The Multiphysics Solution to Maxwell-Hydrodynamic Equations for Modeling Terahertz Generation from Plasmonic Metasurfaces

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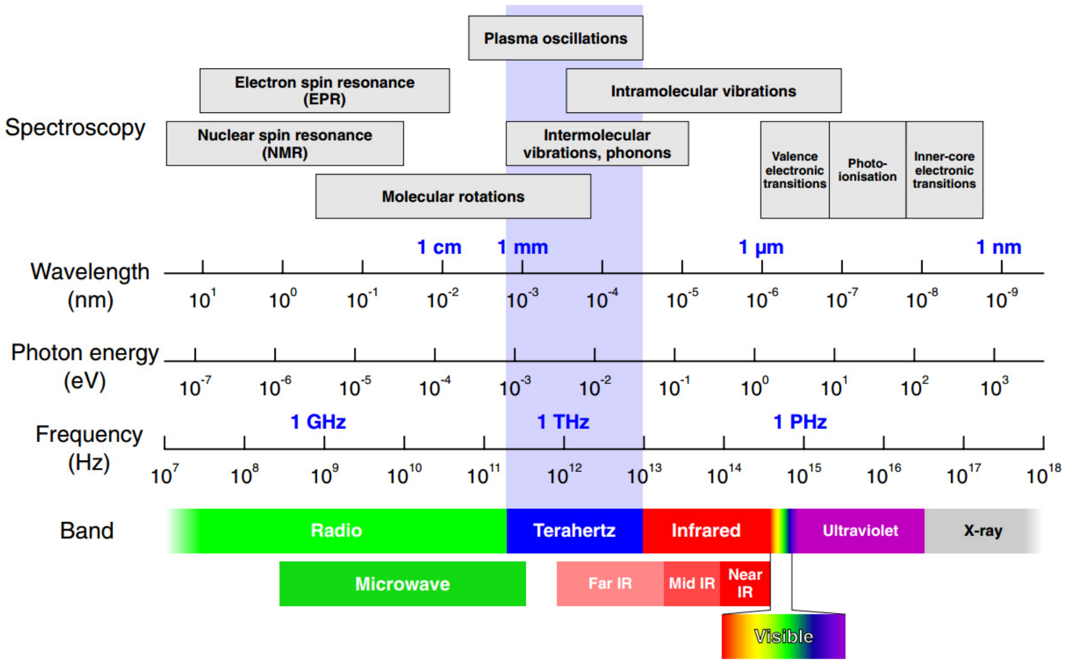
Outline

Broadband Terahertz (THz) Spectroscopy

‘THz gap’

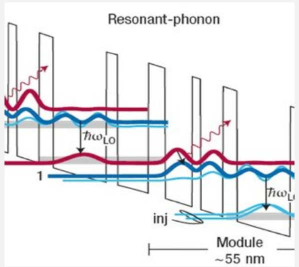
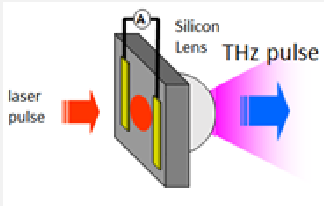
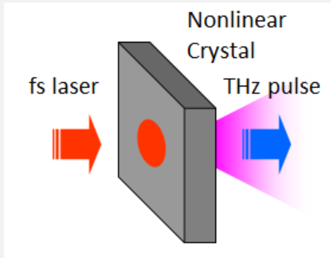
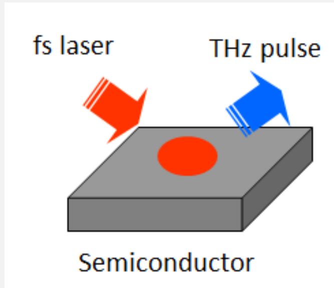
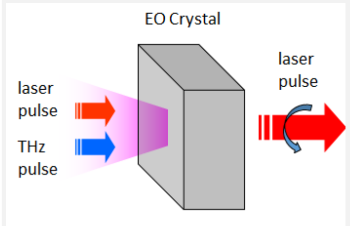


Overview of THz Sources and Detectors

	Generation	Detection
Electronic	• Microwave multiplier chain • Backward-wave oscillator • Gunn diode • Resonant tunnel diodes	• Schottky diode • Backward diode • Rectifying transistor (Tera-FET) **Thermal** • Bolometer, Golay cell, pyroelectric, thermopile
Laser	• Quantum cascade laser • p-type Germanium laser • Molecule gas laser • Free electron laser[1]	
Optical • femtosecond pulse • incoherent multi-mode • two-colour continuous-wave	• Photoconductive switch antenna/photomixer • Optical rectification • Surface emitter • Photo-induced plasma	• Photoconductive switch antenna/photomixer • Electro-optic sampling • Biased-air detection

Ref: W Zouaghi et al. *Eur. J. Phys.* 34: S179, 2013

Generation of THz Waves

Method	Quantum Cascade Laser	Photoconductive Antenna	Semiconductor	Optical Rectification	Electro-optical Sampling
Schematic					

Limited by:

1 Excitation source (bandwidth and center frequency)

2 Operating temperature

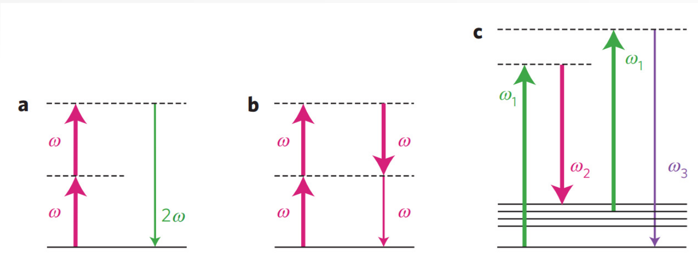
3 Phase matching condition

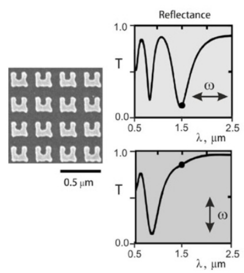
4 Longitudinal optical phonon absorption

