_0'(\varepsilon_{n\vec{k}})]\ \vec{v}_{n\vec{k}}\vec{v}_{n\vec{k}} + i\sum_{n,n',\vec{k}} \frac{\vec{v}_{n,n',\vec{k}}\ \vec{v}_{n',n,\vec{k}}}{\varepsilon_{n,\vec{k}} - \varepsilon_{n',\vec{k}}}\ \frac{f_0\left(\varepsilon_{n,\vec{k}}\right) - f_0\left(\varepsilon_{n',\vec{k}}\right)}{z + \varepsilon_{n,\vec{k}} - \varepsilon_{n',\vec{k}}}$$

$$\overleftrightarrow{\sigma}(z) = \frac{i}{z + M(z)}\sum_{n,\vec{k}}[-f_0'(\varepsilon_{n\vec{k}})]\ \vec{v}_{n\vec{k}}\vec{v}_{n\vec{k}} + i\sum_{n,n',\vec{k}} \frac{\vec{v}_{n,n',\vec{k}}\ \vec{v}_{n',n,\vec{k}}}{\varepsilon_{n,\vec{k}} - \varepsilon_{n',\vec{k}}}\ \frac{f_0\left(\varepsilon_{n,\vec{k}}\right) - f_0\left(\varepsilon_{n',\vec{k}}\right)}{z + M(z) + \varepsilon_{n,\vec{k}} - \varepsilon_{n',\vec{k}}}$$

$$\lim_{\omega \to 0}\lim_{\eta \to 0} M(\omega + i\eta) = i\frac{1}{\tau} \qquad \lim_{\omega \to 0} Re[\overleftrightarrow{\sigma}(\omega + i0^+)] = \overleftrightarrow{\sigma}$$

$$\overleftrightarrow{\sigma} = \tau\sum_{n,\vec{k}}[-f_0'(\varepsilon_{n\vec{k}})]\ \vec{v}_{n\vec{k}}\vec{v}_{n\vec{k}} + \frac{1}{\tau}\sum_{n,n',\vec{k}} \frac{\vec{v}_{n,n',\vec{k}}\ \vec{v}_{n',n,\vec{k}}}{\varepsilon_{n,\vec{k}} - \varepsilon_{n',\vec{k}}}\ \frac{f_0\left(\varepsilon_{n,\vec{k}}\right) - f_0\left(\varepsilon_{n',\vec{k}}\right)}{\left(\frac{1}{\tau}\right)^2 + \left(\varepsilon_{n,\vec{k}} - \varepsilon_{n',\vec{k}}\right)^2}$$

