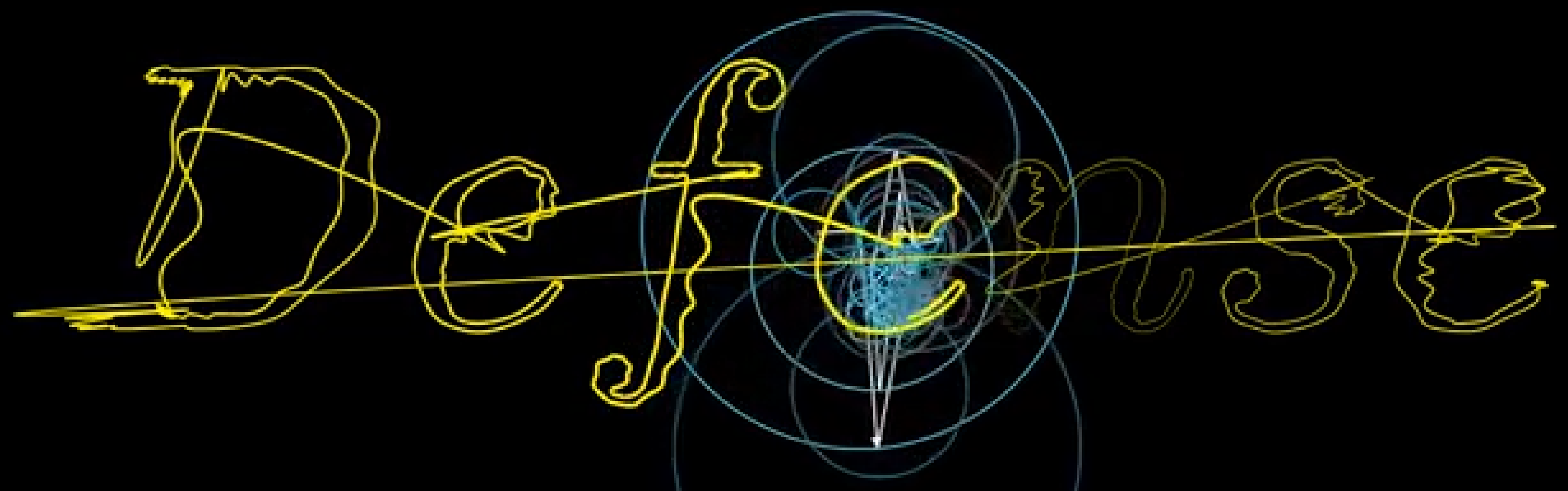
Universal Electromagnetic Response Relations