5 Defect and impurity

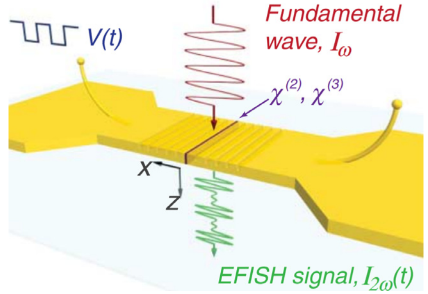
6 Weak nonlinear conversion efficiency

Nonlinear Plasmonics

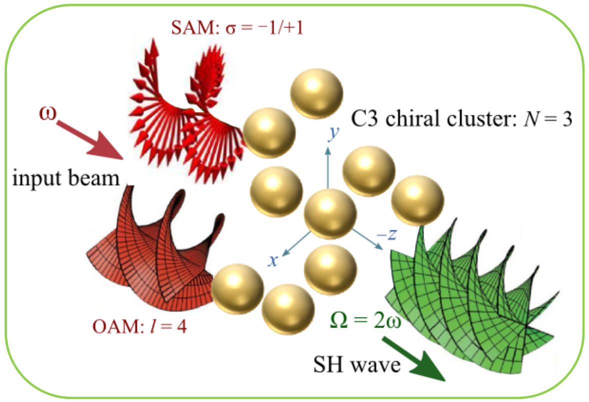




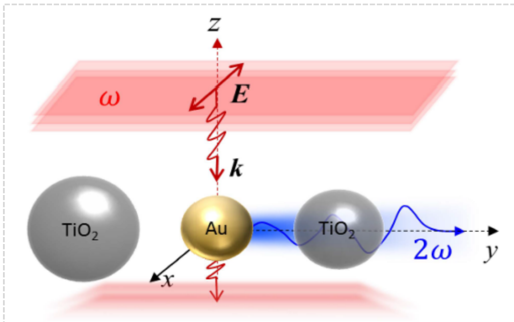
Ref: *Opt. Express* 15: 5238-5247



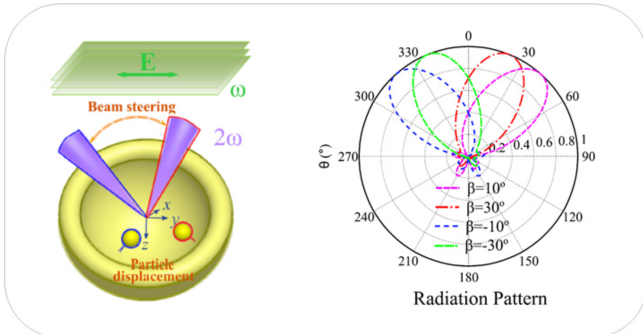
Ref: *Science* 333: 1720-1723



Physical Review B 95: 165432, 2017

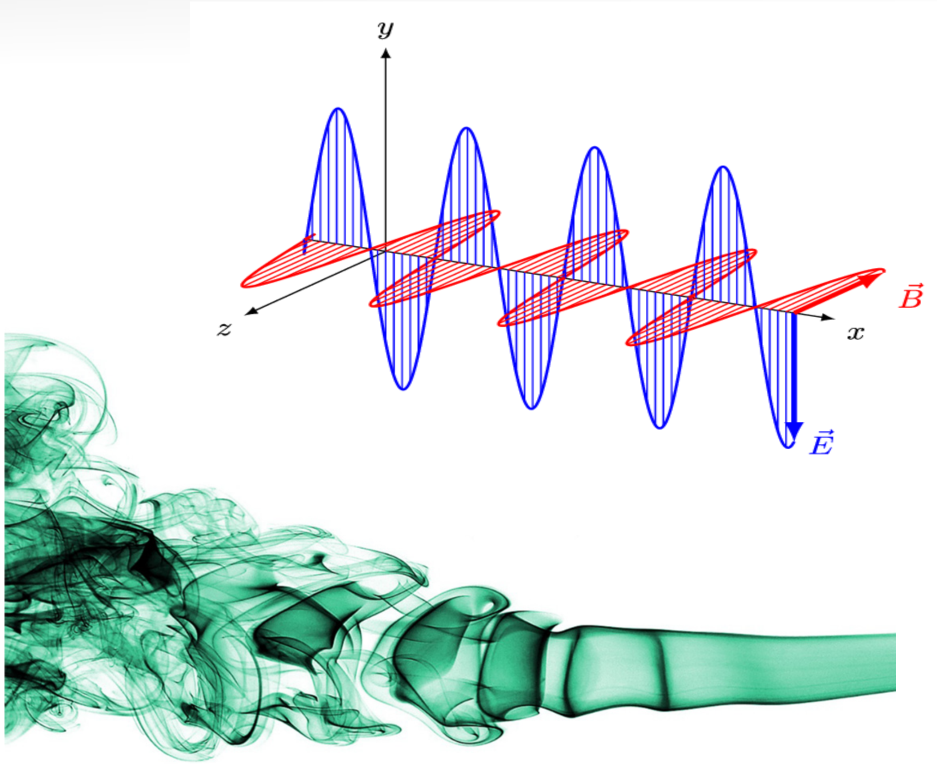


Scientific Reports 6: 18872, 2016



Physical Review A 83: 043824, 2011

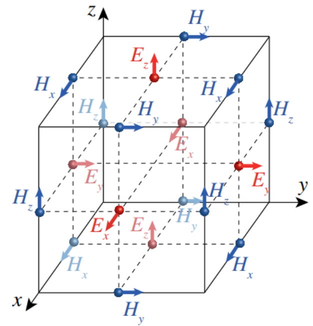
FDTD Implementation of Maxwell-Hydrodynamic Model



