Formation of Bloch and Plasma Oscillations

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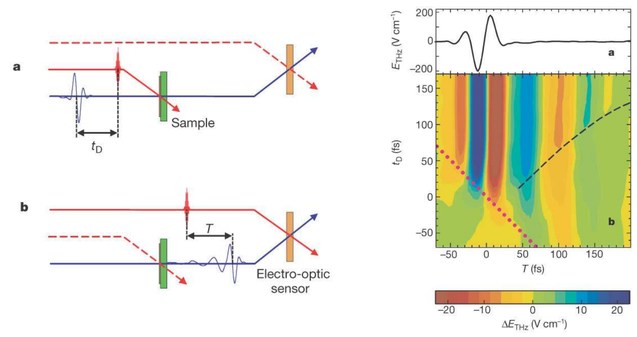
MAX-PLANCK-GESELLSCHAFT

Femtosecond laser irradiation



pump pulse creating charge carriers at time t_0

probe pulse at time t_D later

A. Leitenstorfer, Nature 426(2003)23, R. Huber et al. Nature 414(2001)286

Time and frequency–dependent dynamical response

$$\frac{1}{\epsilon(\omega,t)} = 1 + \frac{e^2}{\epsilon_0 q^2}\int_0^{t-t_0} dT e^{i\omega T}\chi(t,t-T)$$

time delay after probe pulse $T = t - t_D - t_0$

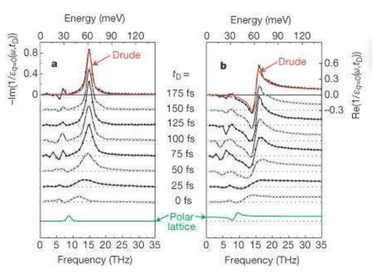
Fourier transformed into frequency

Quantum kinetic equations:

Gartner et al. PRB 66(2002) 075205

Vu and Haug PRB62 (2000) 7179

Kira and Koch PRL 93 (2004) 076402



Solution of meanfield equation

- Linearize kinetic equation to obtain density response $\delta n(q,t) = \int_{t_0}^{t} dt' \chi(t,t') V_q^{\rm ext}(t')$
- one-particle reduced density matrix $\hat\rho$ obeys

$$\dot{\hat\rho} + i[\hat{\mathcal{E}} + \hat V^{\rm ind} + \hat V^{\rm ext}, \hat\rho] = \frac{\hat\rho^{\rm l.e.} - \hat\rho}{\tau}$$

- local equilibrium density matrix $\hat\rho^{\rm l.e.}$ deviates by chemical potential linked to $\delta n(q,t)$ by density conservation
- linearization leads to

$$\chi(t,t') = \Pi(t,t') + \int_{t'}^{t} d\bar t \left[\Pi(t,\bar t)\frac{e^2}{\epsilon_0 q^2} + I(t,\bar t)\right]\chi(\bar t, t')$$

- large-time limit $t + t' \to \infty$ approaches familiar form $\chi = \frac{\Pi^{\rm M}}{1 - \frac{e^2}{\epsilon_0 q^2}\Pi^{\rm M}}$ with Mermin-Das polarization (Mermin PRB 1 (1970) 2362)

Solution of transient time response by one-sided Fourier transform

$$\frac{1}{\epsilon(\omega,t)} = 1 + \frac{e^2}{\epsilon_0 q^2}\int_0^{t-t_0} dT e^{i\omega T}\chi(t,t-T)$$

- limit of long wave lengths $q \to 0$

appreciable simplification $\Pi(t,t') \approx \frac{q^2 n(t')}{m}(t'-t)e^{\frac{t'-t}{\tau}}$ and $I(t,t') \approx \frac{1}{\tau}e^{\frac{t'-t}{\tau}}$

- integral equation into differential one with $n(t) \approx n_0\Theta(t-t_0)$
- Analytic solution K. Morawetz, P. Lipavský, M. Schreiber, Phys. Rev. B 72 (2005) 233203