applied to the free homogeneous electron gas

– PhD Thesis –



René Wirnata

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OUTLINE

Motivation

Functional Approach to ED in Media

- Source Splitting & Field Identifications
- Fundamental Response Tensor & URR

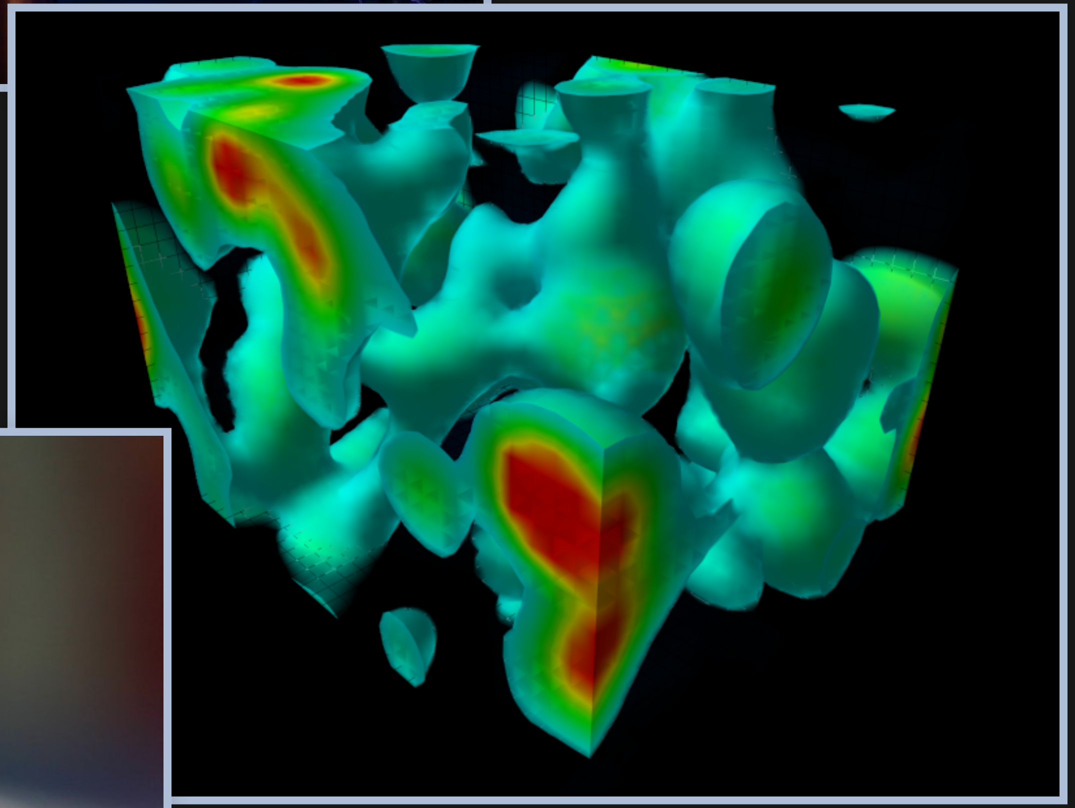
Quantum Field Theory

- Kubo-Greenwood Formalism
- Full Current Operator

Impact on Materials Models

- London Conductivity as Toy Model
- Optical & Magnetic Properties of FEG
- Lindhard Integral Theorem

Summary & Conclusion



MOTIVATION

Goal: Description of optical & magnetic response properties based on microscopic field theories

- Why microscopic theories?
  - most physical effects are genuinely microscopic
  - allows *ab initio* computation of materials properties
    → fundamental insight how matter *really* works

- Possible applications?
  - basically everything related to EM fields in media
  - optical spectroscopy (e.g. refractive index measurements)
  - materials modelling (meta materials, invisibility cloaks, …)

which field theories?

Classical Electrodynamics
Linear Response Theory
Quantum Field Theory

Q: How combine theories and access EM response properties from QM ?

A: Naïvely not possible !
Hang on if you want to find out…

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Functional Approach to Electrodynamics in Media

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SOURCE SPLITTING & FIELD IDENTIFICATIONS

Classical electrodynamics is based on the Maxwell Equations

$$\nabla \cdot \boldsymbol{E}_{\text{ext}} = \varepsilon_0^{-1}\,\rho_{\text{ext}} \qquad\qquad \nabla \cdot \boldsymbol{E}_{\text{ind}} = \varepsilon_0^{-1}\,\rho_{\text{ind}}$$

$$\nabla \times \boldsymbol{B}_{\text{ext}} - \mu_0\varepsilon_0\,\partial_t \boldsymbol{E}_{\text{ext}} = \mu_0\,\boldsymbol{j}_{\text{ext}} \qquad\qquad \nabla \times \boldsymbol{B}_{\text{ind}} - \mu_0\varepsilon_0\,\partial_t \boldsymbol{E}_{\text{ind}} = \mu_0\,\boldsymbol{j}_{\text{ind}}$$

$$\nabla \cdot \boldsymbol{B}_{\text{ext}} = 0 \qquad\qquad \nabla \cdot \boldsymbol{B}_{\text{ind}} = 0$$

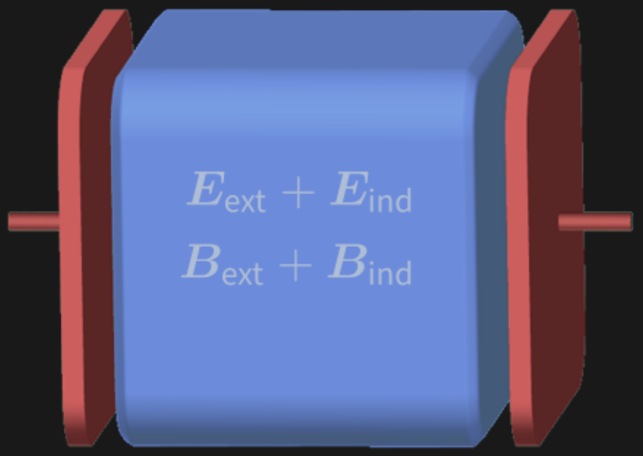
$$\nabla \times \boldsymbol{E}_{\text{ext}} + \partial_t \boldsymbol{B}_{\text{ext}} = 0 \qquad\qquad \nabla \times \boldsymbol{E}_{\text{ind}} + \partial_t \boldsymbol{B}_{\text{ind}} = 0$$

➟ always valid on a fundamental microscopic level!