Maxwell's Equations

$$\nabla \times \mathbf{H} = \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \frac{\partial \mathbf{P}}{\partial t}$$

$$\nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t},$$

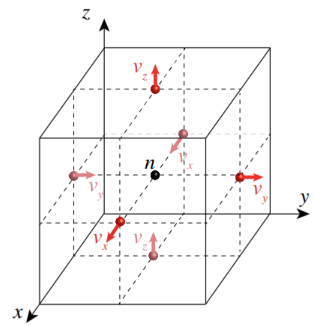


Weakly Coupled by:

$$\frac{\partial n}{\partial t} = -\nabla \cdot (n\mathbf{v}),$$

$$\frac{\partial \mathbf{P}}{\partial t} = -en\mathbf{v}.$$

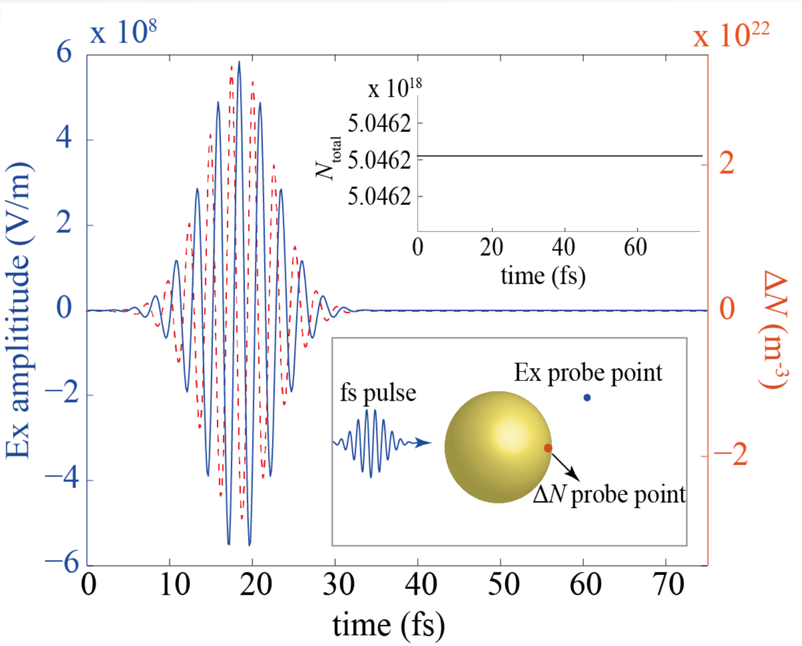
$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{e}{m}(\mathbf{E} + \mu_0 \mathbf{v} \times \mathbf{H}) - \gamma \mathbf{v} - \frac{\nabla p}{n}$$



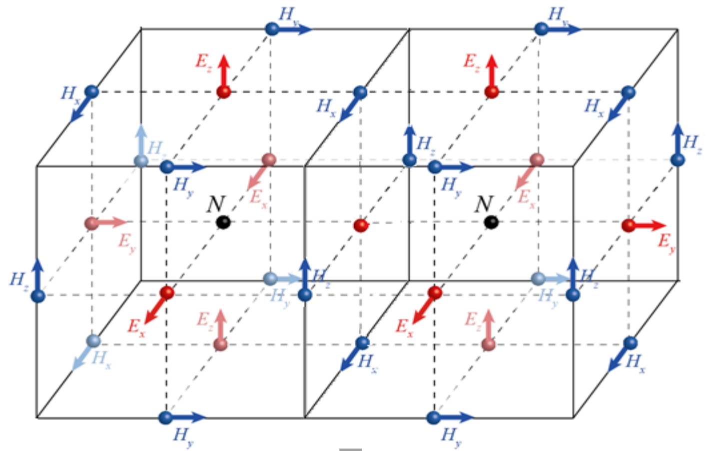
Hydrodynamic Model

The equations are solved by FDTD method with Yee grids.

Charge Conservation



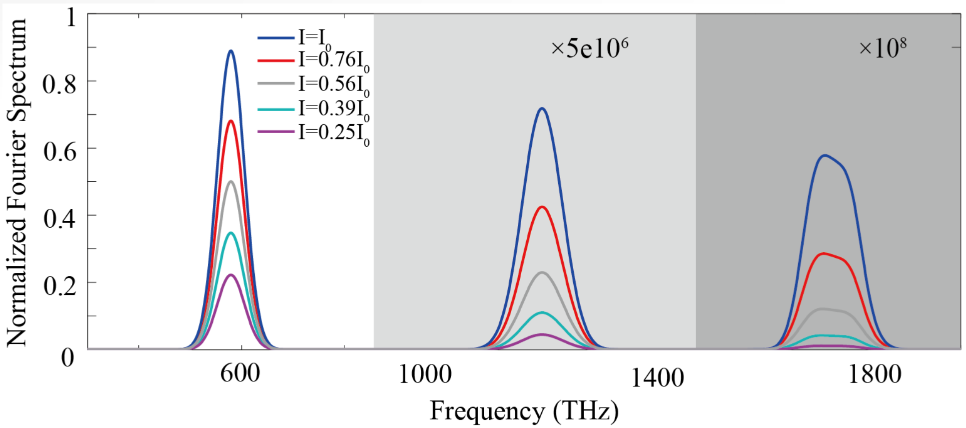
At each point, the electron density fluctuates. However, the total charge within the sphere is conserved.

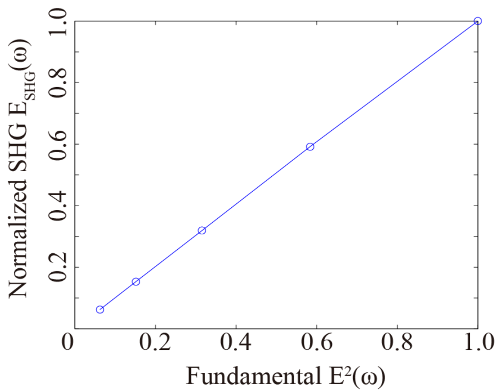


Discretization

$$
\begin{aligned}
n^{l+3/2}(i+1/2, j+1/2, k+1/2) &= n^{l+1/2}(i+1/2, j+1/2, k+1/2) \\
&-\Big[\frac{\Delta t}{\Delta x}\Big(\overline{n}^{l+1/2}(i+1, j+1/2, k+1/2)v_x^{l+1}(i+1, j+1/2, k+1/2)-\overline{n}^{l+1/2}(i, j+1/2, k+1/2)v_x^{l+1}(i, j+1/2, k+1/2)\Big) \\
&+\frac{\Delta t}{\Delta y}\Big(\overline{n}^{l+1/2}(i+1/2, j+1, k+1/2)v_y^{l+1}(i+1/2, j+1, k+1/2)-\overline{n}^{l+1/2}(i+1/2, j, k+1/2)v_y^{l+1}(i+1/2, j, k+1/2)\Big) \\
&+\frac{\Delta t}{\Delta z}\Big(\overline{n}^{l+1/2}(i+1/2, j+1/2, k+1)v_z^{l+1}(i+1/2, j+1/2, k+1)-\overline{n}^{l+1/2}(i+1/2, j+1/2, k)v_z^{l+1}(i+1/2, j+1/2, k)\Big)\Big]
\end{aligned}
$$

