FERMI’S GOLDEN RULE IN THE
SCHRÖDINGER AND WIGNER
PICTURE
INTRODUCTION

Particle trajectories are not only bent by the presence of the crystal. They are changed by collisions with the vibrating crystal lattice.

In these collisions energy between the particles and the lattice is exchanged.

This is modeled by the creation and destruction of pseudo particles (phonons).

In crystals this is by far the most important collision mechanism (more frequent than particle - particle collisions).

The energy exchange is governed by Fermi’s Golden Rule, stating that the amount of particle energy gained / lost in the process is given by the dominant frequency of the lattice.
The exact description of phonon collisions is given by an infinite system of many body Schrödinger for a non-constant number of particles.

The Fermi Golden Rule can be derived (not rigorously) from a long time average of this system.


OVERVIEW

FGR electron - phonon scattering in a crystal.

Discrepancy to experiment, the intra - collisional field effect.

Derivation of the FGR from the Fock - space many body picture.

Infinite collision times; the Levinson and the Barker - Ferry equation.

Local time asymptotics → first order corrections to the FGR.

Numerical results.
FERMI’S GOLDEN RULE (FGR)

Models the interaction of electrons with vibrations of the crystal lattice (pseudo-particles, phonons)

$$\partial_t f(p,t) = Q[f](p,t)$$

$$= \int [S(p,p')f(p',t) - S(p',p)f(p,t)]dp'$$

$f(p,t)$: density of electrons with momentum $p$,

$S(p,p')$: scattering cross section; FGR states specified amount / loss of energy in scattering event

$$S(p,p') = \sum_{\nu=\pm 1} s_\nu(p, p') \delta(\varepsilon(p) - \varepsilon(p') + \nu\hbar\Omega)$$

$\varepsilon(p)$: energy corresponding to momentum $p$;

$\Omega$: dominant eigen-frequency of the phonon lattice.

Derived from a joint density $f_{ep}(p, q, t)$ for electrons with momentum $p$ and phonons with momentum $q$ under some equilibrium assumptions on the phonons.
COLLISIONAL BROADENING

Experiment: Apply electric field to a piece of bulk silicon.

Switch it off instantenously: FGR predicts time constants (relaxation times).

Keep it constant: FGR predicts steady state.

\[ E \cdot \nabla_p f = Q[f] \]

For large fields and small scales both predictions are not quite correct.

Problem: Collisions in FGR are instantenous; quantum mechanics \( \Rightarrow \) collisions take a finite time.
The spatially inhomogeneous case, the Boltzmann equation:

\[ \partial_t f + \nabla_p \varepsilon \cdot \nabla_x f - \nabla_x V \cdot \nabla_p f = Q[f] \]

Remark: Extremely difficult to observe experimentally; argument about relevance
The semi-classical Boltzmann equation

$$\partial_t f_c(x,k,t) + [V(x) + \epsilon(k), f_c]_c = Q^{FGR}[f_c]$$

The quantum Boltzmann equation for the Wigner function

$$\partial_t f(x,k,t) + [V(x) + \epsilon(k), f]_w = Q[f]$$

Quantum phonon operator $Q$ non-local in $x,k,t$. 
DERIVATION OF THE FGR

The Fock-space Schrödinger equation:

$$\psi_m(r, k_1, \ldots, k_m, t)$$

$\psi_m$: wave function for one electron with position $r$ and $m$ phonons with wave vectors $k_1, \ldots, k_m$

$$i\hbar\partial_t \psi = \mathcal{H}\psi, \quad \psi = (\psi_0, \psi_1, \ldots)$$

$$i\hbar\partial_t \psi_m = (\mathcal{H}\psi)_m := H^e\psi_m + H^p\psi_m + \sum_n H^{ep}_{mn}\psi_n$$

$\mathcal{H}$: Fröhlich Hamiltonian

$H^e$: Free particle.

$H^p$: Free phonon.

