Using Ensemble Monte Carlo Methods to Evaluate Non-Equilibrium Green's Functions

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Sunrise over the sea of Cortez

EMC and NEGF

- **EMC (ensemble Monte Carlo) and NEGF (non-equilibrium Green's functions) both had their origins in the 1940s**
- **EMC arose from simulation work at Los Alamos on neutron transport**
- **EMC has been used mostly in classical transport to solve the Boltzmann equation**
- **NEGF began with Julian Schwinger**
- **NEGF has been used mostly in quantum transport to determine correlation functions needed to achieve the distribution function**

Quantum Mechanics with EMC

- Introducing a joint spectral density in place of δ-function in Fermi golden rule: Fischetti (1984), Porod and Ferry (1985), Jauho (and Reggiani, Lugli) (1985,1989,…),
- Bohm and wave functions: Oriols (1998), Chen et al. (1992), Shifren *et al*. (2003)
- Using a quantum kinetic equation with JSD function: Jauho and Wilkins (1982), Jauho (1983,1989)
- Using Wigner equation of motion with JSD: Jauho (1989)
- The JSD is usually approximated by a Lorentzian

None of these use the true NEGF in the EMC!

EMC and NEGF

To my knowledge, these two approaches have never been coupled in studies of semiconductor transport!

Why do We Care?

- **Ensemble Monte Carlo (EMC) techniques provide the most accurate approach to solving the Boltzmann equation, allowing one to focus on the physics of interactions, and letting the computer do the difficult bits**
- **Non-Equilibrium Green's Functions (NEGF) have also been used to determine transport, but are difficult to implement and to evaluate (in fact, most approaches have serious errors[*])**
- **NEGF is now being used by several software houses for semiconductor device simulation; it is slow and difficult!**

[*]D. K. Ferry, J. Weinbub, M. Nedjalkov and S. Selberherr, "A review of quantum transport in field-effect transistors," *Semicond. Sci. Technol*. **37**, 043001 (2022)

What Do These Do?

- EMC techniques are particle-based techniques; the particles used in simulations are correlated with the electrons or holes
- NEGF approaches are based upon wave functions and their evolution in time.
- NEGF has not been associated with particle-based approaches (other than within the Feynman integral approach)
- However, the use of particles for quantum simulations have been known since the beginning (Madelung 1927, Kennard 1928, Bohm 1950)

Non-Equilibrium Green's Functions

The Green's function approach is compute-intensive and has none of the computational simplicity ... of the detailed microscopic picture afforded by the ensemble Monte Carlo method.

J. R. Barker, J. Comp. Electron. 9, 243 (2010)

EMC Techniques are Assured from an Integral Equation

- **The integral equation is developed from the Boltzmann equation and was developed by Kurosawa (1966), Budd (1967) and Rees (1972)**

$$f(\boldsymbol{k},t) = f(\boldsymbol{k},0)e^{-\Gamma_0 t}$$
$$+\int_0^t dt' \int d^3\boldsymbol{k}' P(\boldsymbol{k}' - \frac{e}{\hbar}\boldsymbol{E},\boldsymbol{k}) f\left(\boldsymbol{k}' - \frac{e}{\hbar}\boldsymbol{E}t',\boldsymbol{r},t'\right) e^{-\Gamma_0(t-t\prime)}$$

- **This integral equation allows us to realize how to alternate the processes of *drift* and *scattering* to produce transport**

The distribution function at various times correlates with the ensemble of electrons used in the simulation :

$\boldsymbol{t = 0}$

intermediate time

final time

$$f(\boldsymbol{k},t) = f(\boldsymbol{k},0)e^{-\Gamma_0 t} + \int_0^t dt' \int d^3\boldsymbol{k}' P\left(\boldsymbol{k}' - \frac{e}{\hbar}\boldsymbol{E},\boldsymbol{k}\right) f\left(\boldsymbol{k}' - \frac{e}{\hbar}\boldsymbol{E}t',\boldsymbol{r},t'\right) e^{-\Gamma_0(t-t')}$$

The Transport Physics in Action

Loss of information about the initial condition

Probability that carrier has not been scattered; drift time t-t'

$$f(\boldsymbol{k},t) = f(\boldsymbol{k},0)e^{-\Gamma_0 t}$$

$$+\int_0^t dt' \int d^3\boldsymbol{k}' P(\boldsymbol{k}' - \frac{e}{\hbar}\boldsymbol{E}t, \boldsymbol{k})\, f\left(\boldsymbol{k}' - \frac{e}{\hbar}\boldsymbol{E}t', \boldsymbol{r}, t'\right) e^{-\Gamma_0 (t-t')}$$

Probability to scatter from k' to k

Particles in Quantum Transport

- As mentioned, particles have been suggested for quantum mechanics since the beginning: Madelung 1927, Kennard 1928, Bohm 1950
- Even Feynman, with his path integral method, considered the "paths" to be those of particles (1948); attempts to use this for transport by Thornber and Feynman eventually used a QKE
- Nevertheless, there have been many approaches to put QM into EMC

The problem lies with the very difficult, complicated equation that must eventually be solved for $G^<$

$$G^{r,a} = G_0^{r,a} + G_0^{r,a}\Sigma^{r,a}G_0^{r,a}$$
$$G^< = G_0^< + G_0^r\Sigma^r G^< + G_0^r\Sigma^< G^a + G_0^<\Sigma^a G^a$$

Each product is a convolution integral in the double time, double space coordinates

A.-P. Jauho, Physica 134B, 148 (1985)

- It has long been known that one can use any set of basis functions to solve the Schrödinger equation
- This allows one to chose a basis set that is suited to the problem at hand
- Most people have encountered Airy functions in their quantum mechanics course with a triangular potential well
- In a high electric field, Airy functions, or more properly the Airy transform, is best suited to the Schrödinger equation
- Here, the Airy transform will be used for the NEGFs

ASU

Airy Transforms

The Airy transform of a function *f(ρ,z)* and some reduced parameters are given by:

$$F(k_\perp, s) = \int \frac{dxdy}{2\pi} \int \frac{dz}{L} e^{ik_\perp \cdot \rho} Ai\left(\frac{z-s}{L}\right) f(\rho, z)$$

$$\rho = (x, y)$$
$$L = \sqrt[3]{\hbar/2mF}$$

$$G^r(k,s,s',\omega) = G_F^r(k,s,\omega)[\delta(s-s').$$
$$+\int ds_2 \Sigma^r(k,s,s_2,\omega)G^r(k,s_2,s',\omega)]$$

$$G_F^r(k,s,t) = -i\theta(t)exp\left(-\frac{iE_{ks}t}{\hbar}\right)$$

What we need is the self-energy. The spectral density isn't a Lorentzian due to the very nonlinear nature of the self energy

$$\Sigma^r(s,\omega) = \frac{2\pi|M|^2}{\hbar}\sum_{\eta=\pm 1}\left(N+\frac{1}{2}+\frac{\eta}{2}\right)F(s,\omega)\,, \quad \Theta = \sqrt[3]{\frac{3(e\hbar F)^2}{2m}}\,,$$

$$Re[F(s,\omega)] = \frac{2\pi m^{3/2}\sqrt{\Theta}}{\sqrt{2}\hbar^2}\left[Ai'(\zeta)Bi'^{(\zeta)} - \zeta Ai(\zeta)Bi(\zeta) - \frac{\sqrt{\zeta}}{\pi}\right]$$

$$Im[F(s,\omega)] = \frac{2\pi m^{3/2}\sqrt{\Theta}}{\sqrt{2}\hbar^2}[Ai'^2(\zeta) - \zeta Ai^2(\zeta)]$$