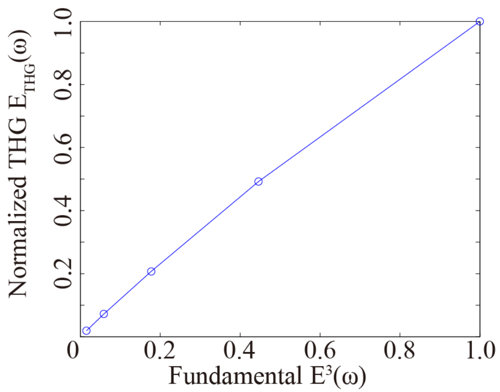
Energy Conservation/Conversion





$$E_{SHG}(2\omega)\sim|E(\omega)|^{2}$$

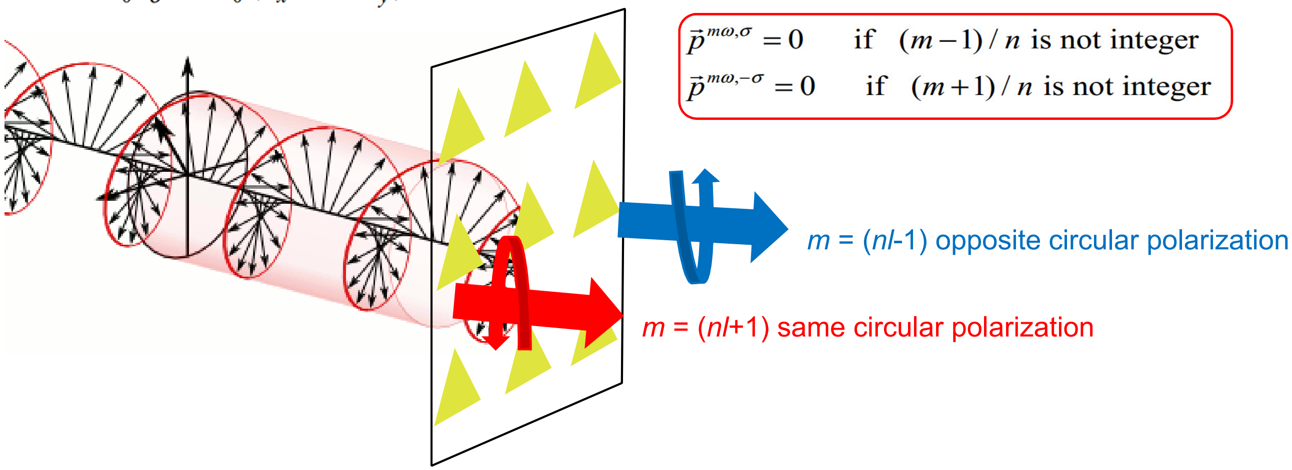
$$E_{THG}(3\omega)\sim|E(\omega)|^{3}$$



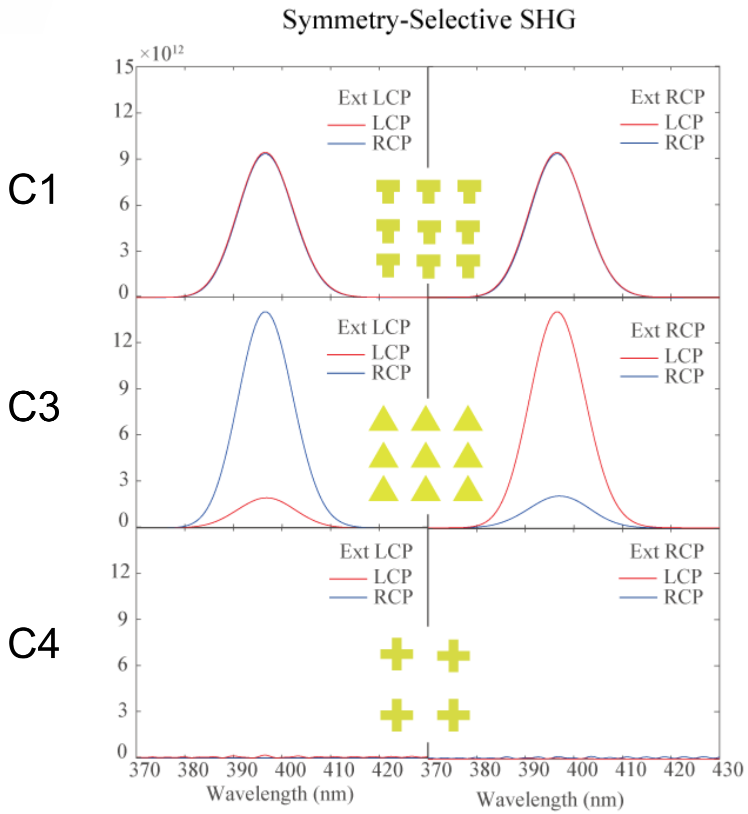
Angular Momentum Conservation (1)

n fold rotational symmetry and m[th] harmonics

$$\vec{E}^{\sigma} = \tilde{E}_0 \hat{e}_{\sigma} = \tilde{E}_0 (\hat{e}_x + i\sigma \hat{e}_y)/\sqrt{2}$$



$$\vec{p}^{\,m\omega,\sigma} = 0 \quad \text{if} \quad (m-1)/n \text{ is not integer}$$
$$\vec{p}^{\,m\omega,-\sigma} = 0 \quad \text{if} \quad (m+1)/n \text{ is not integer}$$