$H^{ep}_{mn}$ Interaction of electron with phonon (generation, destruction).
Hamiltonians

Free electron Hamiltonian, acts only on $r$; $V$: mean field potential

$$H^e = \varepsilon(-i \nabla_r) + V(r), \quad \mathcal{E}(r, k) = \frac{\hbar^2}{2m}|k|^2 + V(r)$$

Free phonon Hamiltonian (acts only on $k^m = (k_1, .., k_m)$

$$H^p \psi_m(r, k^m) = \int H^p(k^m, s^m) \psi_m(r, s^m) ds^m$$

$H^e$ and $H^p$ are diagonal elements in the Fröhlich Hamiltonian $\mathcal{H}$
Electron phonon interaction Hamiltonian

\[ H_{mn}^{ep} = H_{mn}^{ep+} + H_{mn}^{ep-} \]

Creation of a phonon:

\[ H_{mn}^{ep+} \psi_n(r, k^m) = \delta_{m-n-1} \hbar \sum_{l=1}^{m} F(k_l) e^{ir \cdot k_l} \psi_n(r, k^m_{l-}) \]

\[ k^m_{l-} = (k_1, \ldots, k_{l-1}, k_{l+1}, \ldots, k_m) \]

Destruction of a phonon: \( \mathcal{H} \) self adjoint

\[ \sum_{m=0}^{\infty} \int \phi_m(r, k^m) \psi_m(r, k^m) * (\mathcal{H} \Psi)_m(r, k^m) dr dk^m \]

\[ = \sum_{m=0}^{\infty} \int \psi_m(r, k^m) \psi_m(r, k^m) * (\mathcal{H} \Phi)_m(r, k^m) dr dk^m \]
$H_{mn}^{ep-}$ is the adjoint of $H_{n}^{ep+}$

$$H_{mn}^{ep-} \psi_n(r, k^m) = \delta_{m-n+1} \hbar \sum_{l=1}^{n} \int F(s)^* e^{-ir \cdot s} \psi_n(r, k^m_{l+}(s)) ds$$

$k^m_{l+}(s) = (k_1, .., k_{l-1}, s, k_l, .., k_m)$
THE PHONON TRACE

The density matrix corresponding to $\Psi$

$$\rho_{mn}(r, k^m, r', k'^n) = \psi_m(r, k^m)^* \psi_n(r', k'^n)$$

Find equation for phonon trace:

$$(Tr_p \rho)(r, r') = \sum_{m=0}^{\infty} \int \rho_{mm}(r, k^m, r', k^m)dk^m$$

using asymptotics $\rightarrow$ quantum Boltzmann equation for single electron density matrix.
Time Reversibility

PROBLEM:
Quantum mechanics is time reversible

\[ G(\Psi)_m(r, k^m, t) = \psi_m(r, -k^m, -t)^* \]

\[ G(i\hbar \partial_t \Psi) = i\hbar \partial_t G\Psi, \quad G(H\Psi) = H G(\Psi) \]

⇒ know \( \Psi(t = T) \); solve same equation backward in time to compute \( \Psi(t = 0) \).

FGR not time reversible; loss of information by building the phonon trace.
APPROACHES

1. Start from simplified physical model; phonons as bath of harmonic oscillators (Caldeira, Legget); mathematical justification incomplete (Erdos); derive quantum Fokker-Planck operator (Arnold, Markowich)

2. Start with randomized interaction potential (Papanicolao, Shi Jin et al); derive FGR; weak theory.

3. Direct weak e-p interaction asymptotics (Levinson, Argyres, Barker & Ferry); mathematical justification incomplete (Frommlet, Markowich & Ringhofer); arrive at Levinson (Barker - Ferry) equation → FGR.

4. Direct weak e-p interaction asymptotics theory complete; arrive at Pauli master equation (Castella, Degond)
WEAK ELECTRON - PHONON INTERACTIONS

\[ i\hbar \partial_t \rho_{mn} - [H^e + H^p, \rho_{mn}] = \]

\[ H_{m,m-1}^{ep} \rho_{m-1,n} + H_{m,m+1}^{ep} \rho_{m+1,n} \]

\[ -\rho_{m,n-1} H_{n-1,n}^{ep} - \rho_{m,n+1} H_{n+1,n}^{ep} \]

Notation:

\[ \partial_t \rho_{mn} - A \rho_{mn} = (B \rho)_{mn} \]

A diagonal in \( m, n \), \( \Rightarrow \) commutes with taking the phonon trace

\[ \sum_{m=0}^{\infty} \int (A \rho)_{mm} dk^m = [H^e, (Tr_p \rho)] \]

\( \rightarrow \) free streaming operator acting on \( Tr_p \rho \)
Fixed point argument:
Assume $B$ small and iterate, $S_A(t)$ semigroup operator

$$\rho^{j+1} = S_A(t)(\rho^I) + \int_0^t S_A(t - \tau)(B\rho^j)(\tau)d\tau,$$

$$j = 0, 1, ...$$

Not rigorous:

Formulate in Wigner picture and assume classical transport operator.