$$-\zeta = eFs - \hbar(\omega - \eta\omega_0)$$

R. Bertoncini, A. M. Kriman and D. K. Ferry, Phys. Rev. B 40, 3371 (1989)

Working through the math for G< allows us to find that the Kadanoff and Baym ansatz is satisfied, and that an integral equation can be found for the distribution function as

$$G^{<}(k,s,\omega) = -A(k,s,\omega)\,\Sigma^{<}(s,\omega)/2Im\{\Sigma^{r}(s,\omega)\}$$

$$f(s,\omega) = \int ds' K(s,s';\omega-\eta\omega_0) f(s';\omega-\eta\omega_0)$$

$$K(s,s';\omega-\eta\omega_0) = \frac{\frac{1}{L^2} Ai^2\left(\frac{s-s'}{\sqrt[3]{3}L}\right)}{Im[\Sigma^r(s,\omega)]} \times \left(\frac{2\pi^2}{\hbar}\right)^2 |M|^2 2\sqrt{3}\left[\frac{\pi}{2} + tan^{-1}\left(\frac{\hbar\omega - eFs' - Re[\Sigma^r(s',\omega)]}{Im[\Sigma^r(s',\omega)]}\right)\right]$$

R. Bertoncini, A. M. Kriman and D. K. Ferry, Phys. Rev. B 41, 1390 (1990)

Effective drift distance, or energy gain during the drift; velocity obtained from this ΔE

$$K(s, s'; \omega - \eta\omega_0) = \frac{\frac{1}{L^2} Ai^2\left(\frac{s - s'}{\sqrt[3]{3}L}\right)}{Im[\Sigma^r(s, \omega)]}$$

$$\times\left(\frac{2\pi^2}{\hbar}\right)^2 |M|^2 2\sqrt{3}\left[\frac{\pi}{2} + tan^{-1}\left(\frac{\hbar\omega - eFs' - Re[\Sigma^r(s', \omega)]}{Im[\Sigma^r(s', \omega)]}\right)\right]$$

Scattering function arising from $\Sigma^<$

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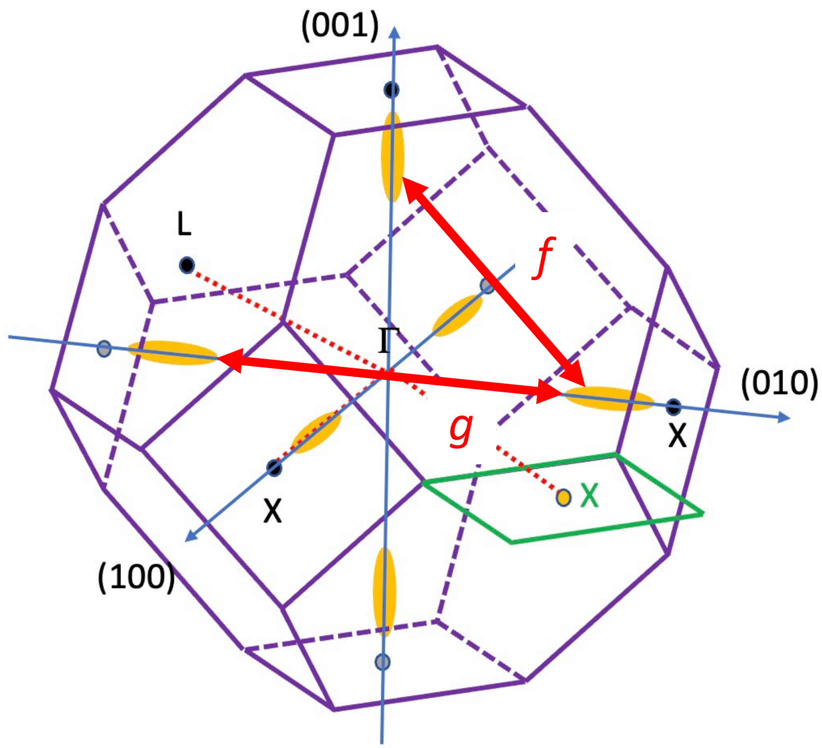
Test Case: Bulk Si at 300 K

- Two effective phonons: 1 high energy for optical intervalley modes and 1 mid energy for acoustic intervalley modes (Long, PR 120, 2024; Ferry, PRB 14, 605)
- The non-polar intervalley phonons are q-independent, which means that they are highly localized in real space, thus not expected to generate any correlations and high-order diagrams
- Analytic non-parabolic energy bands, 10^5 particles
- Field parallel to (111) direction so all valleys make same angle with the field