M. Fang, W.E.I. Sha, et al. *Progress In Electromagnetics Research* 157: 63–78, 2016. (Invited Paper)

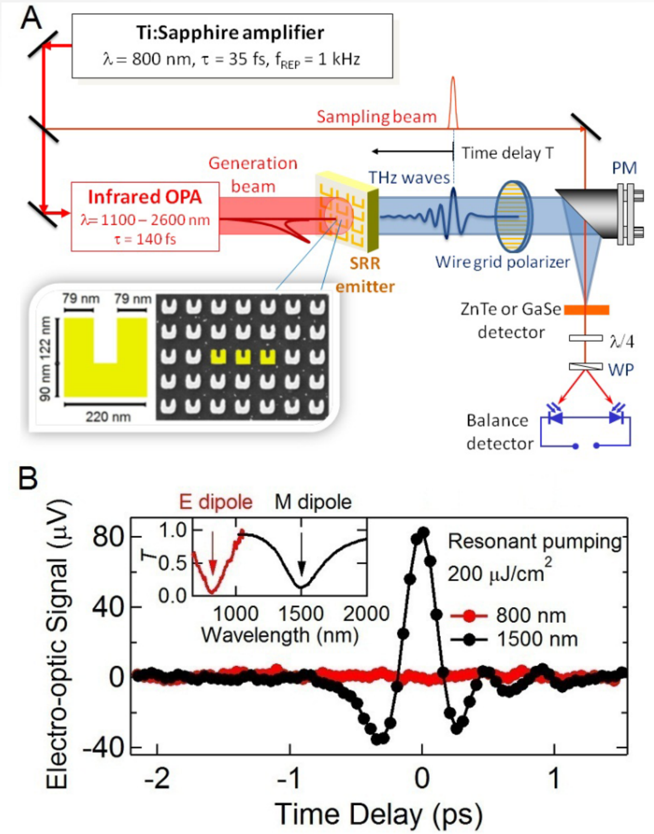
Angular Momentum Conservation (2)

Discretization of Hydrodynamic Equation

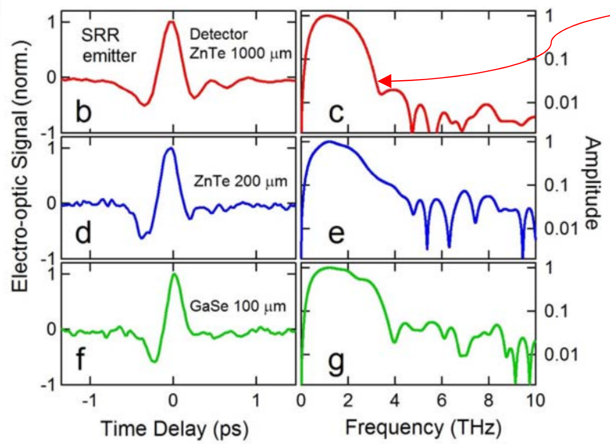
$$
\begin{aligned}
v_x^{l+1}(i,j+1/2,k+1/2) &= v_x^l(i,j+1/2,k+1/2) - \Delta t \gamma v_x^l(i,j+1/2,k+1/2) - \frac{\Delta t e}{m} E_x^{l+1/2}(i,j+1/2,k+1/2) \\
&- \left[\frac{\Delta t}{2\Delta x}\left(v_x^l(i,j+1/2,k+1/2)\cdot v_x^l(i+1,j+1/2,k+1/2) - v_x^l(i,j+1/2,k+1/2)\cdot v_x^l(i-1,j+1/2,k+1/2)\right)\right. \\
&+ \frac{\Delta t}{2\Delta y}\left(\bar{v}_y^l(i,j+1/2,k+1/2)\cdot v_x^l(i,j+3/2,k+1/2) - \bar{v}_y^l(i,j+1/2,k+1/2)\cdot v_x^l(i,j-1/2,k+1/2)\right) \\
&\left.+ \frac{\Delta t}{2\Delta z}\left(\bar{v}_z^l(i,j+1/2,k+1/2)\cdot v_x^l(i,j+1/2,k+3/2) - \bar{v}_z^l(i,j+1/2,k+1/2)\cdot v_x^l(i,j+1/2,k-1/2)\right)\right] \\
&- \frac{\Delta t \mu_0 e}{m}\left(\bar{v}_y^l(i,j+1/2,k+1/2)\bar{H}_z^{l+1/2}(i,j+1/2,k+1/2) - \bar{v}_z^l(i,j+1/2,k+1/2)\bar{H}_y^{l+1/2}(i,j+1/2,k+1/2)\right)
\end{aligned}
$$

spatial interpolation is adopted to force all the physical quantities to be the same locations. The interpolation scheme is crucial to maintain the angular momentum conservation of nonlinear process in metals.

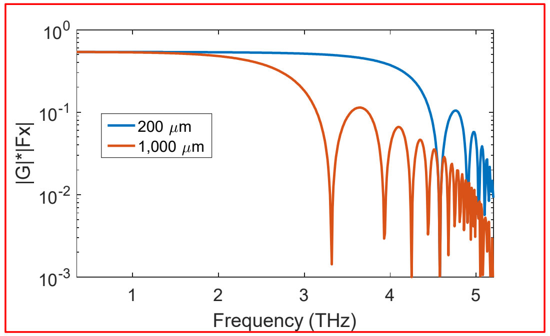
Broadband Metasurface THz Emitter: Experiments in Literature