Assume parabolic bands.

Corresponds to assuming quadratic potentials.

Use characteristics.
THE LEVINSON (BARKER-FERRY) EQUATION

Formulated in terms of the Wigner function (classical equivalent to the density function in the Boltzmann equation)

$$f(x, k, t) = \int Tr_p \rho(x - \frac{1}{2}y, x + \frac{1}{2}y, t) e^{iy \cdot k} dy$$

**Remark:** Since we iterated the semigroup operator the L-B-F equation will be non-local in time.

$$\partial_t f(x, k, t) + [\varepsilon + V, f]_w =$$

$$\int_0^t dt' \int dk' [S(k, k', t - t') f(x, k', t') - S(k', k, t - t') f(x, k, t')]$$

**Remark:** The semigroup operator is expressed in terms of tracing back characteristics in the Wigner picture. (Only true for linear potentials $V$.)
The scattering cross section

Write everything in terms of momentum \( p = \hbar k \)

\[
S(p, p', t) = \sum_{\nu=\pm1} a_{\nu} \cos \left[ \frac{1}{\hbar} \int_0^t \left( \varepsilon(q(p, \tau)) - \varepsilon(q(p', \tau)) + \nu \hbar \Omega \right) d\tau \right]
\]

\[
q(k, \tau) := p - \tau \nabla_x V, \quad \varepsilon(p) = \frac{|p|^2}{2m}
\]

\( \Omega \): eigen-frequency of the lattice

**Remark:** The collisions are never completed! The integral kernel is highly oscillatory for \( \hbar \rightarrow 0 \).

The zero field case \((V = const)\)

\[
S(p, p', t) = \sum_{\nu = \pm 1} a_{\nu} \cos \left[ \frac{t}{\hbar} (\varepsilon(p) - \varepsilon(p') + \nu \hbar \omega) \right]
\]
THE SPATIALLY HOMOGENEOUS ZERO - FIELD LEVINSON EQUATION

Scaling and dimensionless formulation:

\[ \varepsilon(p_0) = KT, \quad t_0 = \frac{1}{\Omega\lambda}, \quad \lambda = O(\hbar) \]

\[ \partial_t f(p, t) = Q_\lambda[f](p, t) = \int_0^t dt' \int dp' \times \]

\[ \frac{1}{\lambda} [S(p, p', \frac{t-t'}{\lambda}) f(p', t') - S(p', p, \frac{t-t'}{\lambda}) f(p, t')] \]

dimensionless cross section

\[ S(p, p', t) = \sum_{\nu = \pm 1} a_\nu \cos[t(\varepsilon(p) - \varepsilon(p') + \nu\Omega)] \]

\[ a_\nu = O(1) \text{ and } \Omega \text{ (scaled emission energy)} = O(1). \]
FERMI’S GOLDEN RULE - A HEURISTIC ARGUMENT

\[ Q_\lambda[f](p, t) = \int_0^t dt' \int dp' \times \]
\[ \frac{1}{\lambda} \left[ S(p, p', \frac{t-t'}{\lambda}) f(p', t') - S(p', p, \frac{t-t'}{\lambda}) f(p, t') \right] \]

Assume: \( \lim_{t \to \infty} S(p, p', t) = 0 \)

\[ Q_\lambda[f](p, t) \to \int dp' \left[ S_0(p, p') f(p', t) - S_0(p', p) f(p, t) \right] \]

\[ S_0(p, p') = \int_0^\infty S(p, p', t) dt \]
cross section:

\[ S(p, p', t) = \sum_{\nu = \pm 1} a_{\nu} \cos[t(\varepsilon(p) - \varepsilon(p') + \nu\Omega)] \]

\[ \int_{0}^{\infty} \cos(zt) \, dt = \delta(z) \] yields FGR.

