Electrical Conductivity from Static Disorder Beyond the Relaxation-Time Approximation

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Our plan for today

- General overview of the transport process
- Methods to evaluate
  - Drude
  - Boltzmann
  - Kubo
- The memory function approach

Linear response

$$j(t) = \int_{-\infty}^{t} \sigma(t - t')\, E(t') dt'$$

Linear response

Causality

$$j(t) = \int_{-\infty}^{t} \sigma(t - t')\, E(t') dt'$$

Linear response

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$$f(\omega) = \int_{-\infty}^{\infty} e^{i\omega t}\, f(t)$$

$$j(\omega) = \sigma(\omega)\, E(\omega)$$

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$$j(\omega) = \sigma(\omega)\, E(\omega)$$

$\omega \rightarrow 0$

$$j = \sigma_{dc}\, E$$

Ω

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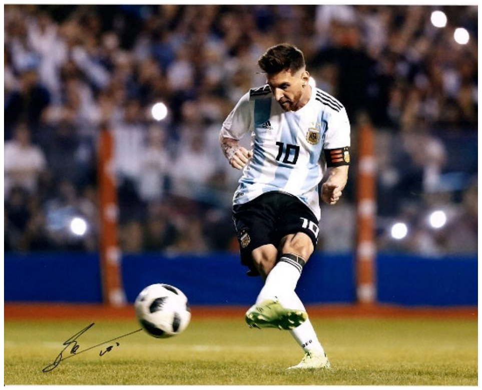

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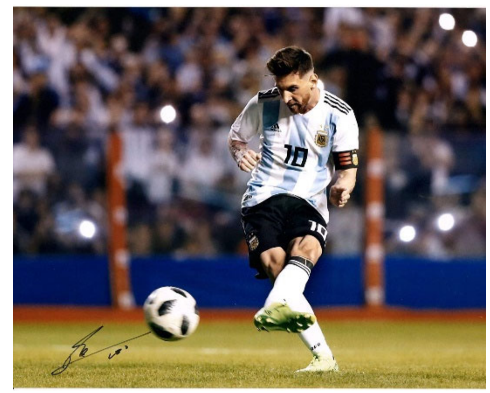

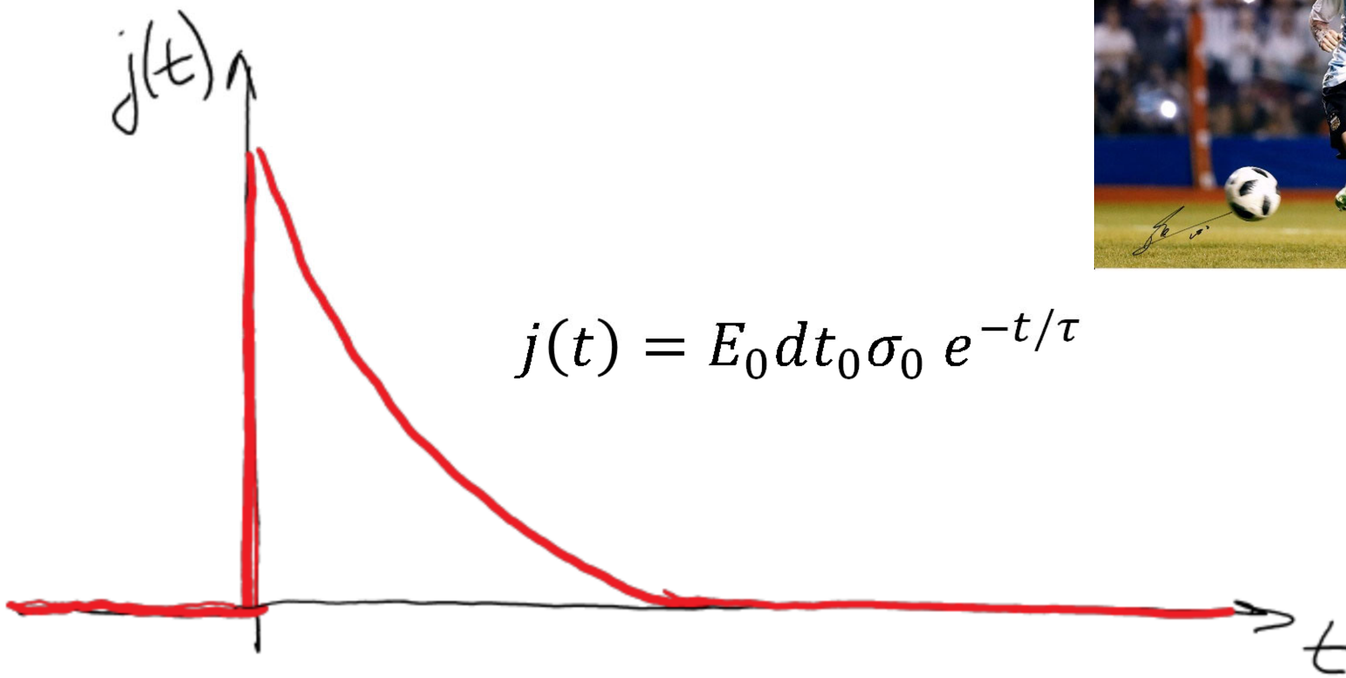

$$j(t) = E_0 dt_0 \sigma_0 \, e^{-t/\tau}$$

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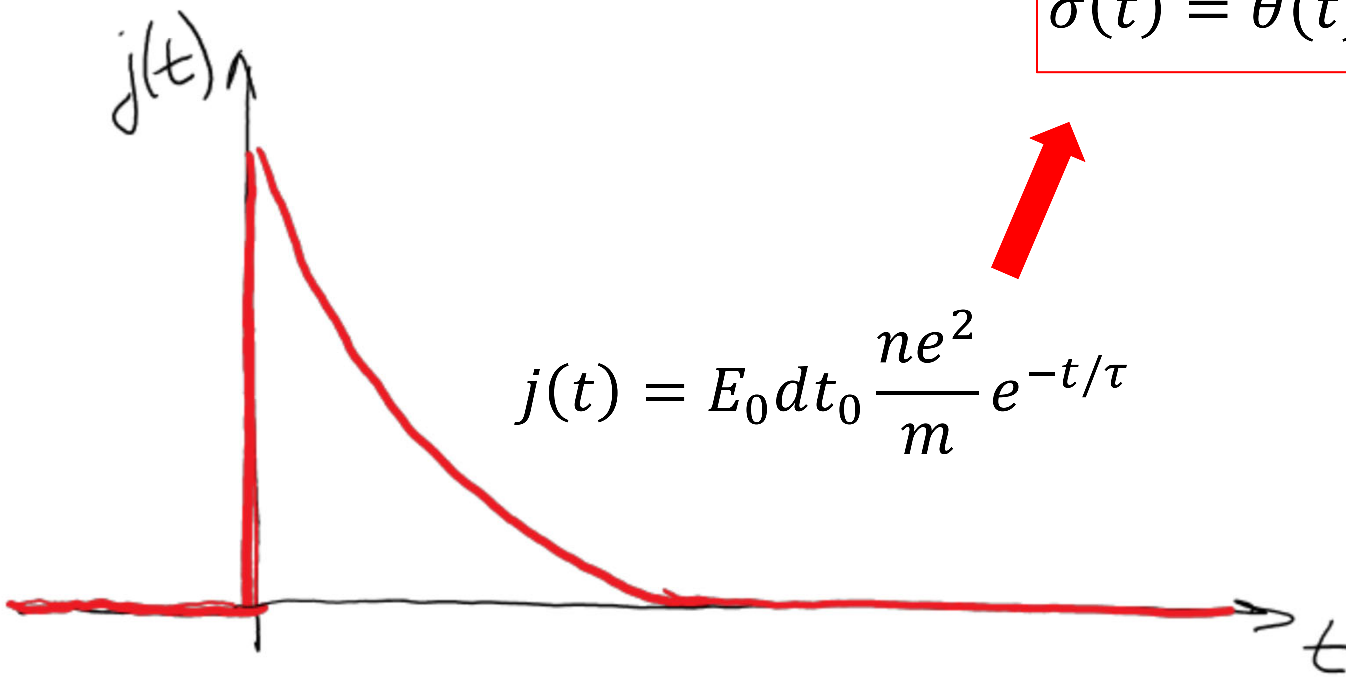