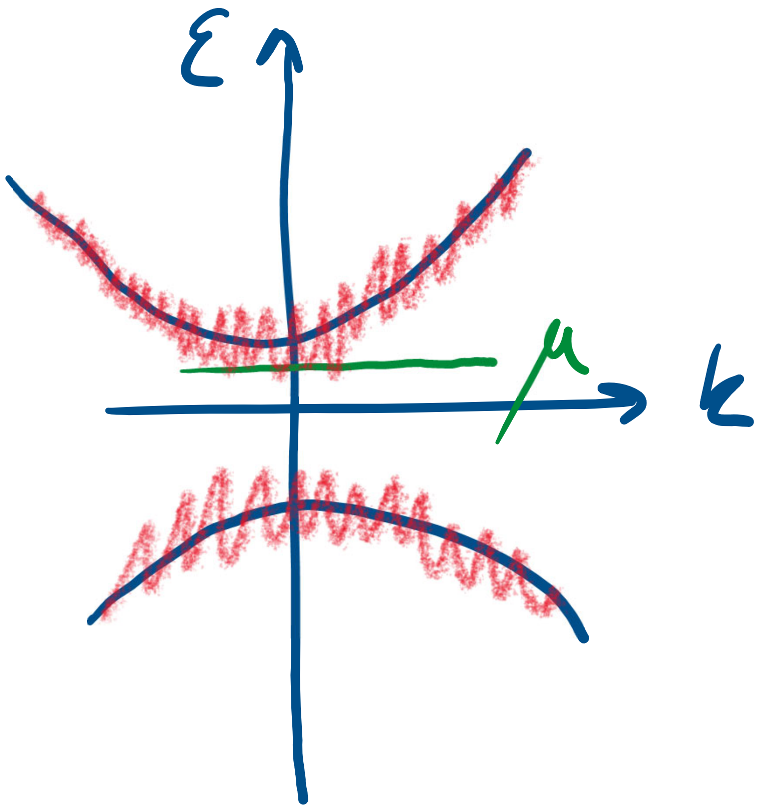
PENNSTATE

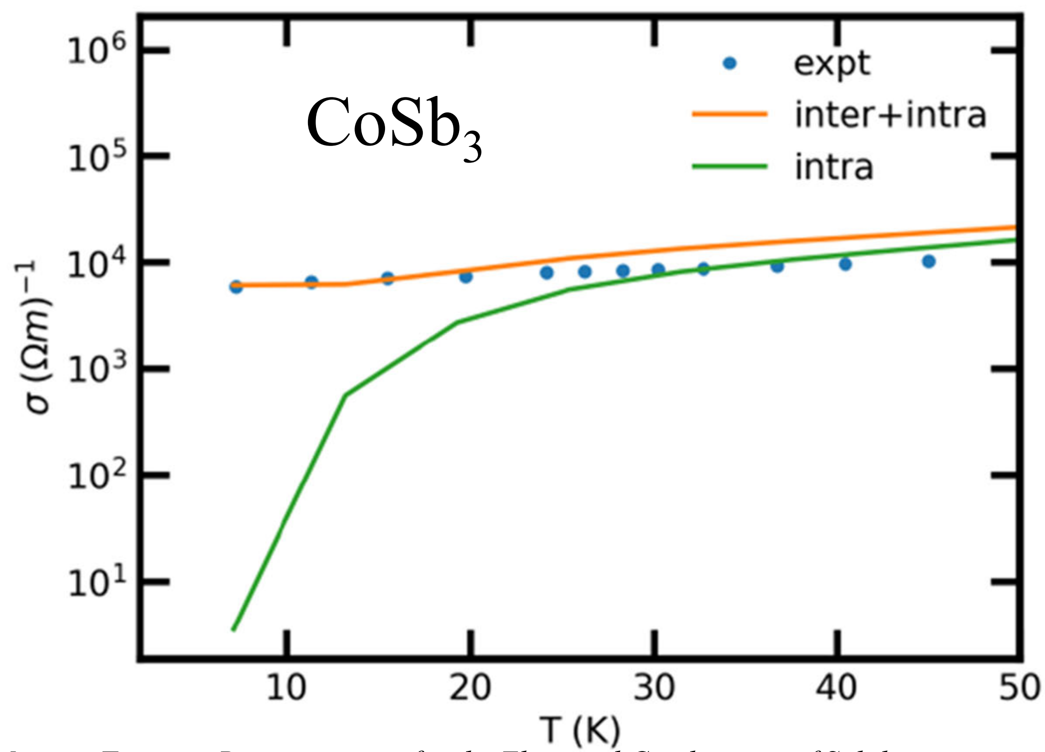
With the memory function approach…

Coherence — Only at low T

$$\overleftrightarrow{\sigma} = \tau \sum_{n,\vec{k}} [-f_0'(\varepsilon_{n\vec{k}})]\ \vec{v}_{n\vec{k}}\vec{v}_{n\vec{k}} + \frac{1}{\tau}\sum_{n,n',\vec{k}} \frac{\vec{v}_{n,n',\vec{k}}\ \vec{v}_{n',n,\vec{k}}}{\varepsilon_{n,\vec{k}}-\varepsilon_{n',\vec{k}}}\ \frac{f_0\left(\varepsilon_{n,\vec{k}}\right) - f_0\left(\varepsilon_{n',\vec{k}}\right)}{\left(\frac{1}{\tau}\right)^2 + \left(\varepsilon_{n,\vec{k}}-\varepsilon_{n',\vec{k}}\right)^2}$$