(001)
L
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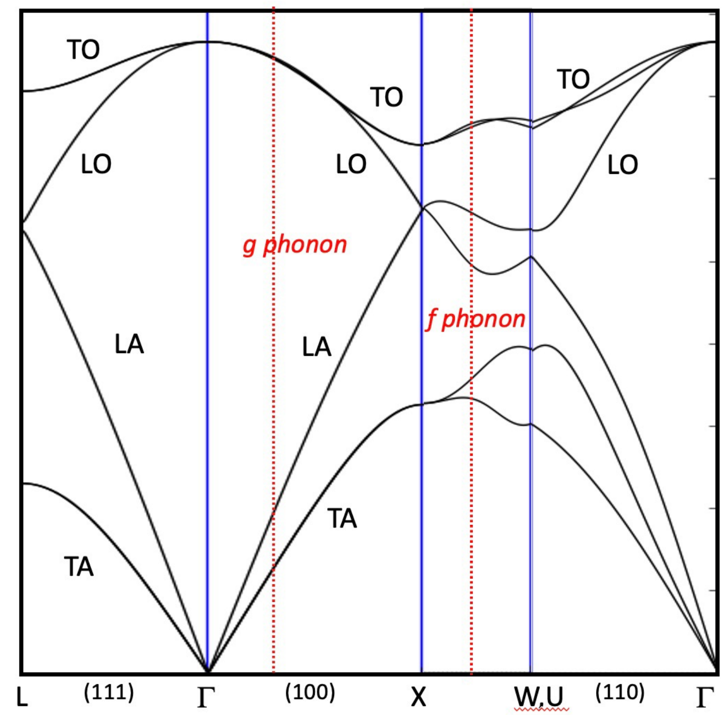
TO
TO
TO
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LO
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g phonon
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LA
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(111)
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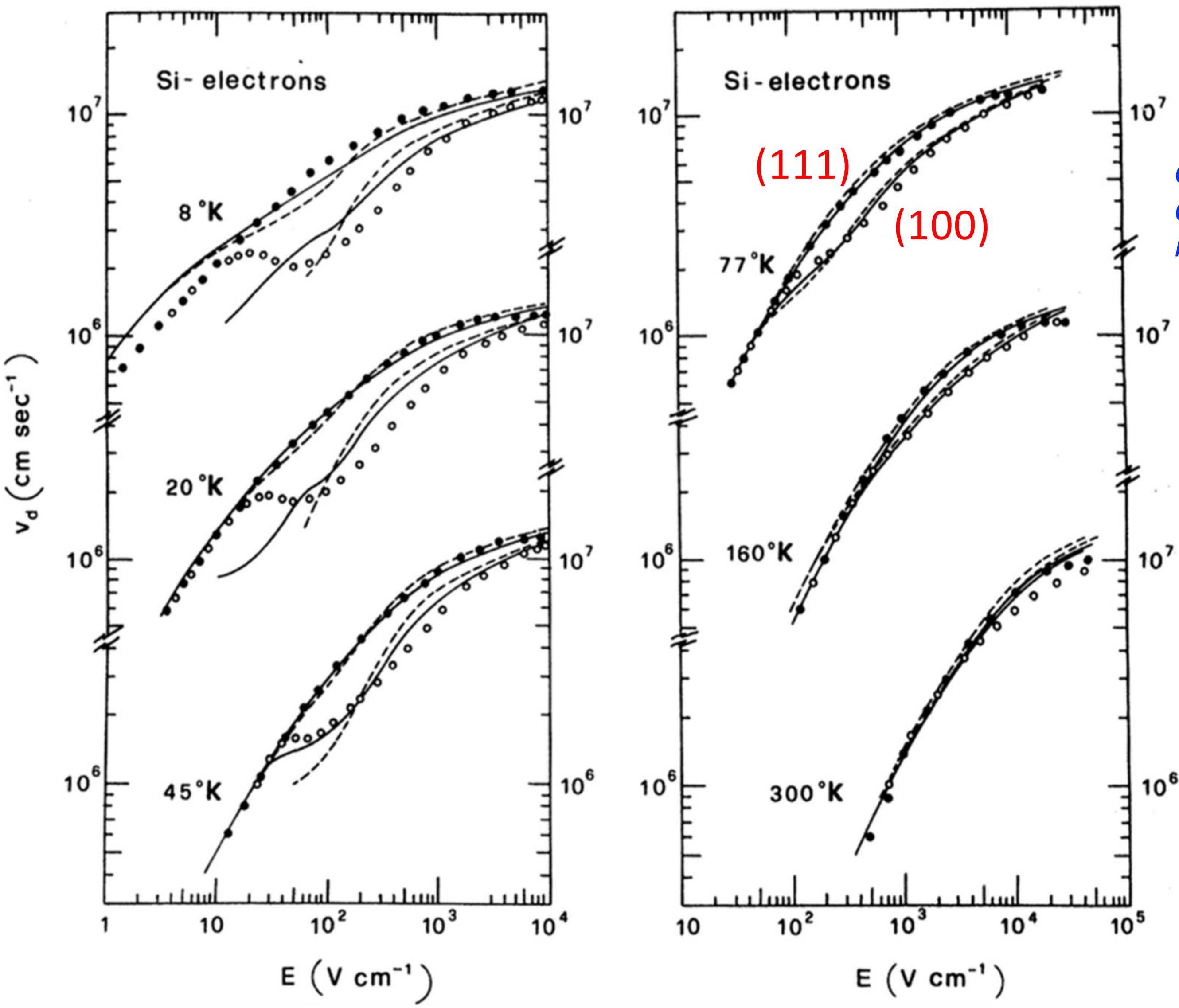
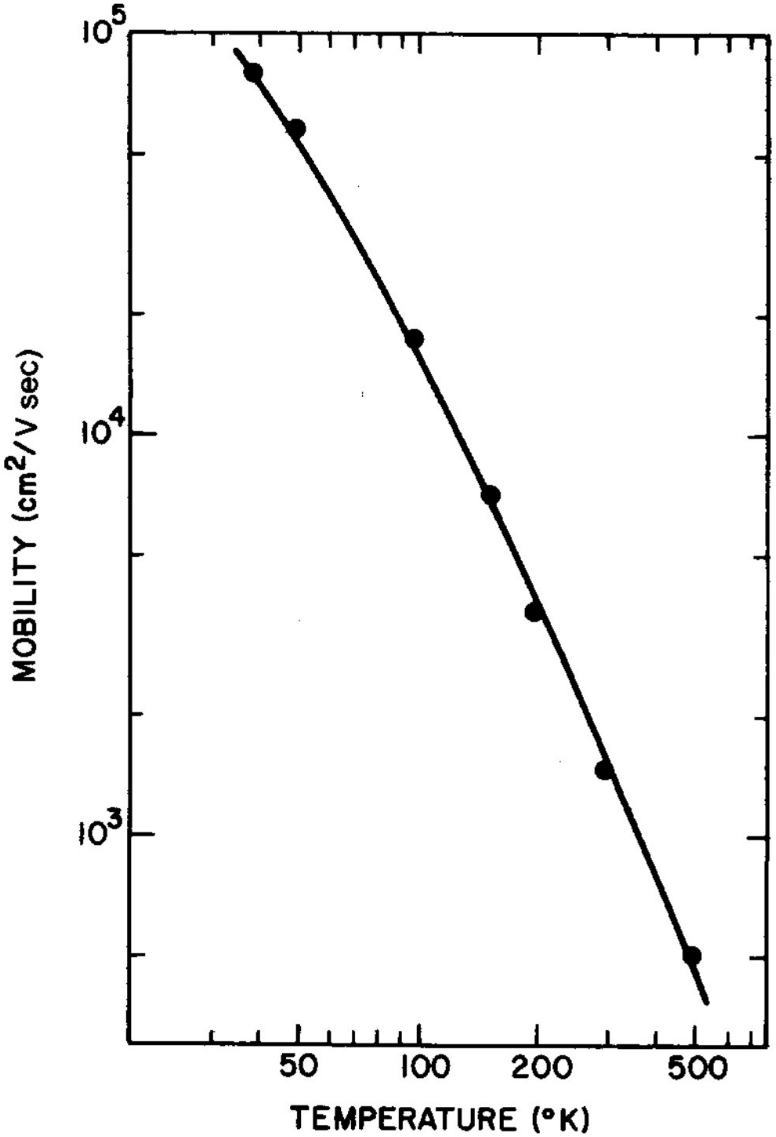
W,U
(110)
Γ



C. Canali, C. Jacoboni, F. Nava, G. Ottaviani, and A. Alberigi-Quaranta, Phys. Rev. B 12, 2265 (1975)



1 high-energy phonon, 0-order coupled

1 low-energy phonon, 1-order coupled

D. K. Ferry, Phys. Rev. B 14, 1605 (1976)

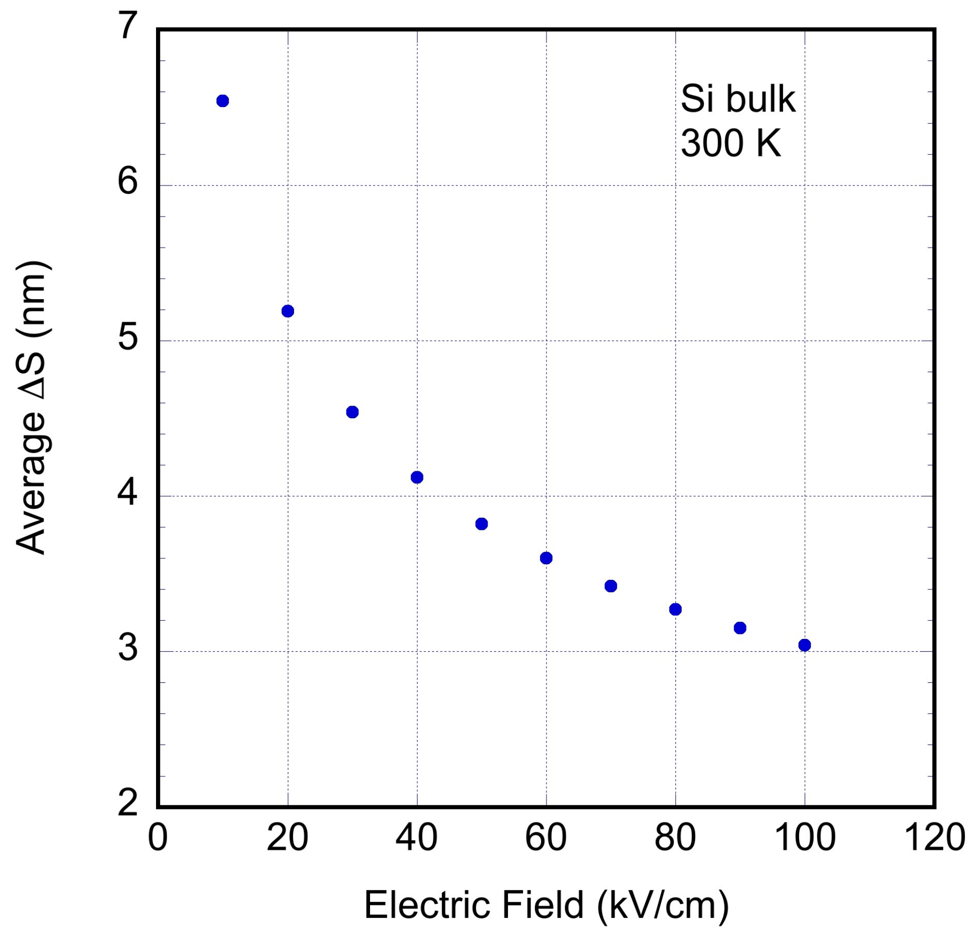
Effective drift distance, or energy gain during the drift; velocity obtained from this ΔE