Absorption Gaps



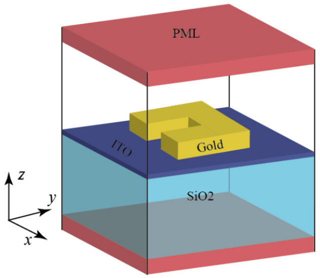
Response Function

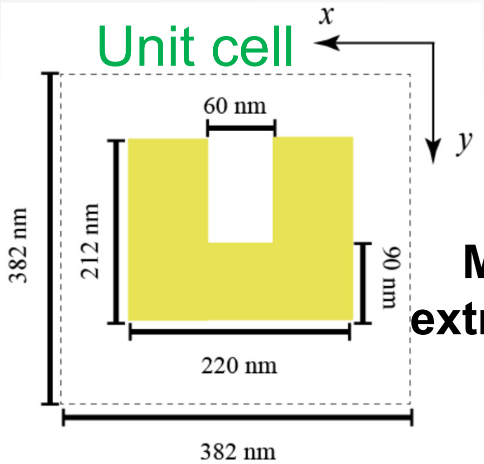


Thickness Dependent THz Detection

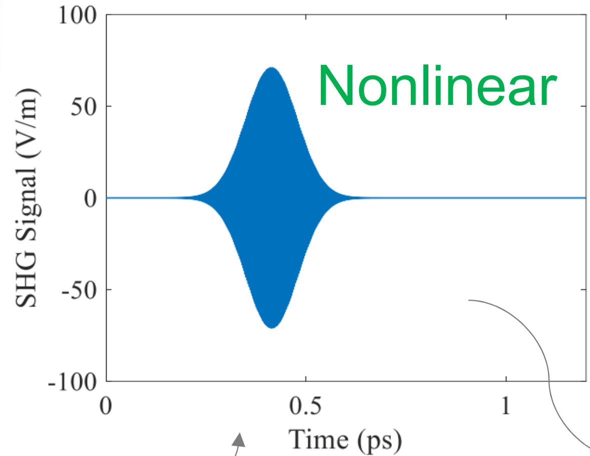
*Ref: L. Luo, et al. *Nature Communications* 5: 3055, 2014