Broadening — Optical transition



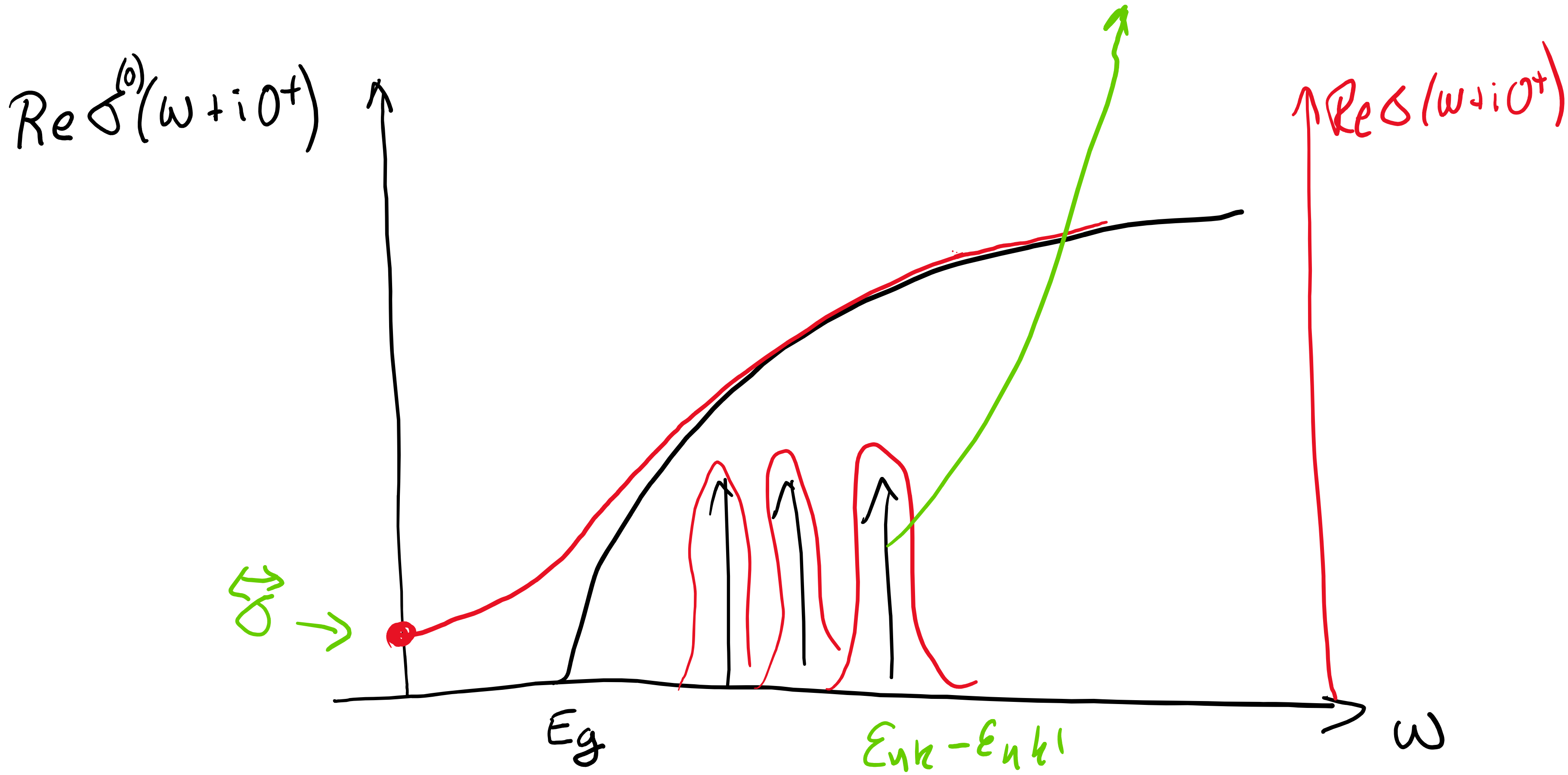


B. R. Green, M. Troppenz, S. Rigamonti, C. Draxl, and J. O. Sofo, *Memory Function Representation for the Electrical Conductivity of Solids*, ArXiv:2110.02859 [Cond-Mat] (2021).