$$K(s, s'; \omega - \eta\omega_0) = \frac{\frac{1}{L^2} Ai^2\left(\frac{s - s'}{\sqrt[3]{3}L}\right)}{Im[\Sigma^r(s, \omega)]}$$

$$\times \left(\frac{2\pi^2}{\hbar}\right)^2 |M|^2 2\sqrt{3} \left[\frac{\pi}{2} + tan^{-1}\left(\frac{\hbar\omega - eFs' - Re[\Sigma^r(s', \omega)]}{Im[\Sigma^r(s', \omega)]}\right)\right]$$

Scattering function arising from $\Sigma^<$

Average drift distance as a function of electric field



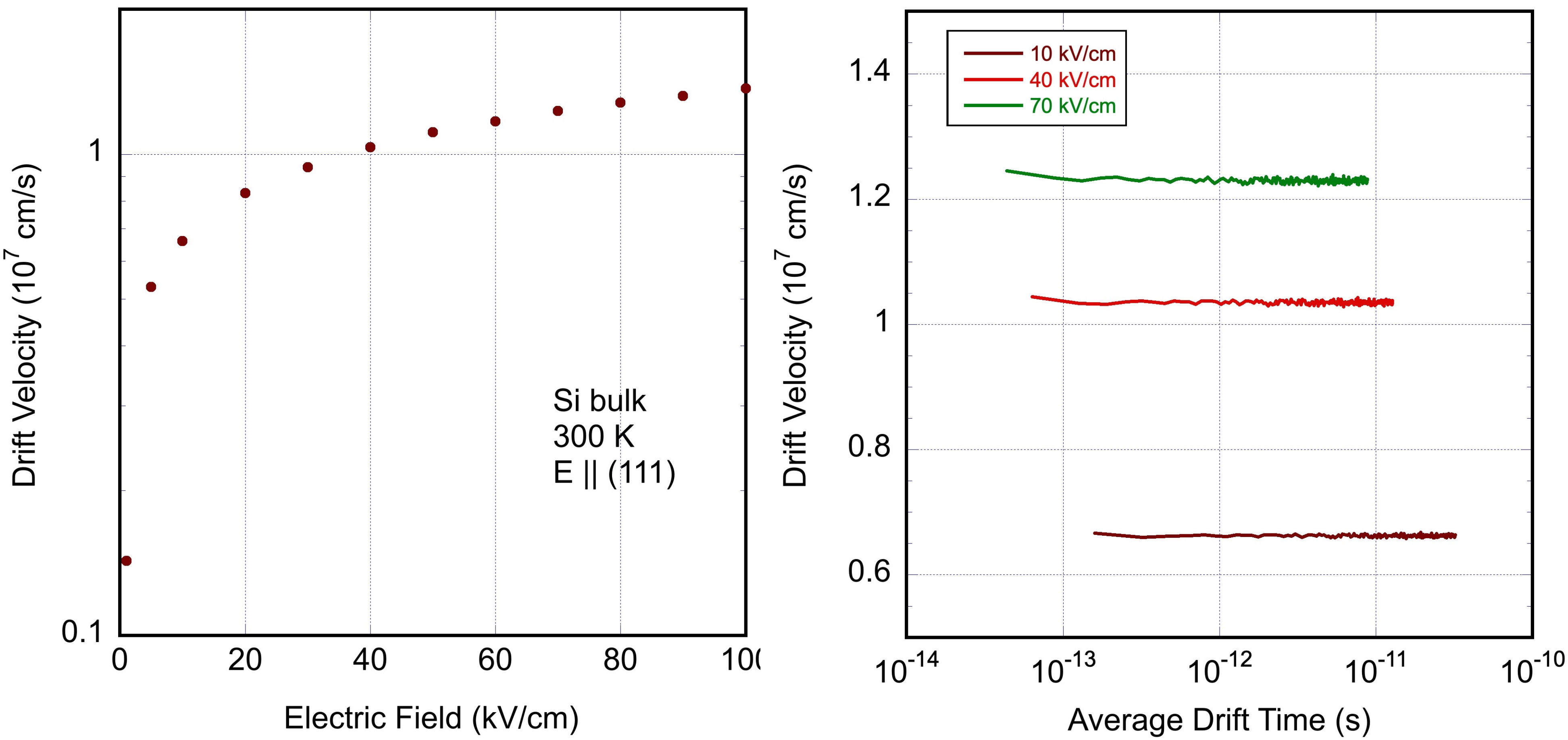
$$Ai^2\left(\frac{s-s'}{\sqrt[3]{3}L}\right)$$

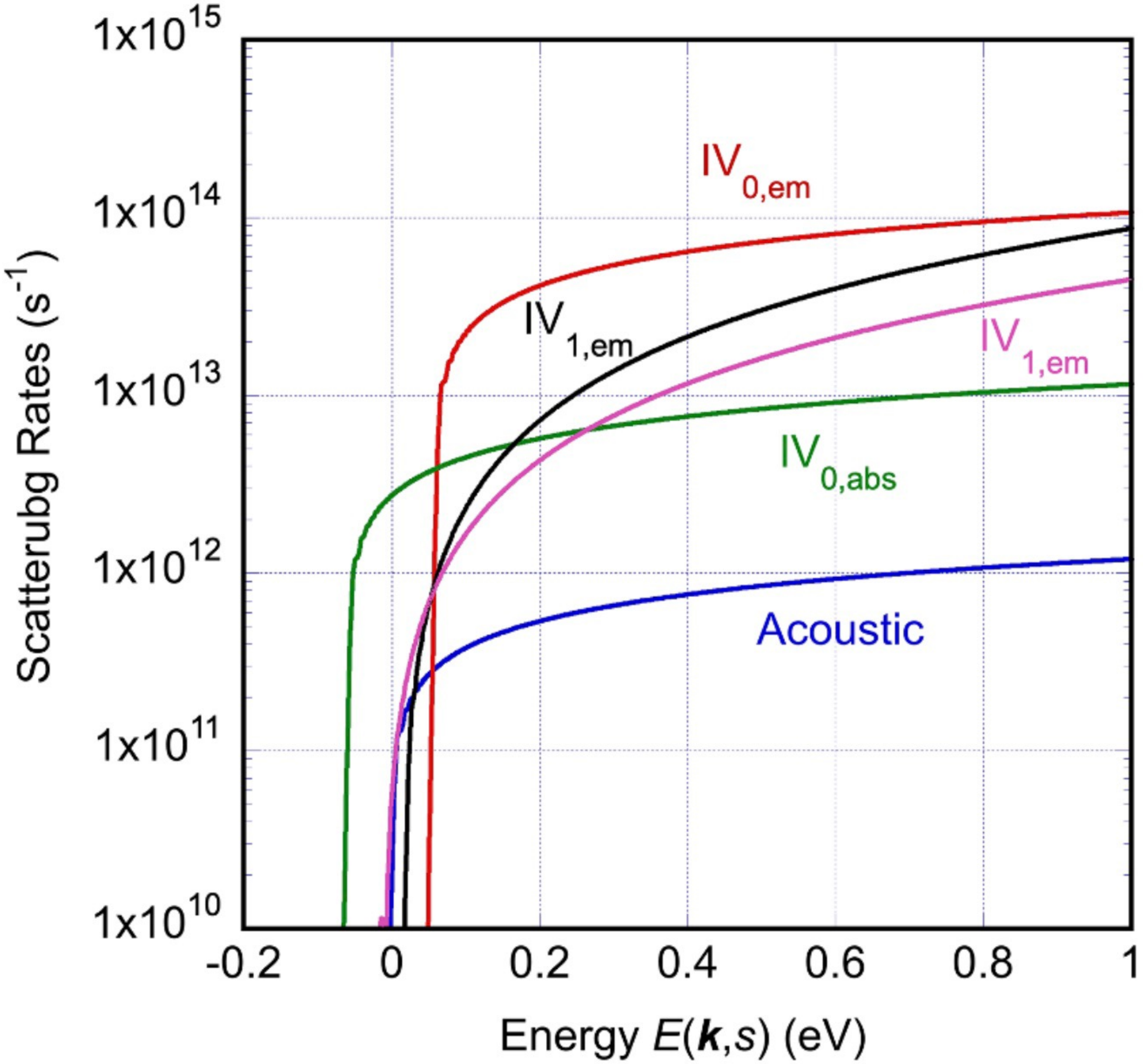
$$L=\left(\frac{\hbar^2}{2m^*eF}\right)^{1/3}$$