Numerical Results of Metasurface THz Emitter by Maxwell-Hydrodynamic (M-H) Model



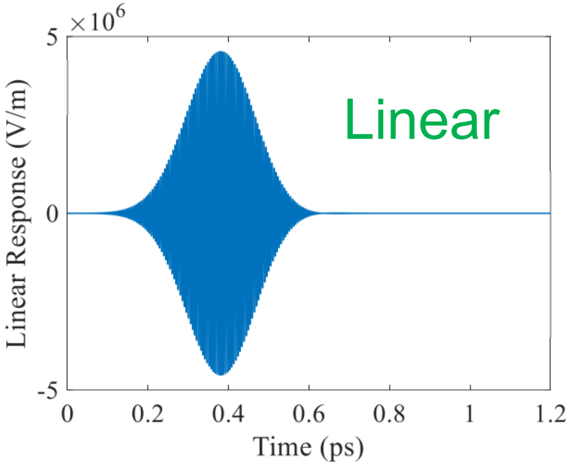


M-H model result extracted by M-Drude model results

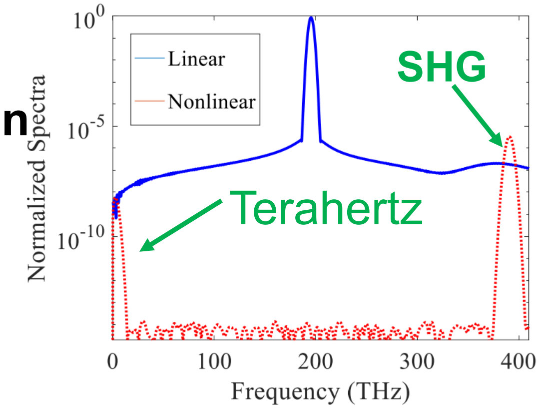


Fourier transform

linear process

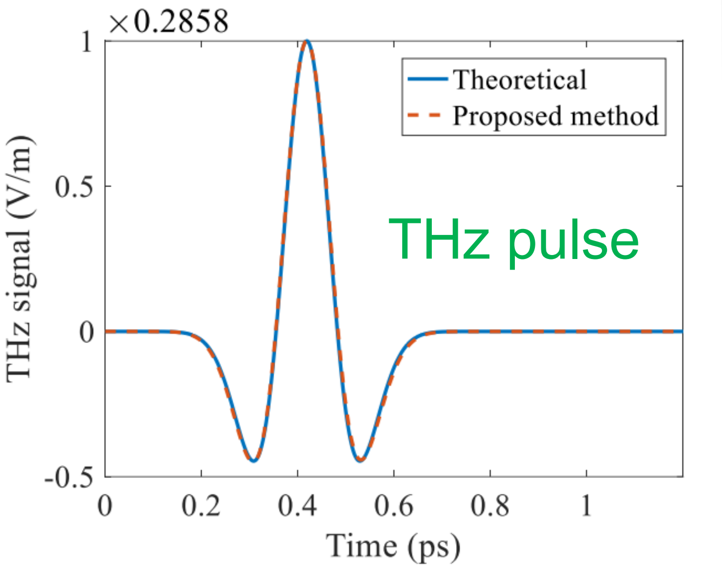


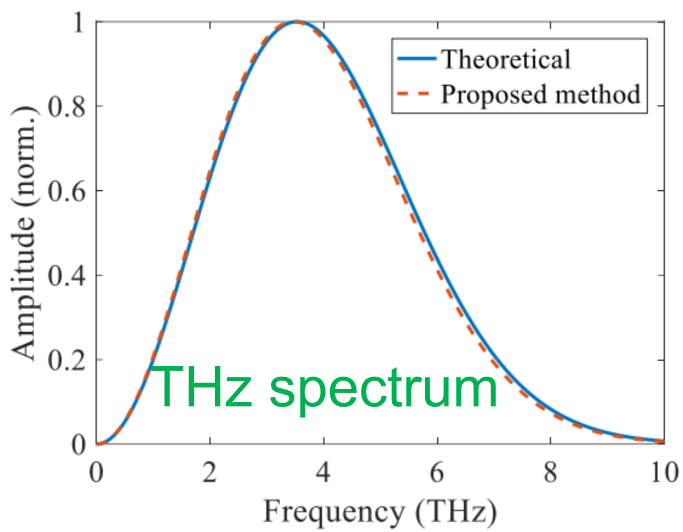
Rectification
SHG
THG
…

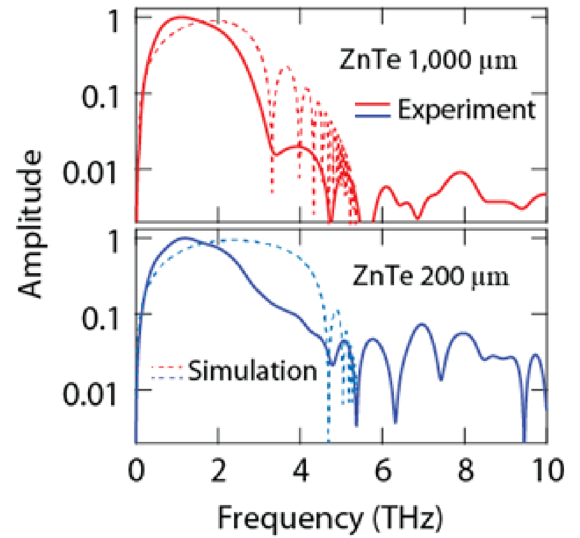


M. Fang, W.E.I. Sha, et al. *IEEE JMMCT* 2: 194-201, 2017

Terahertz Spectrum — Metasurface Generation and ZnTe Crystal Detection



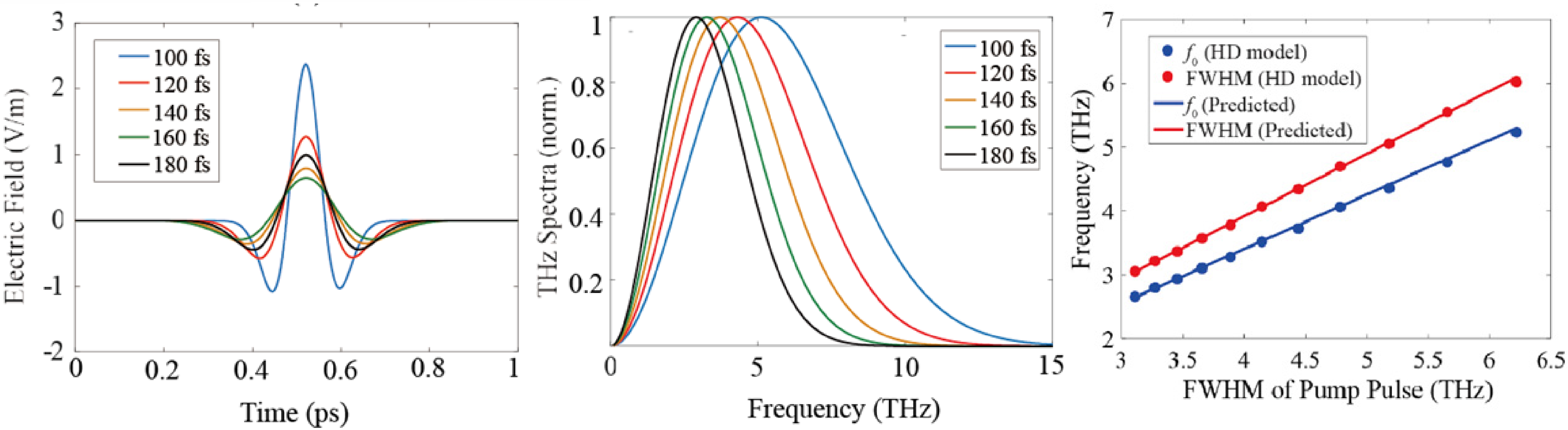




$$E^{(THz)}(\omega) \sim \chi^{(2)}(-i\omega)^2 g_{\frac{1}{\sqrt{2}\sigma}}(\omega) = \chi^{(2)}\omega^2 e^{-\frac{\omega^2}{4\sigma^2}} \Leftrightarrow .$$

$$E^{(THz)}(t) \sim -\chi^{(2)}\partial_t^2 g_{\sqrt{2}\sigma}(t) = \chi^{(2)}\sigma^2(1-2\sigma^2 t^2)e^{-\sigma^2 t^2}$$

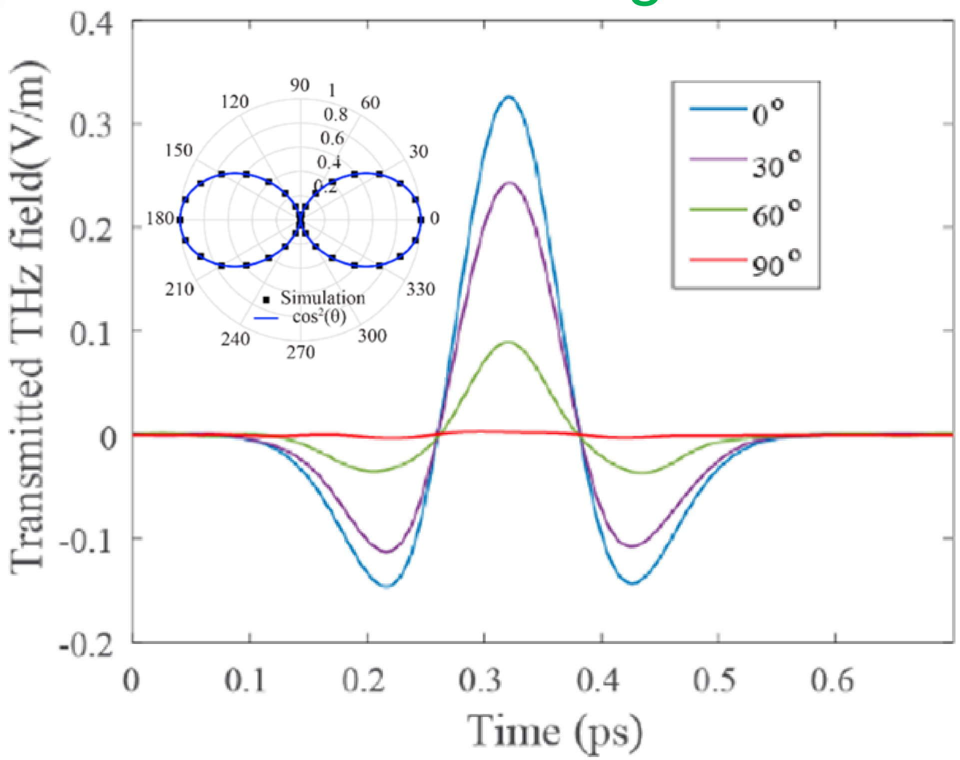
Tunable THz Spectrum by Duration Time or FWHM of Incident Laser Pulse