PENNSTATE

With the memory function approach…

$$\overleftrightarrow{\sigma} = \tau \sum_{n,\vec{k}} [-f_0'(\varepsilon_{n\vec{k}})]\ \vec{v}_{n\vec{k}}\vec{v}_{n\vec{k}} + \frac{1}{\tau} \sum_{n,n',\vec{k}} \frac{\vec{v}_{n,n',\vec{k}}\ \vec{v}_{n',n,\vec{k}}}{\varepsilon_{n,\vec{k}} - \varepsilon_{n',\vec{k}}} \frac{f_0\left(\varepsilon_{n,\vec{k}}\right) - f_0\left(\varepsilon_{n',\vec{k}}\right)}{\left(\frac{1}{\tau}\right)^2 + \left(\varepsilon_{n,\vec{k}} - \varepsilon_{n',\vec{k}}\right)^2}$$



B. R. Green, M. Troppenz, S. Rigamonti, C. Draxl, and J. O. Sofo, *Memory Function Representation for the Electrical Conductivity of Solids*, ArXiv:2110.02859 [Cond-Mat] (2021).

Implemented in “exciting”

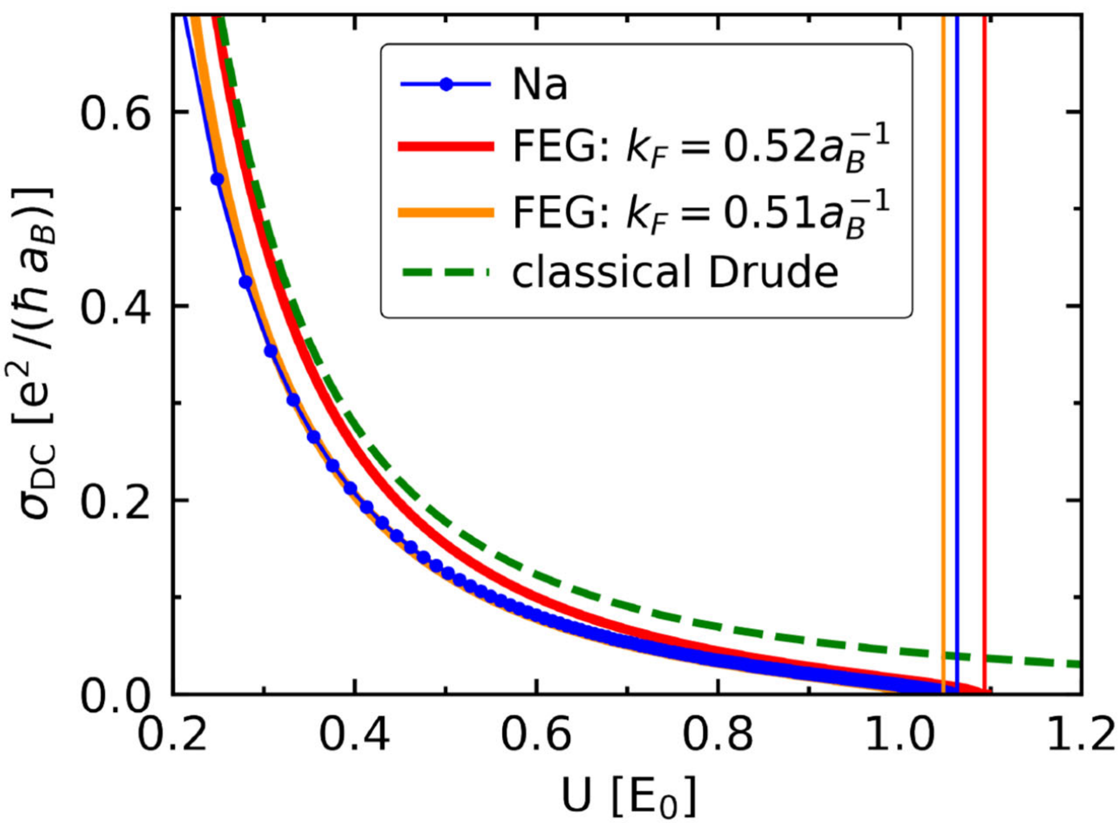
http://exciting-code.org/

Proof of principle: Na (bcc) with random alloy disorder

$$\Phi(\boldsymbol{q},z) = \frac{\Phi^{(0)}(\boldsymbol{q},z+M(\boldsymbol{q},z))}{1 + i\,M(\boldsymbol{q},z)\,\Phi^{(0)}\big(\boldsymbol{q},z+M(\boldsymbol{q},z)\big)/g(\boldsymbol{q})}$$

$$M(q,z) = \frac{1}{N_e m}\sum_{\boldsymbol{q}}\left(\frac{\boldsymbol{q}\cdot\boldsymbol{q}'}{q}\right)^2 |U(\boldsymbol{q}')|^2\Phi(\boldsymbol{q}-\boldsymbol{q}',z)$$