In non-parabolic bands, one connects time and space via

$$\Delta t = \sqrt{\frac{2m_c}{eF}|\Delta s|\left(1 + \frac{E}{E_G} + \frac{eF|\Delta s|}{2E_G}\right)}$$

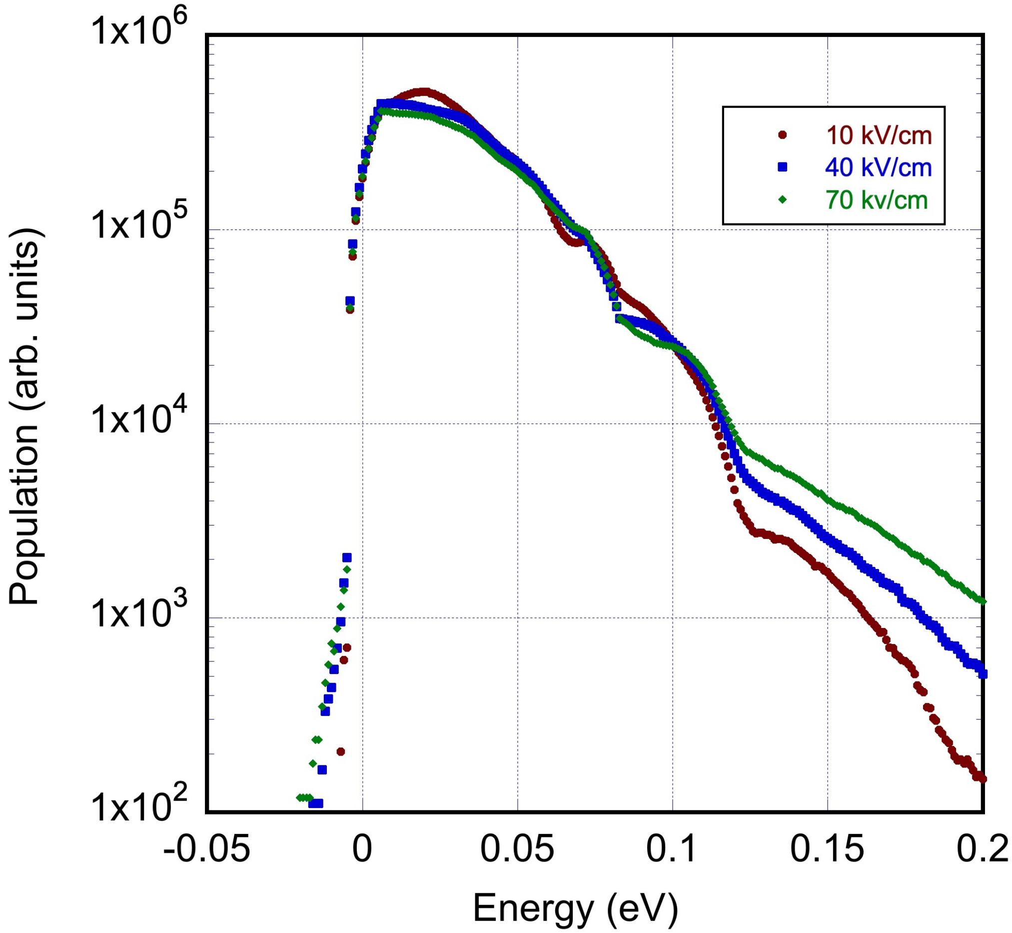
Then, velocity and momentum are determined in the usual manner


Drift Velocity (10^7 cm/s)
1
0.1
0
20
40
60
80
100
Electric Field (kV/cm)
Si bulk
300 K
E || (111)
10 kV/cm
40 kV/cm
70 kV/cm
1.4
1.2
1
0.8
0.6
10^{-14}
10^{-13}
10^{-12}
10^{-11}
10^{-10}
Average Drift Time (s)



1x10^15
1x10^14
1x10^13
1x10^12
1x10^11
1x10^10
Scatterubg Rates (s^-1)
IV0,em
IV1,em
IV1,em
IV0,abs
Acoustic
-0.2
0
0.2
0.4
0.6
0.8
1
Energy E(k,s) (eV)