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Paul Karl Ludwig Drude
1863-1906

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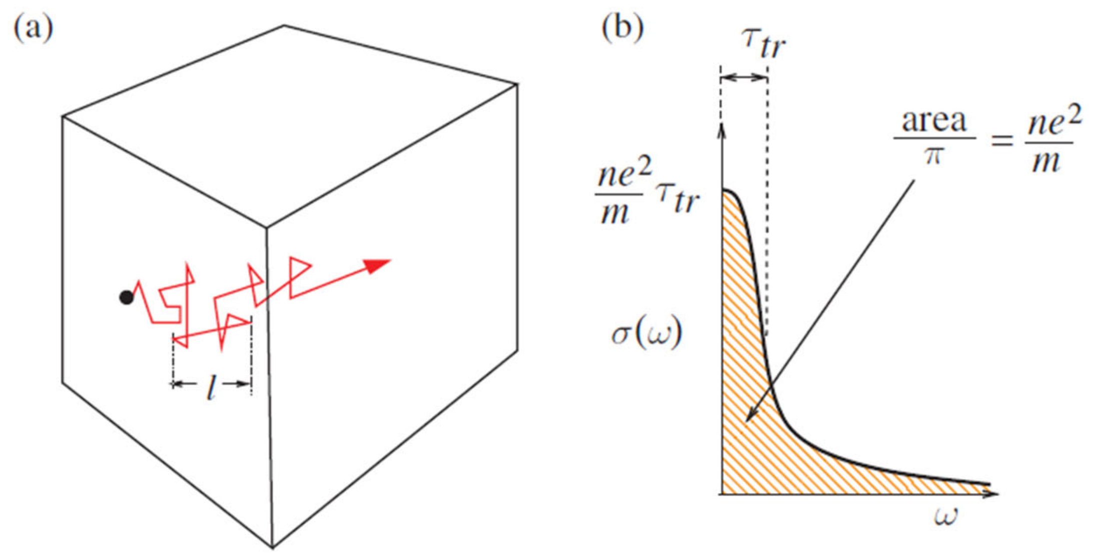
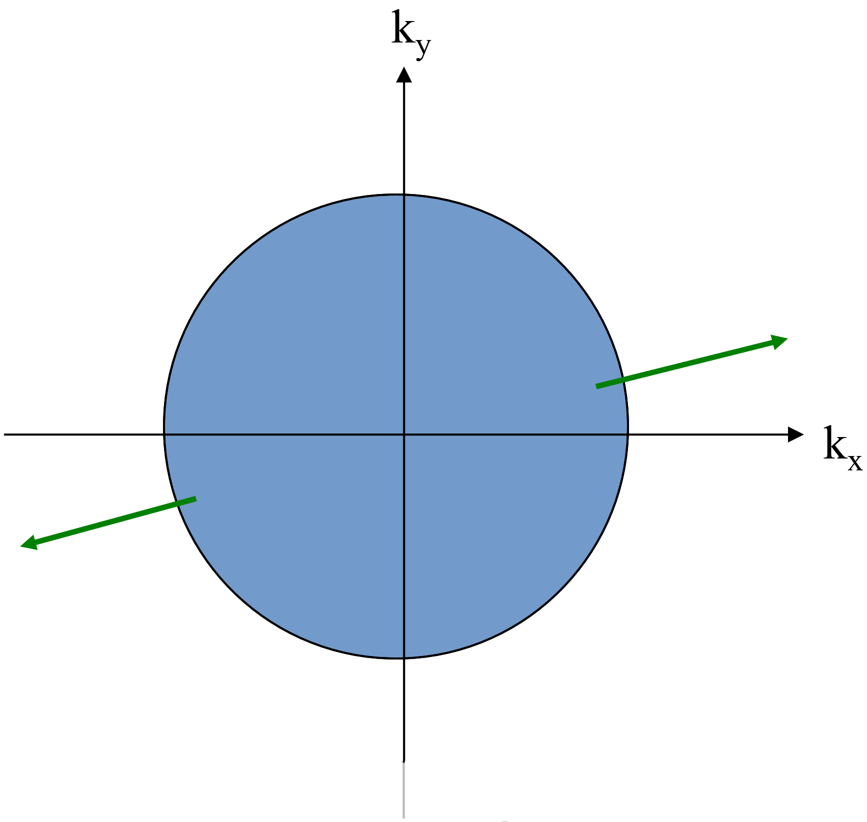
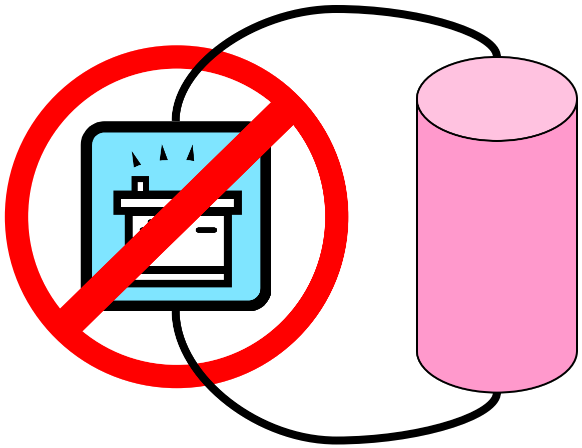


Fig. 10.1 Coleman, Piers. 2015. *Introduction to Many-Body Physics*. Cambridge University Press.

An electric field accelerates electrons





$J = Tr(\rho_0 \hat{J}) = 0$

$J = Tr\left(\rho_E \hat{J}\right) \neq 0$

Need to evaluate the time evolution of the current

(…we know how to do that…)

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Then

$$J = Tr_N\left(\rho\hat{J}\right) = Tr_1\left[(Tr_{N-1}\rho)\hat{J}\right]$$
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$$\langle k_j|\rho_1|k_l\rangle = f_{k_j,k_l} = Tr[\rho c_{k_j} c_{k_j}^{+}]$$

Geography of the single particle density matrix

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- Diagonal elements → Occupations

$$f_{k,k}$$

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- Diagonal elements → Occupations