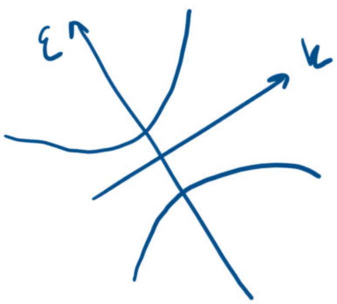
$$\sigma(\boldsymbol{q},z) = \frac{z}{q^2}[z\Phi(\boldsymbol{q},z) - i\phi(\boldsymbol{q},0)]$$

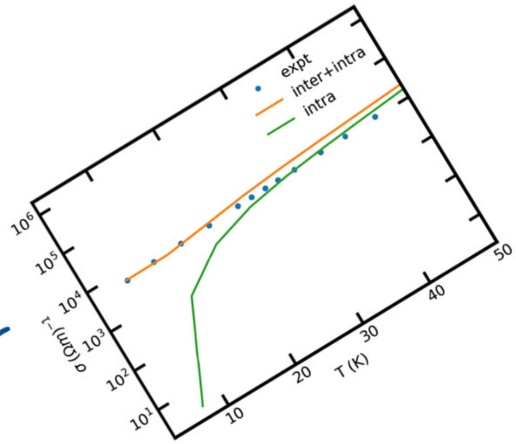


Future…

- Phonons and other bosonic excitations
- Magnetic field (Zak)
- Clear doubts about linear response and electric fields in solids.
- …
- Lifetime of spins and other localized degrees of freedom in solids.

In summary…





$$\widehat{m}(z) = \frac{1}{nm}\sum_{\vec{q}} \langle |U(\vec{q})|^2 \rangle\, \phi(\vec{q},z)$$

$$\phi(\vec{q},z) = \frac{\phi_0(\vec{q},z+\widehat{m}(z))}{1+\widehat{m}(z)\,\phi_0(\vec{q},z+\widehat{m}(z))\,/g(\vec{q})}$$

$$\sigma(\vec{q},z) = i\frac{z}{q^2}[z\,\phi(\vec{q},z) - g(\vec{q})]$$

$$\sigma_{\alpha,\beta}(z) = \sigma^{(0)}_{\alpha,\beta}(z - M(z))$$

$$\sigma^{(\mathrm{dc})}_{\mu,\nu} = \frac{1}{M''}\sum_{n,\boldsymbol{k}}\left(\frac{\partial f}{\partial \varepsilon}\right)_{\varepsilon_{n,\boldsymbol{k}}}\frac{\partial \varepsilon_{n,\boldsymbol{k}}}{\partial k_\mu}\frac{\partial \varepsilon_{n,\boldsymbol{k}}}{\partial k_\nu} - \sum_{n,\boldsymbol{k}\alpha} f(\varepsilon_{n,\boldsymbol{k}})\epsilon_{\mu,\nu,\alpha}\Omega_{n;\alpha}(\boldsymbol{k}) +$$

$$M''\sum_{\substack{n',n,\boldsymbol{k}\\ n\neq n'}} X_{n,n';\mu}(\boldsymbol{k})X_{n',n;\nu}(\boldsymbol{k})\frac{[f(\varepsilon_{n,\boldsymbol{k}}) - f(\varepsilon_{n',\boldsymbol{k}})](\varepsilon_{n,\boldsymbol{k}} - \varepsilon_{n',\boldsymbol{k}})}{M''^2 + (\varepsilon_{n,\boldsymbol{k}} - \varepsilon_{n',\boldsymbol{k}})^2}$$

Thank you!
Send your comments to
sofo@psu.edu