Relative population as a function of energy



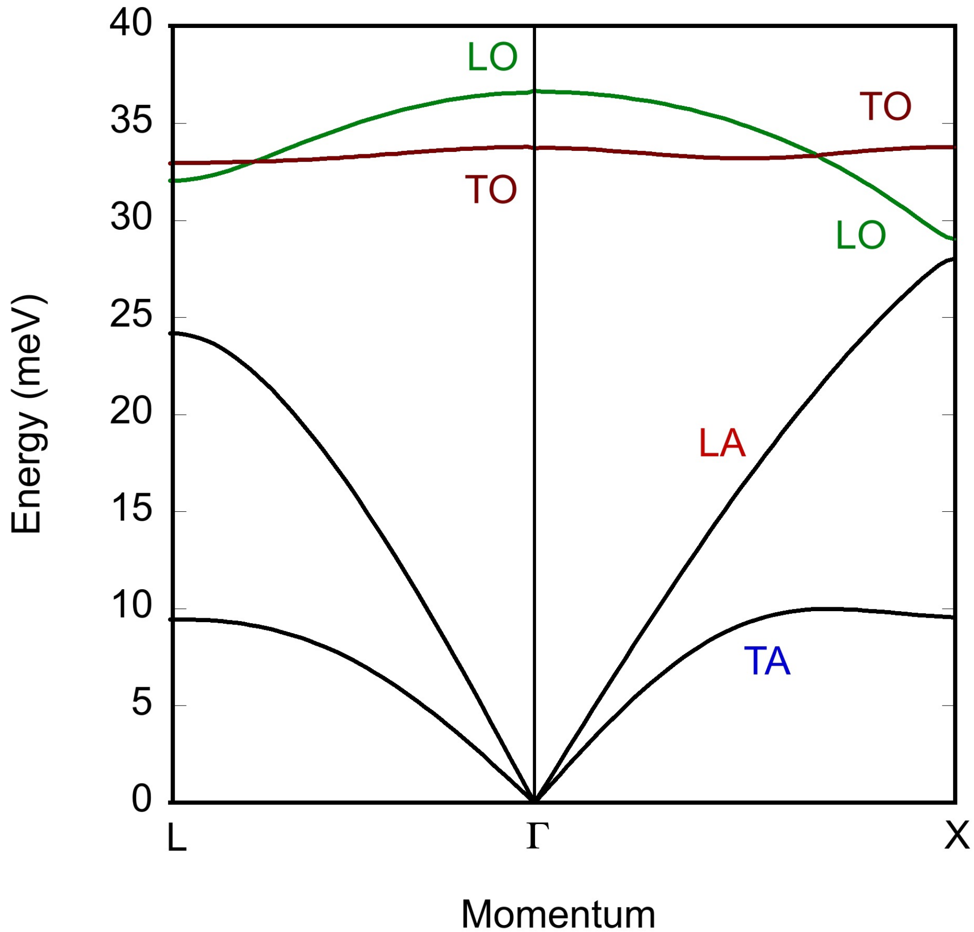
Considering Polar-Optical Modes

- This is a little more problematic—the polar modes are Coulomb fields and may entail long-range correlations; normally requiring two- and three-particle GFs and the Bethe-Salpeter equation for the latter

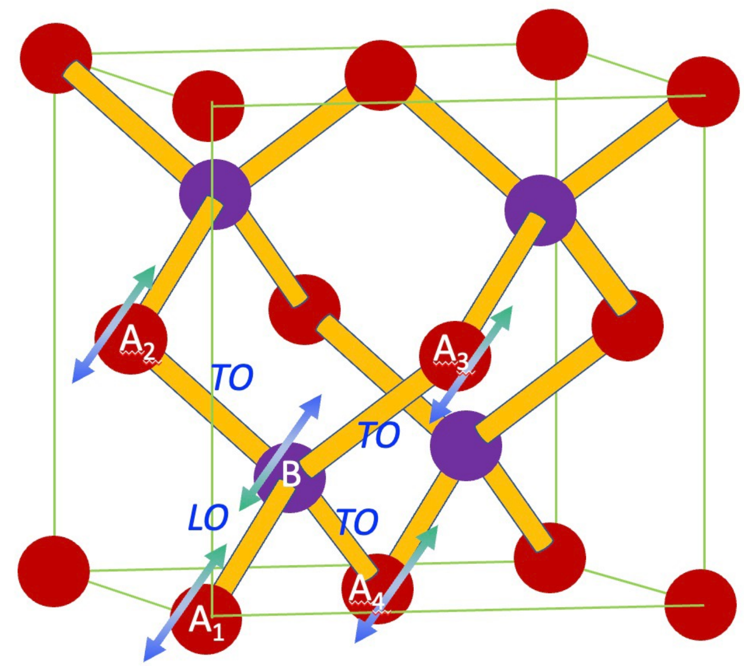
- On the other hand, optical mode scattering has "always" been assumed to be *phase-breaking*, which means the correlations would be broken up by the energy gain/loss in the scattering process.

- We don't know whether this is true, as it has to be evaluated best in real space (see poster on this topic), but we assume it to be true here.