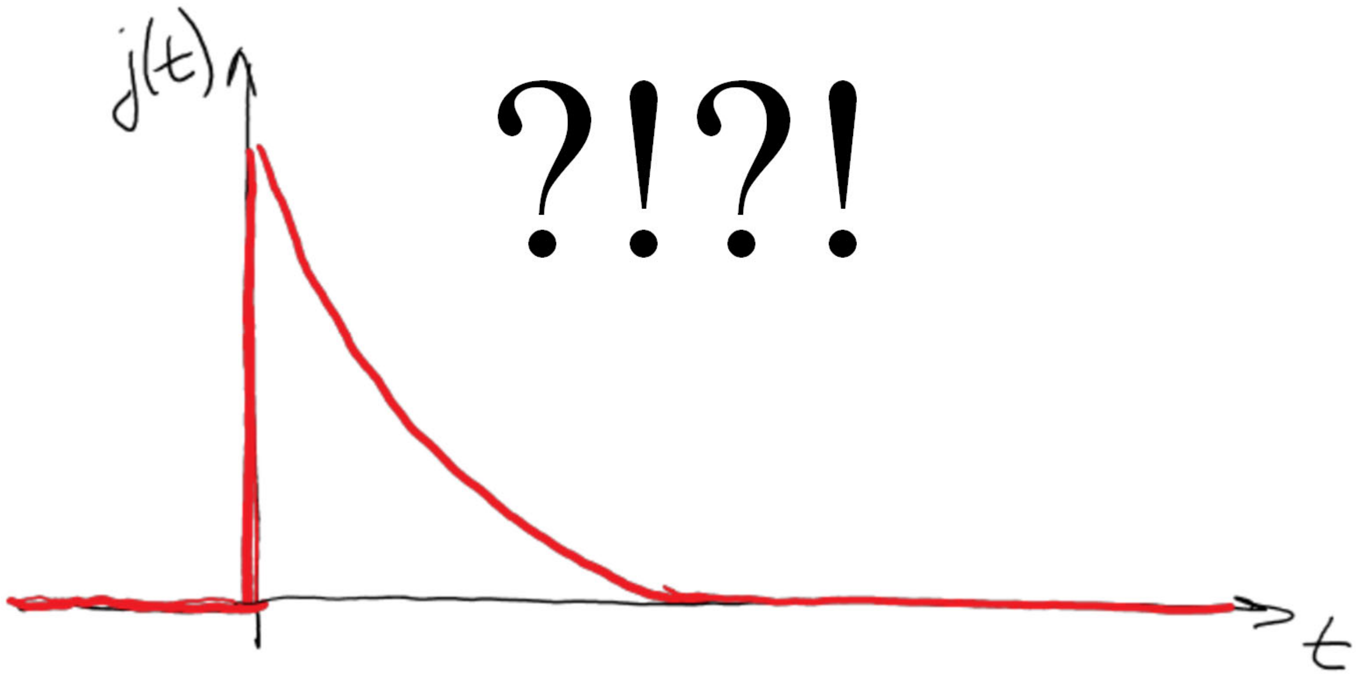
$$f_{k,k}$$

- Non-diagonal elements → Coherences

$$f_{k,k'}$$

Equations of motion and irreversibility

- Equations of motion are time reversible…



The Boltzmann street

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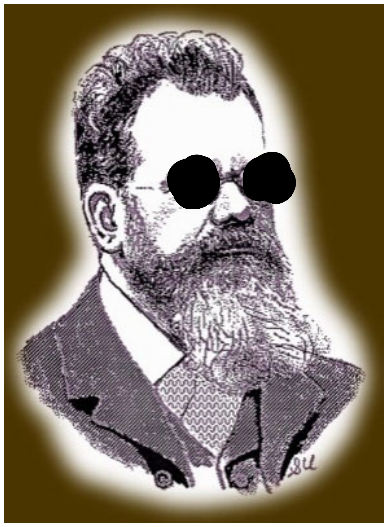
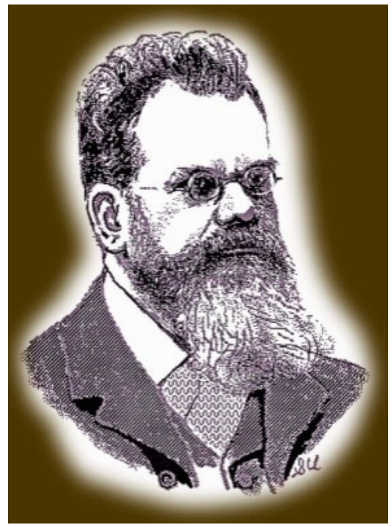


$f_{k,k'}$



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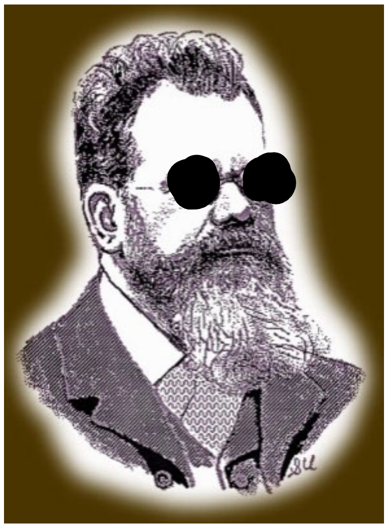


$$f_{k,k'}$$

$$f_{k,k} \equiv f_k$$

$$\left(\frac{df_k}{dt}\right)_{dyn} = C[f_k, f_{k'}]$$

Effects of quantum coherence: Anderson localization

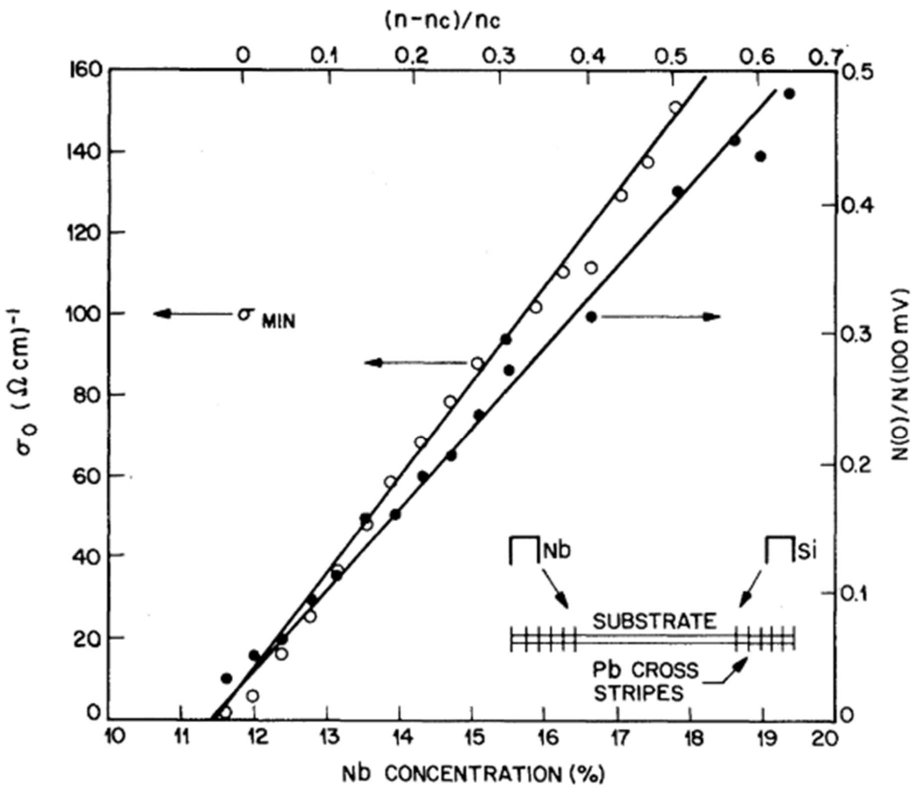


FIG. 1. σ_0 and $N(0)/N(100\text{ mV})$ vs Nb concentration. Inset shows method of sample preparation.

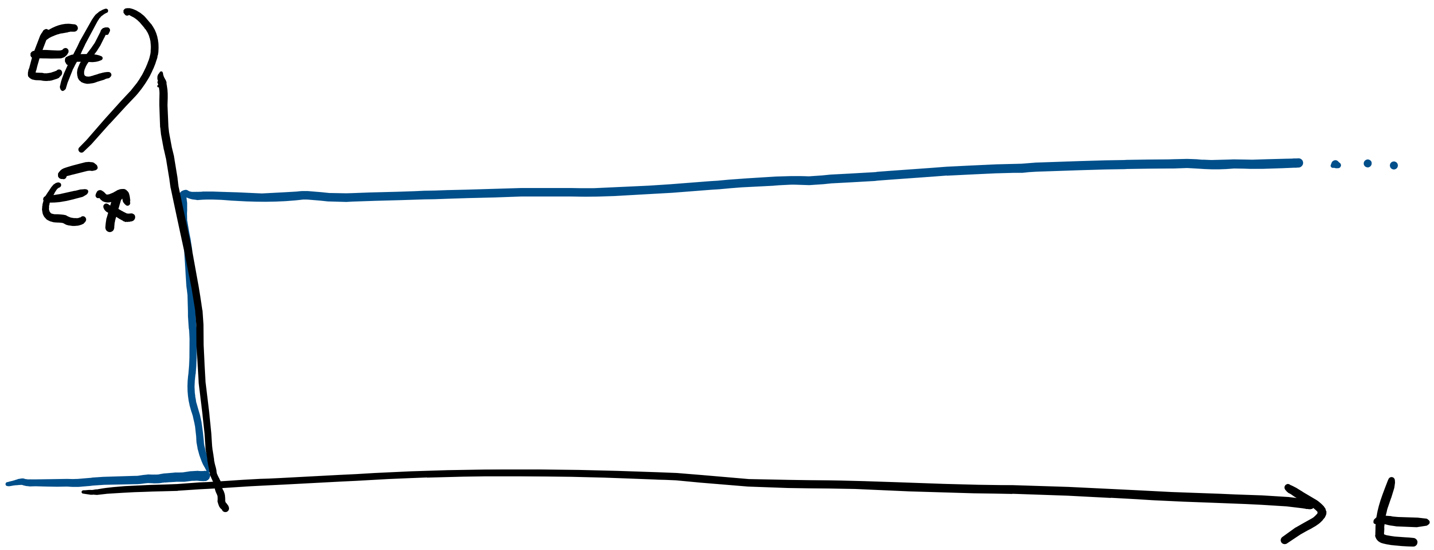
Tunneling and Transport Measurements at the Metal-Insulator Transition of Amorphous Nb: Si
G. Hertel, D. J. Bishop, E. G. Spencer, J. M. Rowell, and R. C. Dynes
Phys. Rev. Lett. **50**, 743 (1983)