Since \( \lim_{t \to \infty} S(p, p', t) \neq 0 \) this becomes a weak limit.
THEOREM 1

Define the functional

\[ Y_\lambda(\phi, f) = \int_0^\infty dt \int dp \{ \phi(p, t) Q_\lambda[f](p, t) \} \]

for smooth, compactly supported test functions \( \phi \). Then

\[ \lim_{\lambda \to 0} Y_\lambda(\phi, f) = \int_0^\infty dt \int dp \{ \phi(p, t) Q_0[f](p, t) \} \]

holds for fixed \( \phi \) with

\[ S_0(p, p') = \sum_{\nu = \pm 1} a_\nu \delta(\varepsilon(p) - \varepsilon(p') + \nu \Omega) \]
THEOREM 2
(first order perturbation)

\[ Y_\lambda(\phi, f) = \int_0^\infty dt \int dp \{ \phi(p,t)(Q_0[f] + \lambda Q_1[\partial_t f])(p,t) \} + o(\lambda) \]

Remark:

- \( Q_1 \) acts on \( \partial_t f \) (non-local in time);
- \( Q_1 \) only defined weakly in \( p \).
Weak formulation of $Q_1[\partial_t f]$: 

$$
\int \phi(p)Q_1[\partial_t f](p)dp = 
$$

$$
- \sum_{\nu=\pm 1} a_{\nu} \int \int \ln(|\varepsilon - \varepsilon' + \nu \Omega|) \frac{d}{d\varepsilon} \frac{d}{d\varepsilon'}[(\phi' - \phi)\partial_t f]dpdp'
$$

$\frac{d}{d\varepsilon}$: directional derivative perpendicular to surfaces of equal energy.

Corresponds (formally) to a first order scattering cross section

$$
S = S_0 + \lambda S_1
$$

$$
S_0(p, p') = \sum_{\nu=\pm 1} a_{\nu} \delta(\varepsilon(p) - \varepsilon(p') + \nu \Omega)
$$

$$
S_1(p, p', \partial_t) = \sum_{\nu=\pm 1} \frac{a_{\nu}}{(\varepsilon(p) - \varepsilon(p') + \nu \Omega)^2} \partial_t
$$
REMARK: Parabolic bands $\varepsilon(p) = \frac{|p|^2}{2}$: polar coordinates and radial derivatives
NUMERICAL VERIFICATION

THEOREM 3: Let $\Gamma$ be a time-direction smoothing operator

$$(\Gamma f)(t) = \int_{0}^{\infty} \gamma(t-t')f(t')dt'.$$

Then

$$\Gamma Q_\lambda[f] = Q_0(\Gamma f) + \lambda Q_1[\Gamma \partial_t f] + o(\lambda)$$

everywhere weakly in $t$ weakly in $p$. 

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Computations

- Parabolic bands $\varepsilon = \frac{|p|^2}{2m}$

- $a_n = \text{const}$: $\delta$– function interaction potential

- Symmetry: $f(p, t) = f(\varepsilon(p), t)$

- Compare smoothed energies: $\int \varepsilon \Gamma Q_\lambda[f] dp$
FIGURE 1
FIGURE 4

- $K^*Q_f$
- $Q_f[K^*\gamma]$
- $Q_{fg}[K^*\gamma]$
FIGURE 5

- \( K^* Q[f] \)
- \( Q_f[K^*] \)
- \( Q_{fg}[K^*] \)

(time vs. energy)
SOLVING THE LEVINSON EQUATION

\[ \partial_t f_\lambda = Q_\lambda[f_\lambda] \]

\[ \partial_t f_{01} = Q_0[f_{01}] + \lambda Q_1[\partial_t f_{01}] \]

REMARK:

- \( f_\lambda \rightarrow f_{01} \) not covered by the theory.

- Extremely difficult to solve; implicit; \( Q_1 \) singular integral kernel
Example:

\[ \partial_t f_{01} = Q_0[f_{01}] + \lambda Q_1[Q_0[f_{01}]] \]

yields an ill posed equation.

Solve for expansion terms directly.

\[ f_{01} = f_0 + \lambda f_1 \]

\[ \partial_t f_0 = Q_0[f_0] \]

\[ \partial_t f_1 = Q_0[f_1] + Q_1[\partial_t f_0] = Q_0[f_1] + Q_1[Q_0[f_0]] \]
FIGURE 7

(time (ps))

(energy (meV))
FIGURE 8

energy (meV)
time (ps)
f filtered
FIGURE 9

Energy (meV) vs. Time (ps)

$f_0 + \lambda f_1$
CONCLUSIONS

- The first order correction produces a significant change in the transient behavior.

- This can explain collisional broadening in actual devices.

Open Problems

- The non-zero field case (→ the intra - collisional field effect).

- Numerics for non - radially symmetric solutions (→ MC).

- How to solve the first order approximation using weighted particle methods.