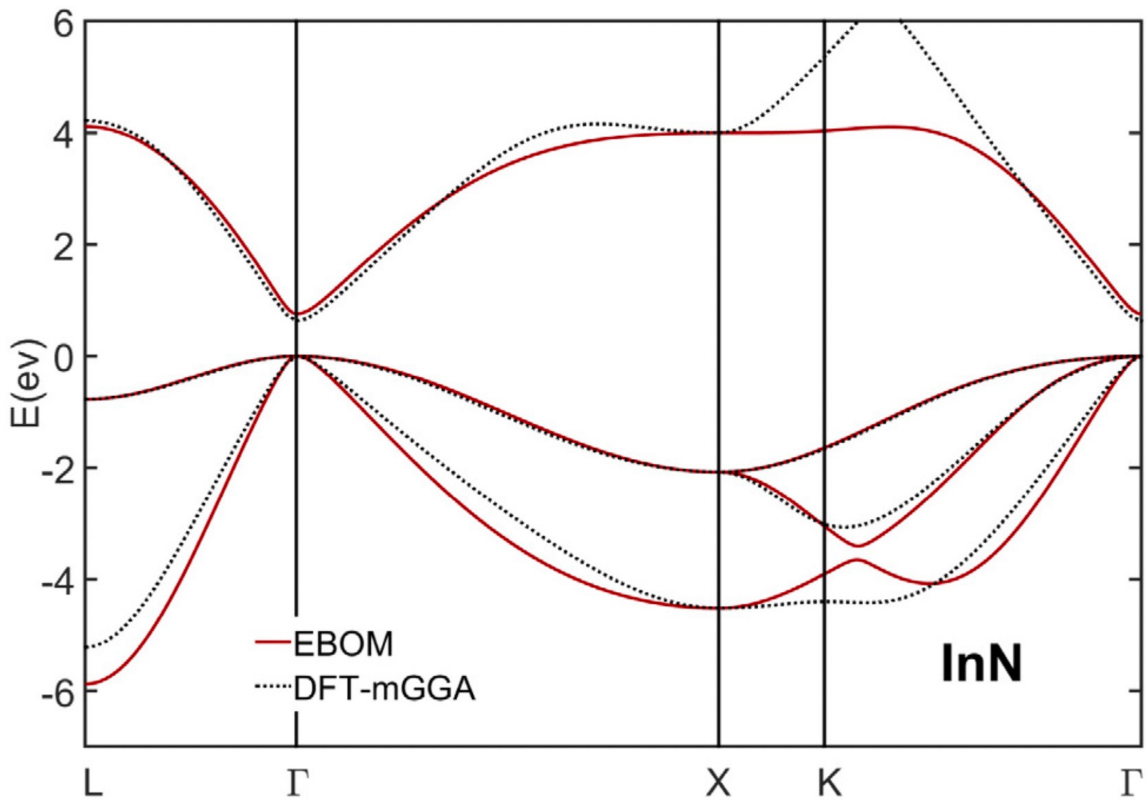
Phonon spectrum of III-V ZB



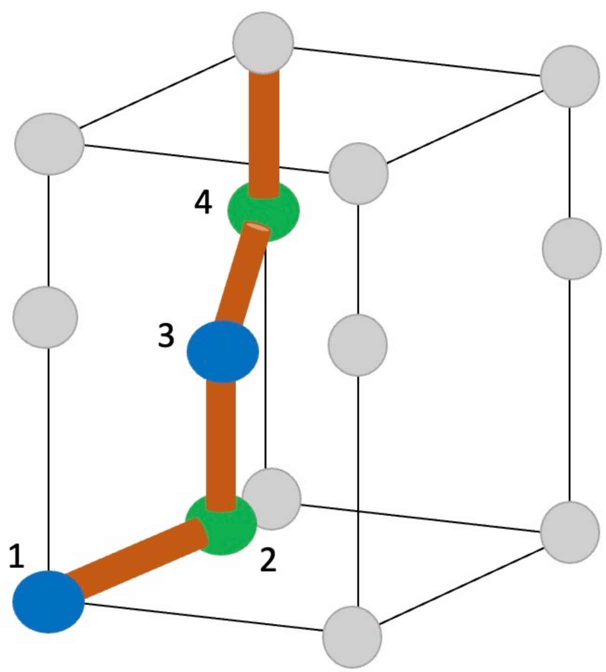
Phonon Motion of III-V ZB



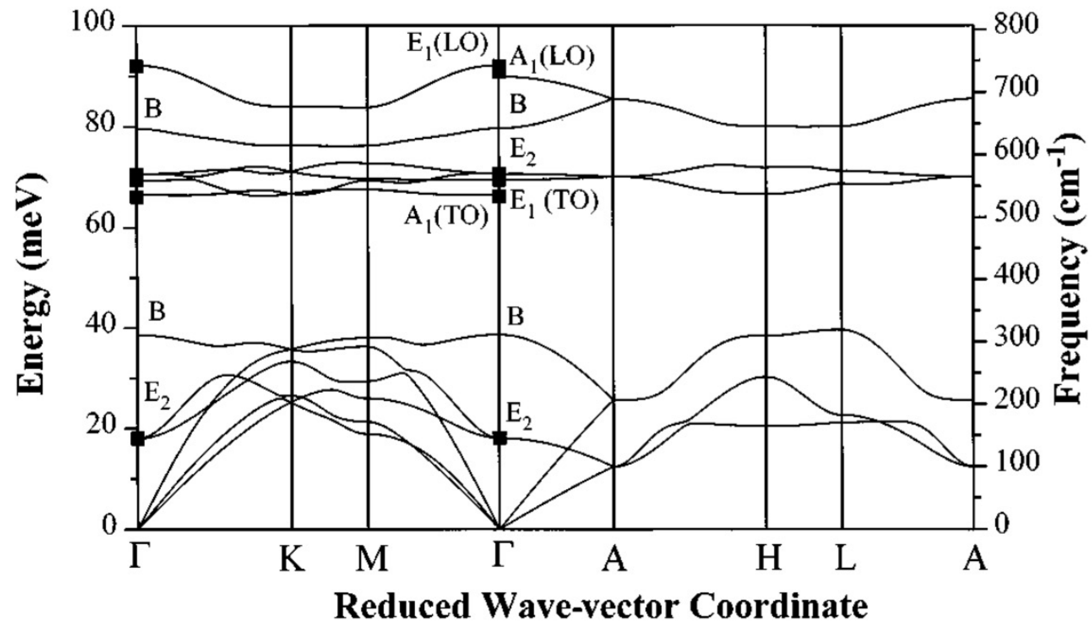
Band Structure of InN from two different approaches