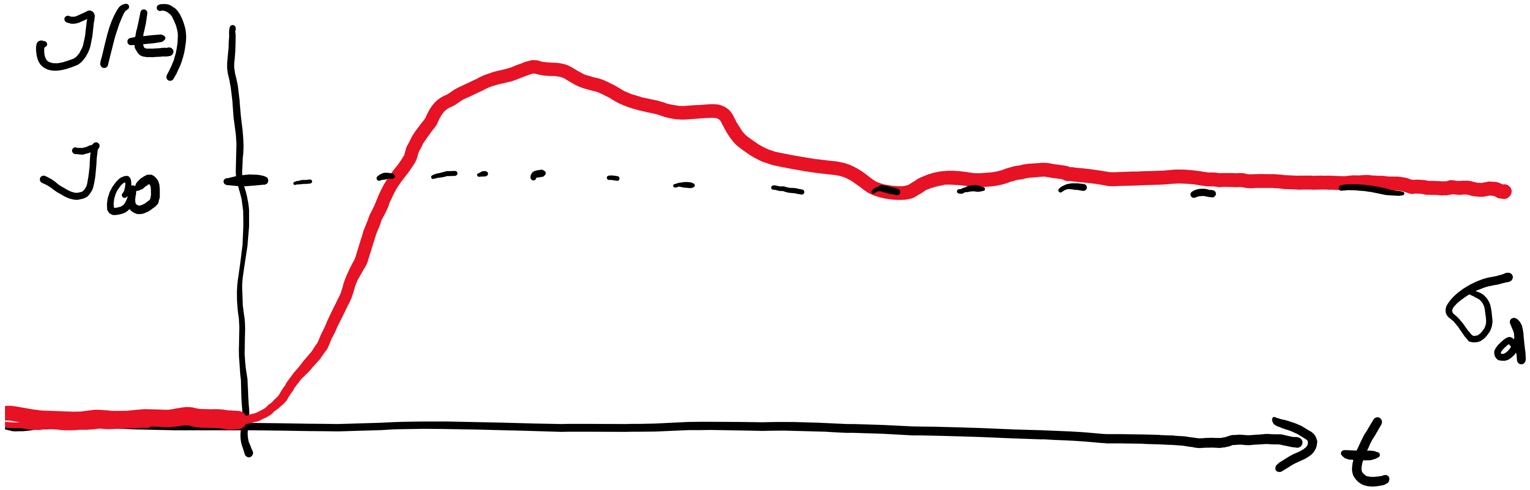
Other methods based on the evolution of the 1 particle density matrix

- Kadanoff and Baym…
- Keldysh and family…

Will ignore them because today, I do not understand them well enough…

Let's do an experiment…





$$\sigma_{dc} = \frac{J_\infty}{E_x}$$

Equilibrium after a long time

$$\langle \hat{J} \rangle = \frac{Tr\left[e^{-\beta(\hat{H}_0 - \hat{P}E_F)}\hat{J}\right]}{Tr\left[e^{-\beta(\hat{H}_0 - \hat{P}E_F)}\right]}$$

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- Kubo identity (disentangling…)

$$e^{-\lambda(\hat{A}+\hat{B})} = e^{-\lambda\hat{A}} - e^{-\lambda\hat{A}} \int_0^{\lambda} e^{-\mu\hat{A}}\hat{B}e^{-\mu(\hat{A}+\hat{B})}$$

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$$\langle \hat{J} \rangle = \langle \hat{J} \rangle_0 + \left(\hat{P}, \hat{J}\right)_0 E_F$$

$$\left(\hat{A}, \hat{B}\right)_0 = \int_0^{\beta} d\mu \left\langle e^{\mu H_0}\left(\hat{A}^+ - \langle \hat{A}^+ \rangle_0\right) e^{-\mu H_0}\left(\hat{B} - \langle \hat{B} \rangle_0\right)\right\rangle_0$$

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$$\langle \hat{J} \rangle(t) = \frac{Tr\left[e^{-\beta \hat{H}_0} e^{it(L_0 - L_P E_F)} \hat{J}\right]}{Tr\left[e^{-\beta \hat{H}_0}\right]}$$

$$L_0 \cdot \; := \left[\hat{H}_0, \cdot\right] \quad L_P \cdot \; := [\hat{P}, \cdot]$$

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$$L_0 \cdot := \left[\widehat{H}_0, \cdot\right] \quad L_P \cdot := [\hat{P}, \cdot]$$

$$\sigma(t) = \left(\hat{J}(t), \hat{J}\right)_0 = i\langle [\hat{J}(t), \hat{P}] \rangle_0$$

Which is the Kubo formula…

The tale of Greenwood and Kubo

$$H_0 = \sum_n \varepsilon_n \, c_n^+ c_n \;\Rightarrow\; \sigma(t) = \left(\hat{J}(t)\middle|\hat{J}\right) = -\sum_{n,s} \frac{f(\varepsilon_n) - f(\varepsilon_s)}{\varepsilon_n - \varepsilon_s} |\langle n|\hat{j}|s\rangle|^2 e^{i(\varepsilon_n - \varepsilon_s)t}$$

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of periodic boundary conditions. The current is therefore given by the last part of (28), i.e.

$$J_x(t) = -2Fe^2\hbar \sum_{m,n} |v_{mn}|^2 \frac{f_n - f_m}{E_n - E_m} \frac{\sin(E_n - E_m)t/\hbar}{E_n - E_m}. \quad \ldots\ldots (29)$$

We write $\pi\boldsymbol{\delta}(E_n - E_m)$ for the 'quasi-δ-function' $\sin\{(E_n - E_m)t/\hbar\}/(E_n - E_m)$ and suppose the nature of the potential to be such that

$$\sum_m |v_{mn}|^2 \boldsymbol{\delta}(E_n - E_m)$$

is insensitive to the width $\hbar/t$ of the peak, provided that a large number of energy levels E_n are included. Then, over times $\hbar/kT \ll t \ll \hbar/\Delta E$, (28) gives a time-independent current, and hence a value for the conductivity,