M. Fang, W.E.I. Sha, et al. *Optics Express*, 26(11): 14241, 2018

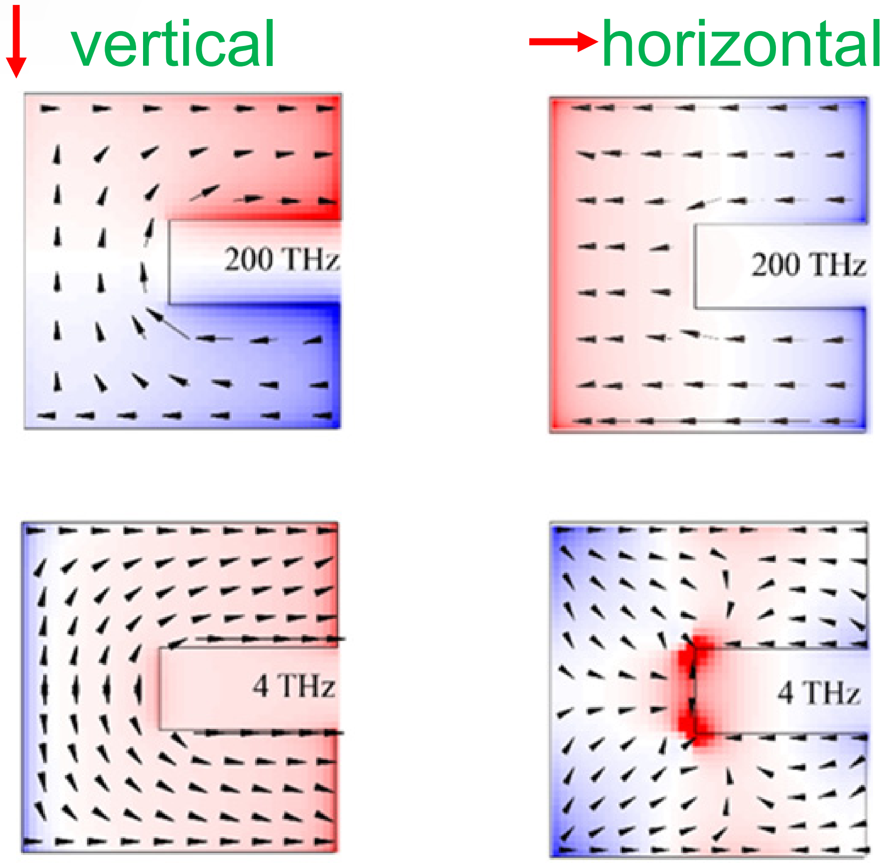
Incident Angle and Polarization Dependent THz Generation

incident angles



vertical

horizontal



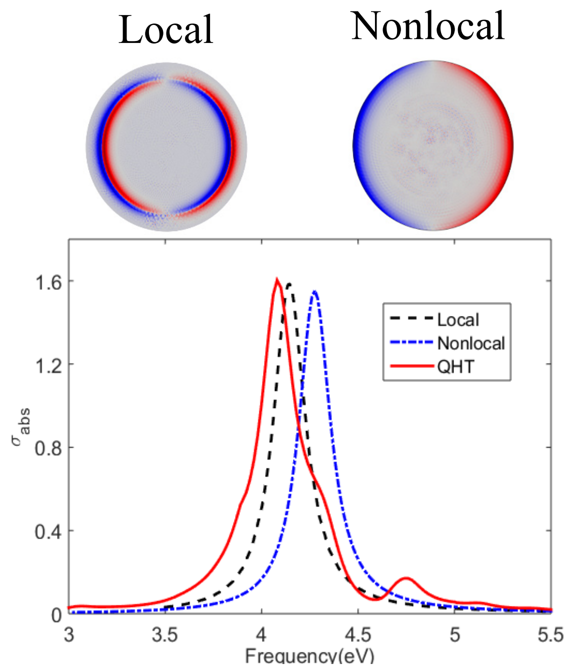
Conclusion

1. A time-domain implementation of Maxwell-hydrodynamic model for conduction electrons in metals has been developed to enable nonperturbative studies of nonlinear coherent interaction between light and plasmonic nanostructures.

2. Numerical method was validated by conservation and conversion laws.

3. We numerically demonstrated a new concept of THz emitter based on a single-layer nonlinear metasurface of nanoscale thickness, representing a new platform for revealing artificial magnetism-induced THz generation.

Outlook



$$\nabla \times \mathbf{H} = \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \frac{\partial \mathbf{P}}{\partial t}$$
$$\nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t},$$

Maxwell's Equations

+

$$mn\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) = -n\nabla\frac{\delta G}{\delta n} + ne(\mathbf{E} + \mathbf{v}\times\mathbf{B})$$
$$\frac{\partial n}{\partial t} = -\nabla\cdot(n\mathbf{v})$$

Hydrodynamic Model

+

$$\frac{\delta G}{\delta n} = \frac{\delta T}{\delta n} + \frac{\delta F_{\mathrm{xc}}}{\delta n} = \frac{\delta T_{\mathrm{TF}}}{\delta n} + \frac{\delta T_{\mathrm{W}}}{\delta n} + \frac{\delta E_{\mathrm{x}}}{\delta n} + \frac{\delta E_{\mathrm{c}}}{\delta n} + \frac{\delta E_{\mathrm{LB94}}}{\delta n}$$

Quantum Corrections