Indium Nitride

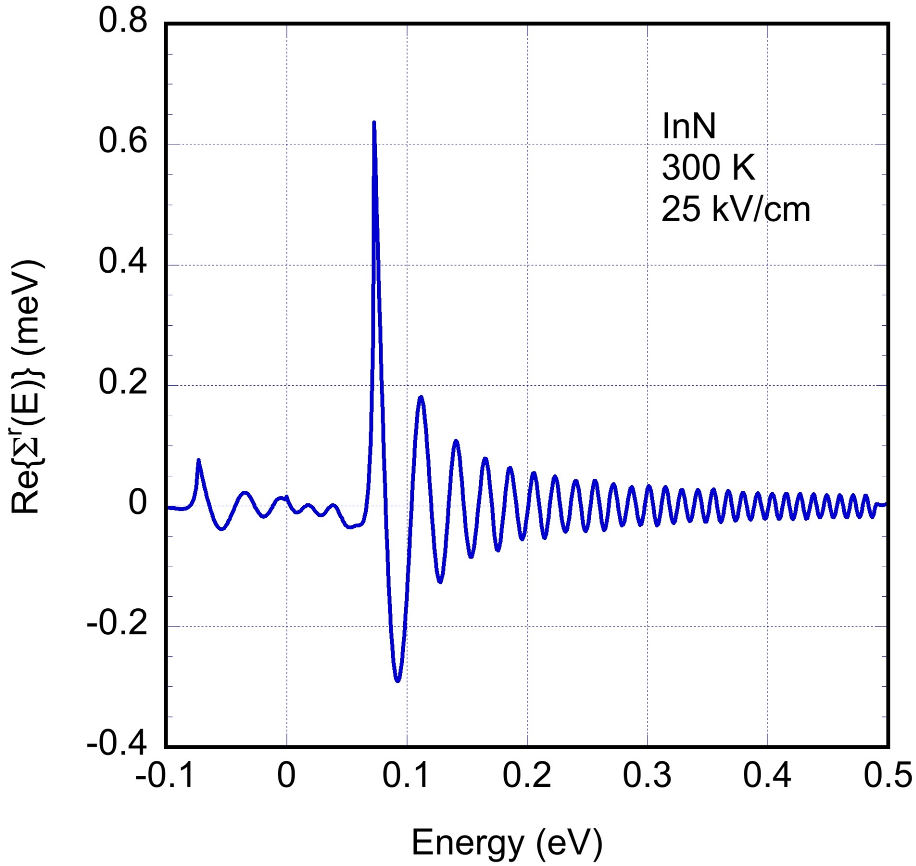


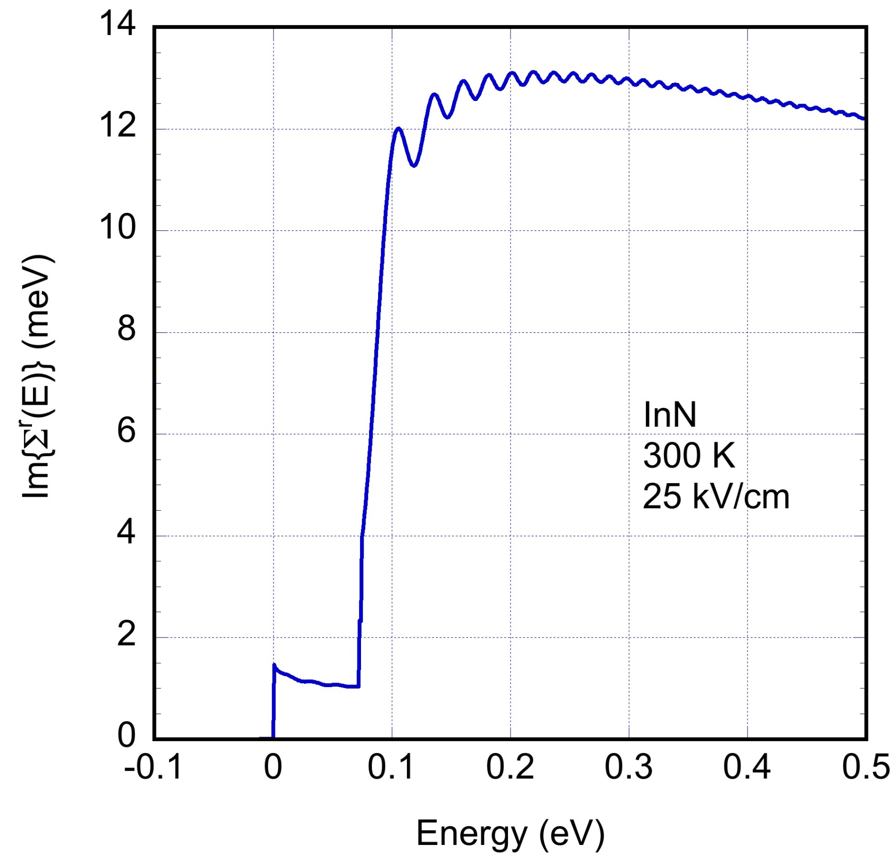
Wurtzite unit cell

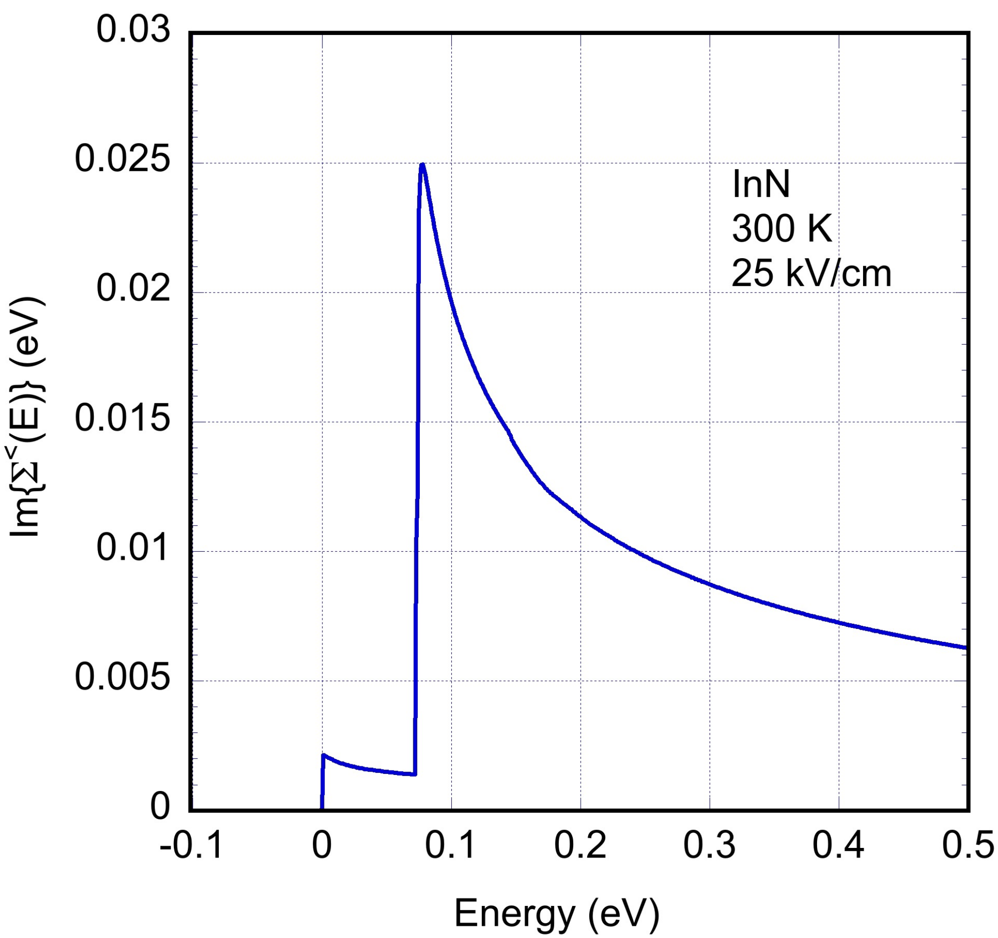


Wurtzite phonon spectrum

Retarded Self-Energy for InN



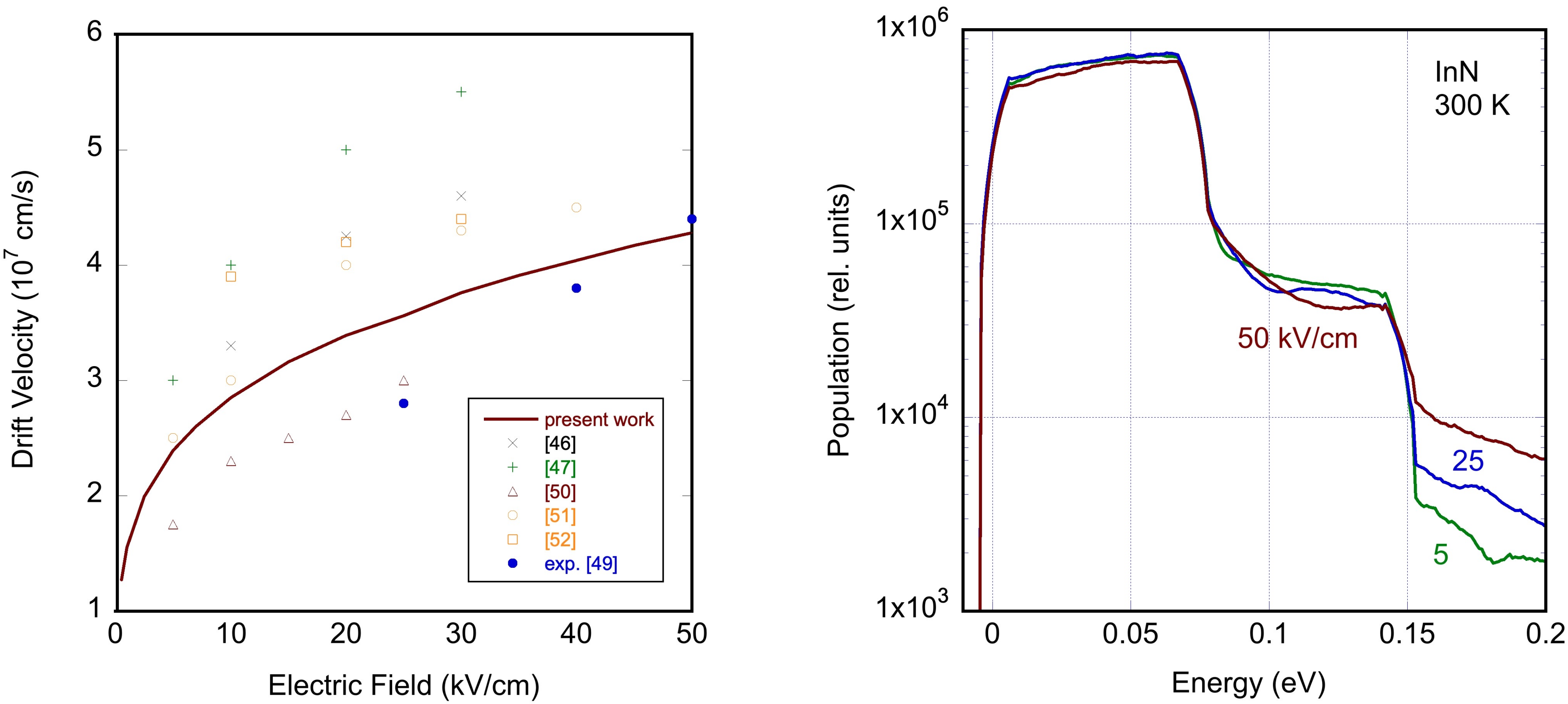




Imaginary part of the less-than self-energy for InN, arising from two polar optical modes (A_1 and E_1) and the acoustic mode.

The large decrease is a result of the nature of POP in quasi-two-dimensions (normally seen in semi-classical approaches)

EMC Results for InN



Summary

- In conclusion, it appears that we have a particle approach that makes NEGF more usable for modeling
- There is no reason this cannot be extended to full-band MC
- A point of significant interest is that determining G^r, A, $\Sigma^<$, $G^<$, and f requires < 2.0 s per field point on my MacBook Pro with the M1 pro chip (this machine). That is a major advantage!

For further information and details:

D. K. Ferry, Semicond. Sci. Technol. ***38*** *055005 (2023)*

D. K. Ferry, Semicond. Sci. Technol. ***38*** *075001 (2023)*

Coming soon, to a bookstore near you:

D. K. Ferry, X. Oriols, and J. Weinbub, Quantum Transport in Semiconductor Devices: Simulation with Particles (IOP Publishing, in press)