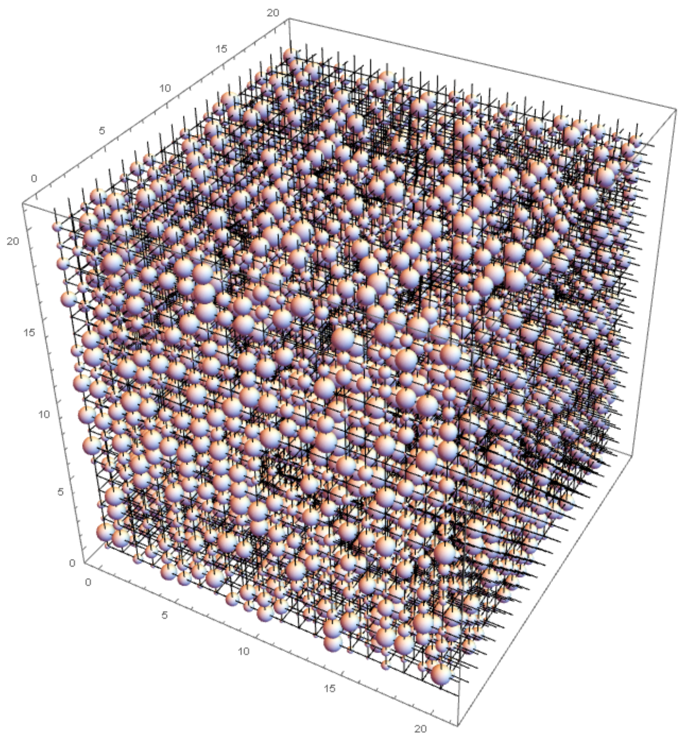
$$\sigma = -2\pi e^2\hbar \sum_{m,n} |v_{mn}|^2 \left(\frac{\partial f}{\partial E}\right)_{E_n} \boldsymbol{\delta}(E_n - E_m), \quad \ldots\ldots (30)$$

which may be rewritten in the form of (21),

$$\sigma = -2\pi e^2\hbar \int \sum_{m,n} |v_{mn}|^2 \boldsymbol{\delta}(E - E_n)\boldsymbol{\delta}(E - E_m) \frac{\partial f}{\partial E} dE. \quad \ldots\ldots (31)$$

Greenwood, D. A. 1958. "The Boltzmann Equation in the Theory of Electrical Conduction in Metals." *Proceedings of the Physical Society of London* 71 (460): 585–96.

Anderson localization



$$H = \sum_{\vec{r}} \varepsilon_{\vec{r}}\, c^{+}_{\vec{r}} c_{\vec{r}} - t \sum_{\vec{r},\vec{\delta}} c^{+}_{\vec{r}+\vec{\delta}} c_{\vec{r}}$$

$$\varepsilon_{\vec{r}} = \mathrm{Random}[-W, W]$$

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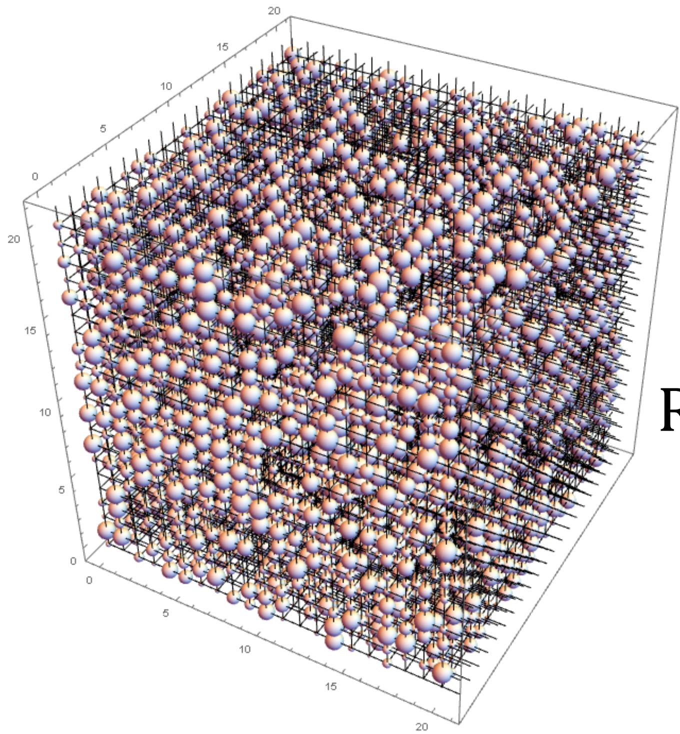
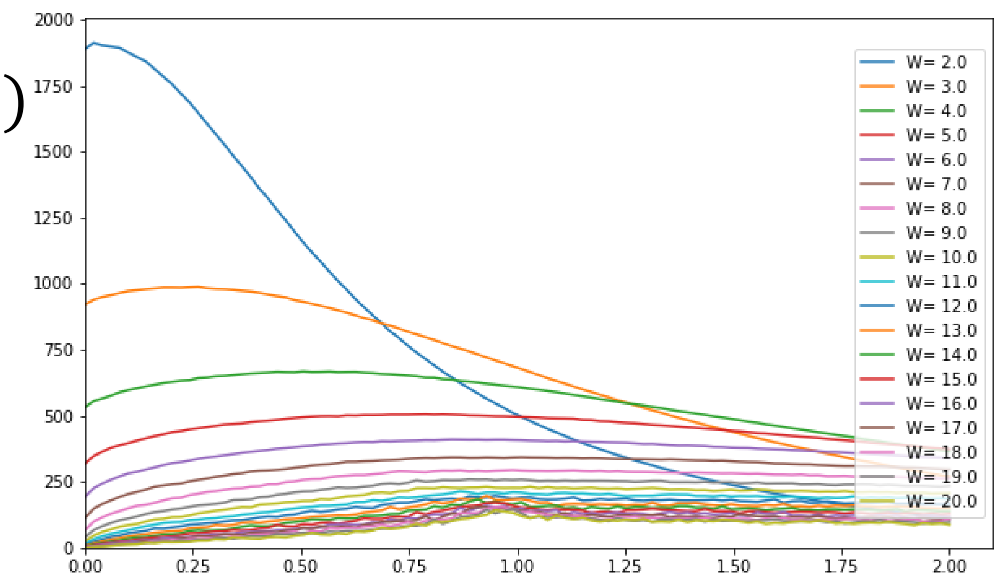


$\mathrm{Re}\sigma(\omega)$



ω

$$\mathrm{Re}\sigma(\omega) = -\sum_{n,s} \frac{f(\varepsilon_n)-f(\varepsilon_s)}{\varepsilon_n-\varepsilon_s} |\langle n|\hat{j}|s\rangle|^2\, \delta(\omega + \varepsilon_n - \varepsilon_s)$$

Kubo and ab-initio

$$\sigma(t) = \left(\hat{J}(t)\middle|\hat{J}\right) = -\sum_{n,s} \frac{f(\varepsilon_n) - f(\varepsilon_s)}{\varepsilon_n - \varepsilon_s} |\langle n|\hat{J}|s\rangle|^2 e^{i(\varepsilon_n - \varepsilon_s)t}$$

$$f(z) = \int_0^\infty e^{izt} f(t)$$

$$\sigma(z) = -i \sum_{n,s} \frac{f(\varepsilon_n) - f(\varepsilon_s)}{\varepsilon_n - \varepsilon_s} \frac{|\langle n|\hat{J}|s\rangle|^2}{z + \varepsilon_n - \varepsilon_s}$$

Periodic boundary conditions $\Longrightarrow$ Always modes that do not decay

Macroscopic limit of LARGE systems and LONG times!!

Memory Function

$$\sigma(t) = \left(\hat{J}(t)\middle|\hat{J}\right) = \left(e^{iLt}\hat{J}\middle|\hat{J}\right)$$

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$$Q = 1 - P = 1 - \left|\hat{J}\right)\left(\hat{J}\right|$$

Projector

Memory Function

$$\sigma(t) = \left(\hat{J}(t)\middle|\hat{J}\right) = \left(e^{iLt}\hat{J}\middle|\hat{J}\right)$$

$$Q = 1 - P = 1 - \left|\hat{J}\right)\left(\hat{J}\right|$$

$$\frac{d\hat{J}(t)}{dt} = -\int_0^t dt'\, \hat{J}(t-t')\frac{\left(e^{iQLt'}QL\hat{J}\middle|QL\hat{J}\right)}{\left(\hat{J}\middle|\hat{J}\right)} + ie^{iQLt}QL\hat{J}$$

Exact!