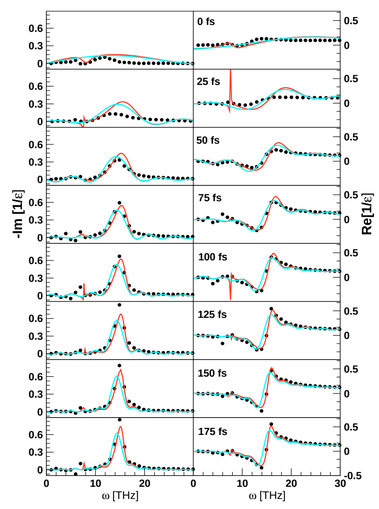
$$\frac{1}{\epsilon(\omega,t)} = 1 - \frac{\omega_p^2}{\sqrt{\omega_p^2 - \frac{1}{4\tau^2}}}\int_0^{t-t_0} dt'\, e^{(i\omega - \frac{1}{2\tau})t'} \sin\left(\sqrt{\omega_p^2 - \frac{1}{4\tau^2}}\, t'\right)$$

Achievement:

long-time limit yields the Drude formula $\lim_{t\to\infty}\frac{1}{\epsilon} = 1 - \frac{\omega_p^2}{\omega_p^2 - \omega(\omega + \frac{i}{\tau})}$

This limit is not so easy to achieve within short-time expansions, e.g. approximate result [ElSayed et al, PRB 49 (1994) 7337] gives $1 - \frac{\omega_p^2}{\omega_p^2 - (\omega + i/\tau)^2}$.

Comparison with experiment



GaAs

Resonance about 8 THz due to optical phonons, adding intrinsic contribution of crystal lattice

$$\epsilon_{\rm GaAs} = \epsilon_\infty\left(\epsilon + \frac{\omega_{\rm LO}^2 - \omega_{\rm TO}^2}{\omega_{\rm TO}^2 - \omega^2 - i\gamma\omega}\right)$$

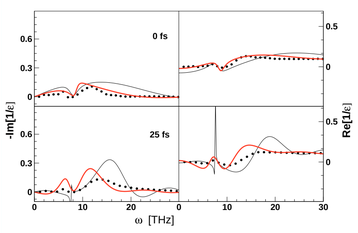
$\frac{\omega_{\rm LO}}{2\pi} = 8.8$ THz, $\frac{\omega_{\rm TO}}{2\pi} = 8.1$ THz lattice damping γ =0.2 ps^{-1} and background polarizability of ion lattice $\epsilon_\infty = 11.0$

Huber et al, phys.stat.sol.(b) 234 (2002) 207

pumb pulse at $t_0 = -40$fs, probe pulse full-width at half-maximum $27fs$, plasma frequency ω_p =14.4 THz, relaxation time $\tau = 85$ fs

Improvement by realistic shape

- too fast build-up of the collective mode at the time $t = 25$ fs
- just the time duration of the experimental pulse
- we have approximated this by the instant jump
- more realistic smooth populating can be modeled by an arctan-function and numerical solution improves the description



First two time evolution steps comparing an instant population of conduction band with a smooth transition.

Hybridization of plasma and Bloch oscillations

Electrons in periodic potential under electric field E show Bloch [Z. Phys. 52 (1928) 555] oscillations given by period of lattice d $\omega_B = \frac{eEd}{\hbar}$, experimentally observed K. Leo, Semicond. Sci. Technol. 13 (1998) 249 .

Question: How do Bloch oscillation and plasma oscillation influence each other and how do they forme time-dependently

Polarization: $\Pi(t,t') = [\frac{nq^2}{m} + o(q^4)]e^{\frac{t'-t}{\tau} - i\frac{\Omega_q^2}{2}(t'-t)^2}$

Mermin correction:$I(t,t') = [\frac{1}{\tau} + o(q^2)]e^{\frac{t'-t}{\tau} - i\frac{\Omega_q^2}{2}(t'-t)^2}$