Mori, Hazime. "Transport, Collective Motion, and Brownian Motion." *Progress of Theoretical Physics* **33,** 423 (1965).

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$$\frac{d\hat{J}(t)}{dt} = +\int_0^t dt'\,\hat{J}(t-t')\,m(t') + f(t)$$

Langevin Eq.

memory

random Force

Memory Function

$$\frac{d\hat{J}(t)}{dt} = -\hat{J}(t)\frac{1}{\tau} + f(t)$$

Short memory.

$$m(t) = -\frac{1}{\tau}\delta(t)$$

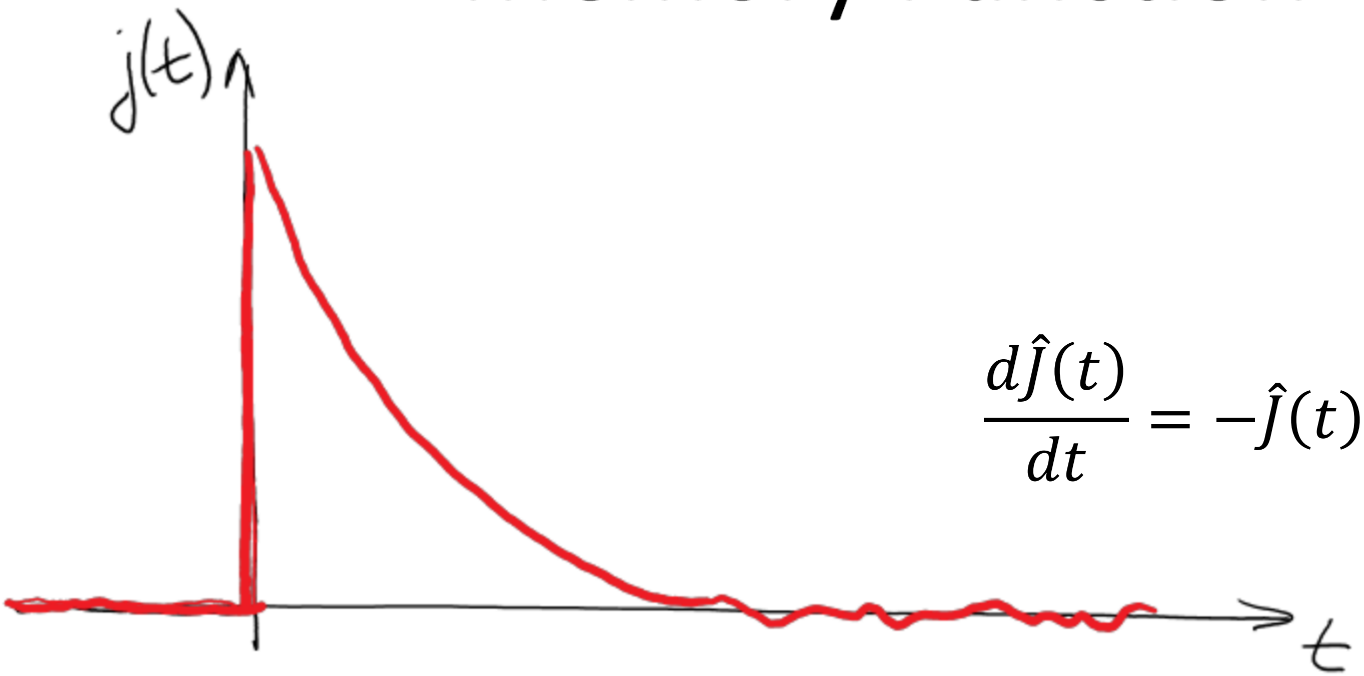
$$\frac{d\hat{J}(t)}{dt} = +\int_0^t dt'\,\hat{J}(t-t')\,m(t') + f(t)$$

Langevin Eq.

memory

random Force

Memory Function



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Langevin Eq.

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Memory Function

$$\frac{d\hat{J}(t)}{dt} = \int_0^t dt'\, \hat{J}(t-t')\, m(t') + f(t)$$

$$\sigma(t) = \left(\hat{J}(t)\middle|\hat{J}\right) = \left(e^{iLt}\hat{J}\middle|\hat{J}\right) \Longrightarrow \quad \frac{d\sigma(t)}{dt} = \int_0^t dt'\, \sigma(t-t')\, m(t')$$

Memory Function

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$$\hat{f}(z) = i \int_0^\infty e^{izt} f(t) dt$$

Laplace transform

$$\hat{\sigma}(z) = \frac{ne^2}{m} \frac{1}{\hat{m}(z) - z}$$

Generalized Drude form

Self-Consistent Current Relaxation (how to calculate $\widehat{m}(z)$)

$$H_0 = \sum_{n,\boldsymbol{k}} \varepsilon_{n,\boldsymbol{k}} \, c^\dagger_{n,\boldsymbol{k}} c_{n,\boldsymbol{k}}$$

$$H_i = \sum_{\boldsymbol{q}} U(\boldsymbol{q}) \rho(-\boldsymbol{q})$$

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

$$\xi_{n',n,\boldsymbol{k}}(\boldsymbol{q}) = c^\dagger_{n',\boldsymbol{k}-\boldsymbol{q}} c_{n,\boldsymbol{k}}$$

$$\rho(\boldsymbol{q}) = \sum_{n',n,\boldsymbol{k}} M_{n',n,\boldsymbol{k}}(\boldsymbol{q}) \, \xi_{n',n,\boldsymbol{k}}(\boldsymbol{q})$$

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

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

Adapted from the free electron gas solution of Götze, Wolfgang. "The Mobility of a Quantum Particle in a Three-Dimensional Random Potential." Philosophical Magazine B **43**, 219 (1981)

Self-Consistent Current Relaxation (how to calculate $\hat{m}(z)$)

$$H_0 = \sum_{n,\boldsymbol{k}} \varepsilon_{n,\boldsymbol{k}}\, c^\dagger_{n,\boldsymbol{k}} c_{n,\boldsymbol{k}} \qquad H_i = \sum_{\boldsymbol{q}} U(\boldsymbol{q})\rho(-\boldsymbol{q}) \qquad \xi_{n',n,\boldsymbol{k}}(\boldsymbol{q}) = c^\dagger_{n',\boldsymbol{k}-\boldsymbol{q}} c_{n,\boldsymbol{k}}$$

$$\begin{aligned}[H_0, \xi_{n',n,\boldsymbol{k}}(\boldsymbol{q})] &= (\varepsilon_{n',\boldsymbol{k}-\boldsymbol{q}} - \varepsilon_{n\boldsymbol{k}})\xi_{n',n,\boldsymbol{k}}(\boldsymbol{q}) \\ &=: \varepsilon_{n',n,\boldsymbol{k}}(\boldsymbol{q})\xi_{n',n,\boldsymbol{k}}(\boldsymbol{q}) \ ,\end{aligned}$$

$$\begin{aligned}&[H_i, \xi_{n',n,\boldsymbol{k}}(\boldsymbol{q})] = \\ &= \sum_{\boldsymbol{q}'} U(\boldsymbol{q}') \sum_{l} \{ M_{l,n'}(\boldsymbol{k}-\boldsymbol{q}, -\boldsymbol{q}')\, \xi_{l,n,\boldsymbol{k}}(\boldsymbol{q}-\boldsymbol{q}') \\ &- \ M_{n,l}(\boldsymbol{k}-\boldsymbol{q}', -\boldsymbol{q}')\, \xi_{n',l,\boldsymbol{k}-\boldsymbol{q}'}(\boldsymbol{q}-\boldsymbol{q}') \} \ .\end{aligned}$$

Adapted from the free electron gas solution of Götze, Wolfgang. "The Mobility of a Quantum Particle in a Three-Dimensional Random Potential." Philosophical Magazine B **43**, 219 (1981)

Self-Consistent Current Relaxation (how to calculate $\widehat{m}(z)$)

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

$$\rho(\boldsymbol{q}) = \sum_{n',n,\boldsymbol{k}} M_{n',n,\boldsymbol{k}}(\boldsymbol{q})\,\xi_{n',n,\boldsymbol{k}}(\boldsymbol{q})$$

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

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

$$\mathcal{P}(\boldsymbol{q})\bullet = \sum_{\alpha} A_{\alpha}(\boldsymbol{q})\,\left(A_{\alpha}(\boldsymbol{q}), \bullet\right)$$

Adapted from the free electron gas solution of Götze, Wolfgang. “The Mobility of a Quantum Particle in a Three-Dimensional Random Potential.” Philosophical Magazine B **43**, 219 (1981)

Self-Consistent Current Relaxation (how to calculate $\widehat{m}(z)$)

$$\Phi(\boldsymbol{q}, z) = (\rho(\boldsymbol{q}), \mathcal{R}(z)\rho(\boldsymbol{q})) \qquad g(\boldsymbol{q}) := (\rho(\boldsymbol{q}), \rho(\boldsymbol{q}))$$

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

$$M(\boldsymbol{q}, z) := M_{1,1}(\boldsymbol{q}, z) = (\mathcal{L}_i A_1(\boldsymbol{q}), \mathcal{R}(z)\mathcal{L}_i A_1(\boldsymbol{q}))$$

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

Adapted from the free electron gas solution of Götze, Wolfgang. "The Mobility of a Quantum Particle in a Three-Dimensional Random Potential." Philosophical Magazine B **43**, 219 (1981)

Self-Consistent Current Relaxation (how to calculate m(z))

Model of disorder:
alloy, solvent, …

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

Charge relaxation of the ordered
system from DFT code

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

M. Troppenz, B. Green, S. Rigamonti, C. Draxl, JS, "Memory Function Approach for the Impurity Limited Electrical Conductivity of Solids", in preparation.

Self-Consistent Current Relaxation (how to calculate m(z))

PENNSTATE 1855

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

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

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

$$\sigma(\omega) = \lim_{\eta\to 0}\lim_{\boldsymbol{q}\to 0}\sigma(\boldsymbol{q},\omega+i\eta)$$

M. Troppenz, B. Green, S. Rigamonti, C. Draxl, JS, “Memory Function Approach for the Impurity Limited Electrical Conductivity of Solids”, in preparation.

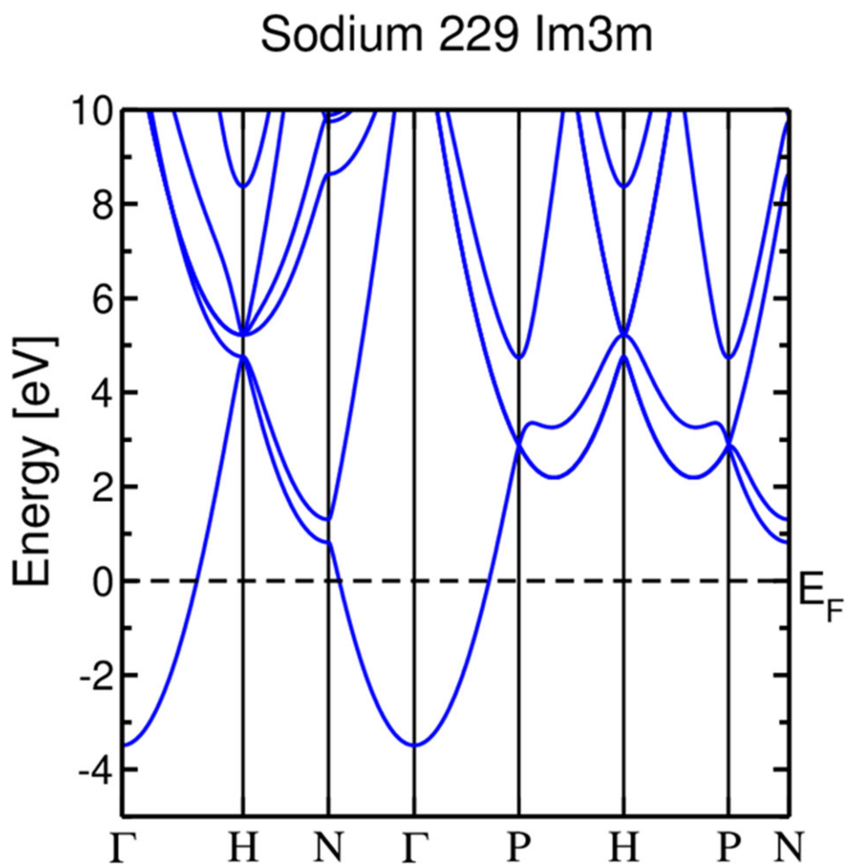
exciting

PENNSTATE

http://exciting-code.org/

Implemented in "exciting"

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



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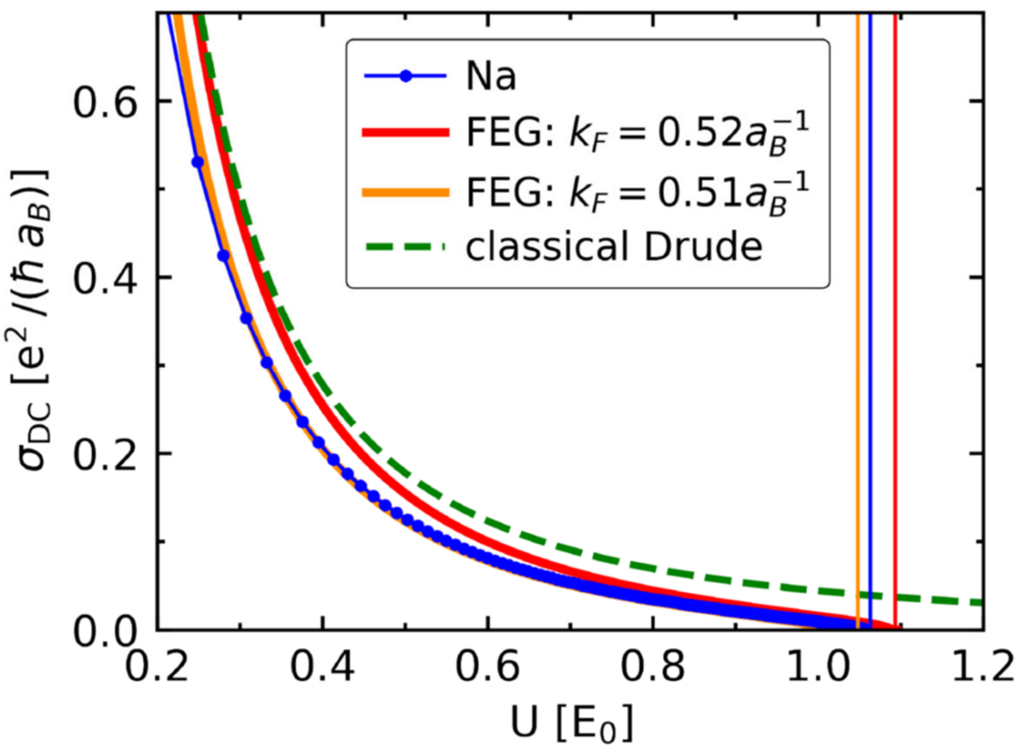
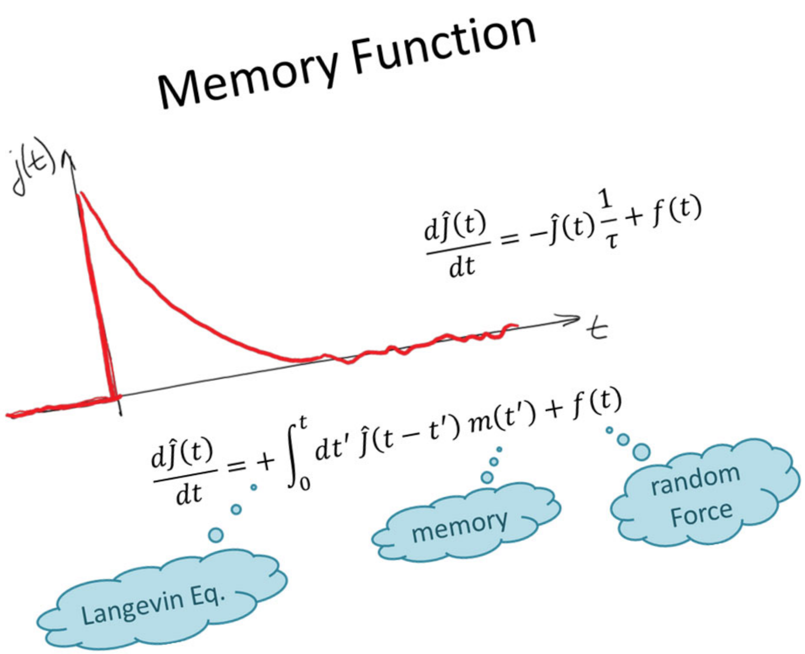