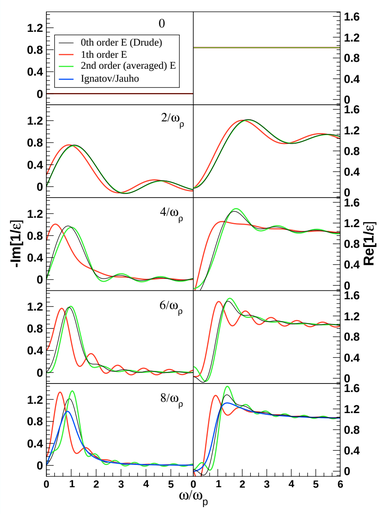
with field and wave vector dependence

$$\Omega_q^2 = \frac{e\mathbf{Eq}}{m\hbar} = \omega_B\omega_p\frac{q_{||}v_0}{\hbar\omega_p}$$

plasma frequency: $\omega_p^2 = 4\pi e^2 n/T$, maximal electron velocity: $v_0 = \hbar/md$

If electrons in resonance with plasma frequency, $q_{||}v_0 \to \hbar\omega_p$

Results



Time evolution of response function

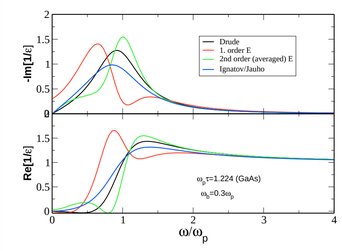
Large times (equilibrium):

$$\epsilon(\omega,\infty) = 1 - \frac{\omega_p^2}{\omega(\omega + \frac{i}{\tau})}\left[1 + i\Omega_q^2\frac{3\omega + \frac{i}{\tau}}{\omega(\omega + \frac{i}{\tau})^2} + \Omega_q^4\frac{\frac{1}{\tau^2} - i\frac{6}{\tau}\omega - 15\omega^2}{\omega^2(\omega + \frac{i}{\tau})^4}\right] + \mathcal{O}(\Omega_q^6) + \mathcal{O}(q^2)$$

No collisions $\tau \to \infty$ linear field effect reported in K. Morawetz, A. P. Jauho, Phys. Rev. E 50 (1994) 474

Resonant waves compare with: A. A. Ignatov, A. P. Jauho, J. Appl. Phys. 85 (1999) 3643, Y. A. Kosevich, Phys. Rev. B 63 (2001) 205313

Comparison with equilibrium



Response function for large times compared with the Drude response and Ignatov/Jauho result

$$\epsilon_{\rm IJ}(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega + \frac{i}{\tau})}\left[1 - \omega_b^2\frac{\omega^2\tau^2 + 3i\omega\tau - 3}{(\omega + \frac{i}{\tau})^2}\right] + \mathcal{O}(\omega_b^4)$$

If no mean-fields ? → Levinson equation

Time diagonal part of Kadanoff/Baym equation $\Delta_E = \frac{k^2 + p^2 - (k-q)^2 - (p+q)^2}{2m}$

$$\frac{\partial\rho_k}{\partial t} = \frac{2}{\hbar^2}\sum_{pq} V_q^2 \int_0^t d\bar t \cos\left\{\frac{t-\bar t}{\hbar}\Delta_E\right\}\left(\rho'_{k-q}\rho'_{p+q}(1-\rho_p)(1-\rho_k) - \rho_p\rho_k(1-\rho'_{k-q})(1-\rho'_{p+q})\right)_{\bar t}$$

time-dependent Fermi's Golden Rule and memory effects

Properties:

- density conservation $\frac{\partial}{\partial t}n = 0$ • momentum conservation $\frac{\partial}{\partial t}\langle p_1\rangle = 0$
- Time variation of kinetic energy $\frac{\partial}{\partial t}(\langle\frac{p_1^2}{2m}\rangle + \langle V_{12}\rangle) \equiv 0$

Phys. Lett. A 199 (1995) 241 , Eur. Phys. J. A (1999) 291-305, Phys. Rev. C 64 (2001) 024613

The inclusion of memory effects produces the full energy conservation.