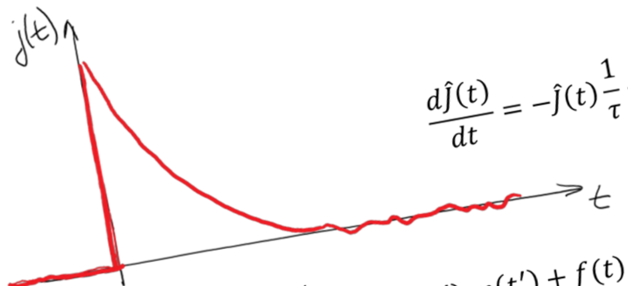
In summary…



Memory Function
j(t)
t
$\frac{d\hat{j}(t)}{dt} = -\hat{j}(t)\frac{1}{\tau} + f(t)$
$\frac{d\hat{j}(t)}{dt} = +\int_0^t dt'\, \hat{j}(t-t')\, m(t') + f(t)$
Langevin Eq.
memory
random Force

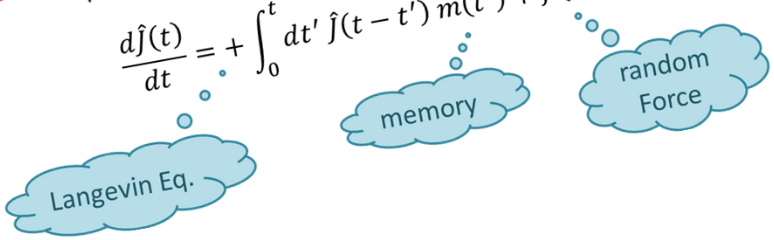
In summary…

Memory Function



$$\frac{d\hat{J}(t)}{dt} = -\hat{J}(t)\frac{1}{\tau} + f(t)$$

$$\frac{d\hat{J}(t)}{dt} = +\int_0^t dt'\, \hat{J}(t-t')\, m(t') + f(t)$$



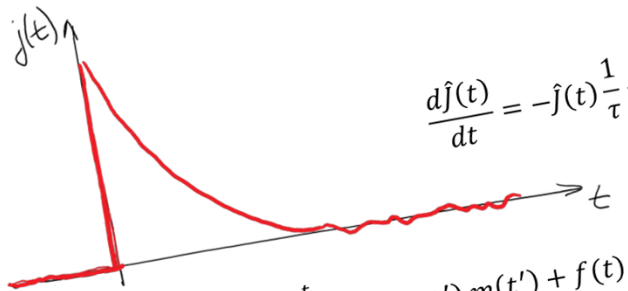
$$\hat{m}(z) = \frac{1}{nm}\sum_{\vec{q}} \langle |U(\vec{q})|^2 \rangle\, \phi(\vec{q}, z)$$

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

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

In summary…

Memory Function



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Langevin Eq.

memory

random Force

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

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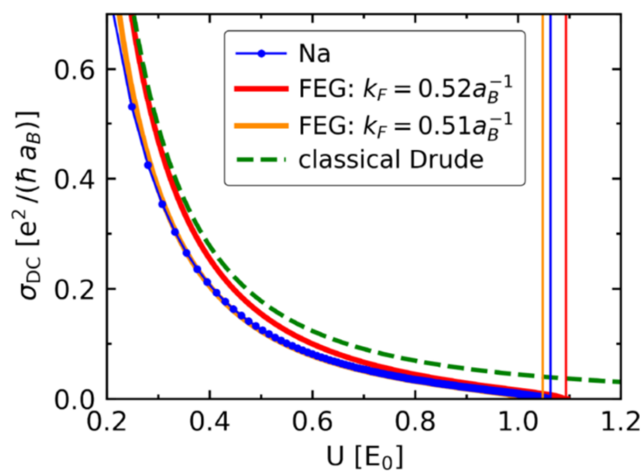
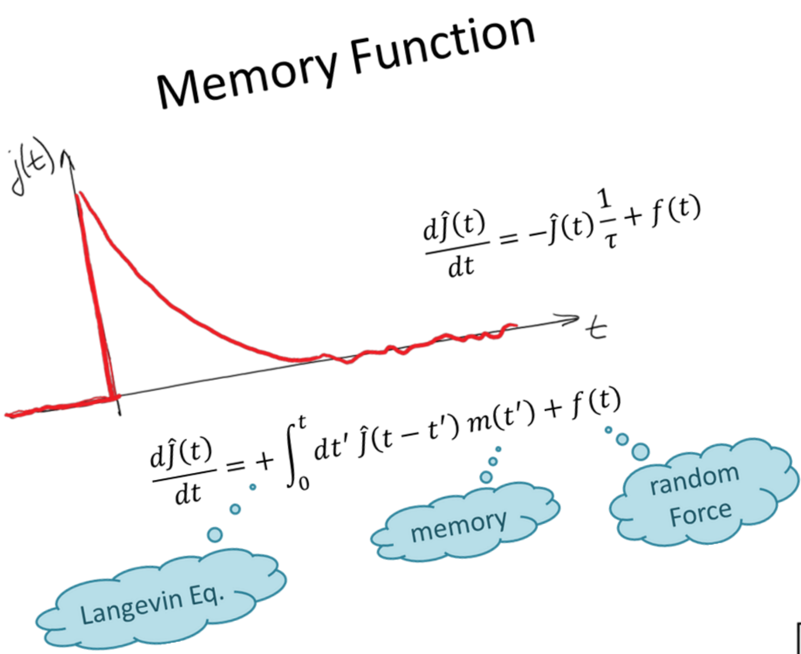
$$\sigma(\vec{q},z) = i\frac{z}{q^2}\left[z\,\phi(\vec{q},z) - g(\vec{q})\right]$$



In summary…

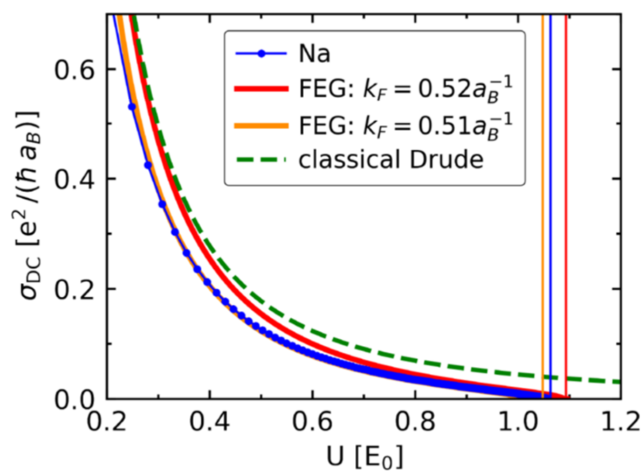


$$\hat{m}(z) = \frac{1}{nm}\sum_{\vec{q}} \langle |U(\vec{q})|^2 \rangle\, \phi(\vec{q}, z)$$

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

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

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



Reflection…

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

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

"Hold Infinity
in the palm of your hand
And Eternity
in an hour"

Auguries of Innocence,
William Blake