But, several effects hidden:

Off-shell tails in ρ, renormalization of scattering rates and wave function, quasiparticle energies, collision delays: Ann. Phys. (NY) 294 (2001) 135

Better: neglect memory effects, only time-dependent Fermi's Golden Rule: e.g. Maxwellian plasma [Phys. Lett. A 246 (1996) 311; Phys. Rev. E 63 (2001) 20102]

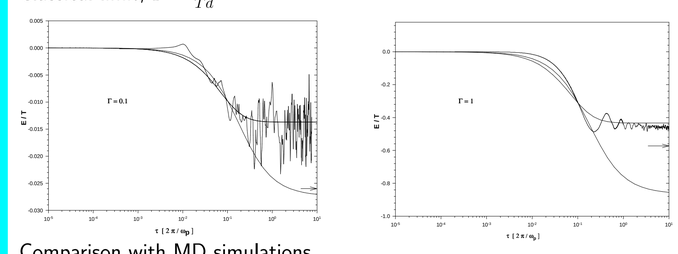
static Debye $z = \omega_p\sqrt{t^2 - it\frac{\hbar}{T}}$:

$$\dot E_{\rm corr}(t) = -\frac{e^2 n\kappa T}{2\hbar}{\rm Im}\left[(1 + 2z^2)e^{z^2}(1 - {\rm erf}(z)) - \frac{2z}{\sqrt{\pi}}\right]$$

dynamical screening $z_1 = \omega_p\sqrt{2t^2 - it\frac{\hbar}{T}}$:

$$\dot E_{\rm corr}^{\rm dynam}(t) = -\frac{e^2\kappa T}{\hbar}{\rm Im}\left[e^{z_1^2}(1 - {\rm erf}(z_1))\right]$$

Classical limit, $\Gamma = \frac{e^2}{Td}$



Comparison with MD simulations

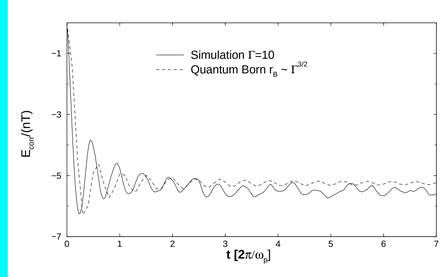
Dense classical plasma by quantum approximation

On a correspondence between classical and quantum particle systems, Phys. Rev. E 66 (2002) 022103

Quantum-Born [Eur. Phys. J. A (1997) 291]:

$$\frac{E_{\rm corr}^T(t) - E_{\rm corr}^0(t)}{nT} = \frac{1}{(36\pi^4)^{1/6}}\frac{r_s^3}{\Gamma}\left(\frac{\sin y\tau}{y\tau} - 1\right)\left(\frac{1}{b_l}\arctan(\frac{1}{b_l}) + \frac{1}{b_l^2 + b_l^4}\right)$$

Bruckner parameter $r_s = \frac{d}{a_B}$, $b_l = \frac{\hbar\kappa}{2p_f} = \sqrt{\Gamma}(48\pi^2)^{-1/6}$, time in plasma periods $\tau = \frac{2\pi}{\omega_p}t$ or $y\tau = 4\epsilon_f t/\hbar = (2)^{4/3}\pi^{5/3}3^{5/6}\tau/\sqrt{r_s}$



Simulation of dense classical plasma [G. Zwicknagel]

best fit ($\hbar \sim T$):

$$r_s^{\rm fit} = \frac{1}{2}\sqrt{\frac{3}{8}}\Gamma^{3/2}$$

$$\lambda^2 = \frac{d}{\kappa} = \frac{d^2}{(3\Gamma)^{1/2}} \approx d^2$$

Summary

- collisions have no time to happen yet (only mean-fields are formed)
- separate gross feature of the formation of collective modes at transient times which are due to mean-field fluctuations
- simple analytic formula for time dependence of the dielectric function
- hybridization of plasma and Bloch oscillations, formed on same time scale

But: relaxation time needed and what if no mean-fields (quasi-neutrality) ?

- Short time behavior by time-dependent Fermi's golden rule ≡ Finite duration approximation of non-Markovian collision integrals

  -low temperature value is universal; ratio $\sim \hbar/\epsilon_F$ (formation of quasi-particles), high temperature limit $\sim 1/\omega_p$

  -analytical results for dynamical screening, static screening leads to 1/2 correlation energy

  -good agreement with molecular dynamics

  -strong coupling by equivalence: N classical particles ↔ $N-1$ quantum particles