Source splitting in ab initio theory:

$$\rho_{\text{tot}} = \rho_{\text{ext}} + \rho_{\text{ind}}$$

$$\boldsymbol{j}_{\text{tot}} = \boldsymbol{j}_{\text{ext}} + \boldsymbol{j}_{\text{ind}}$$



Convert to traditional naming scheme via fundamental field identifications

$$\boldsymbol{P} = -\varepsilon_0 \boldsymbol{E}_{\text{ind}} \qquad \boldsymbol{M} = \mu_0^{-1} \boldsymbol{B}_{\text{ind}}$$

$$\boldsymbol{D} = +\varepsilon_0 \boldsymbol{E}_{\text{ext}} \qquad \boldsymbol{H} = \mu_0^{-1} \boldsymbol{B}_{\text{ext}}$$

$$\boldsymbol{E} = \boldsymbol{E}_{\text{tot}} \qquad \boldsymbol{B} = \boldsymbol{B}_{\text{tot}}$$

FUNDAMENTAL RESPONSE TENSOR (1)

Basis of (linear) Response Theory:

Induced fields can be regarded as functionals of external ones.

Lorentz 4-vector notation:

$$j^\mu = \begin{pmatrix} c\rho \\ \boldsymbol{j} \end{pmatrix}, \quad A^\mu = \begin{pmatrix} \varphi/c \\ \boldsymbol{A} \end{pmatrix}$$

Fields & Potentials:

$$\boldsymbol{E} = -\nabla\varphi - \partial_t \boldsymbol{A}$$

$$\boldsymbol{B} = \nabla \times \boldsymbol{A}$$

Q: Which functional is the "correct" one?

$$\boldsymbol{E}_{\text{ind}}[\boldsymbol{E}_{\text{ext}}, \boldsymbol{B}_{\text{ext}}], \quad \boldsymbol{j}_{\text{ind}}[\boldsymbol{E}_{\text{ext}}], \quad \boldsymbol{B}_{\text{ind}}[\rho_{\text{ext}}, \boldsymbol{j}_{\text{ext}}], \ \ldots ?$$

A: Postulate of Functional Approach: $j^\mu_{\text{ind}} = j^\mu_{\text{ind}}[A^\nu_{\text{ext}}]$

Linear response tensor:

$$\boxed{\chi^\mu{}_\nu(x, x') = \frac{\delta j^\mu_{\text{ind}}(x)}{\delta A^\nu_{\text{ext}}(x')}}$$

2nd order tensor $\chi^\mu{}_\nu$ contains complete information on EM response.

FUNDAMENTAL RESPONSE TENSOR (2)

Continuity equation and gauge invariance imply the constraints:

$$\partial_\mu \chi^\mu{}_\nu(x,x') = \partial'^\nu \chi^\mu{}_\nu(x,x') = 0$$

$$x^\mu = \begin{pmatrix} ct \\ \boldsymbol{x} \end{pmatrix} \qquad \partial^\mu = \begin{pmatrix} -\partial_t \\ \nabla \end{pmatrix} \qquad k^\mu = \begin{pmatrix} \omega/c \\ \boldsymbol{k} \end{pmatrix}$$

⇒ at most 9 independent linear response functions!

For homogeneous systems: $\chi(x,x') = \chi(x-x')$

Equivalently in Fourier space: $\chi(k,k') = \chi(k)\,\delta(k-k')$

this implies in 3+1 formalism

$$\chi^\mu{}_\nu(\boldsymbol{k},\omega) = \begin{pmatrix} -\dfrac{c^2}{\omega^2}\,\boldsymbol{k}^\mathrm{T}\,\overleftrightarrow{\chi}\,\boldsymbol{k} & \dfrac{c}{\omega}\,\boldsymbol{k}^\mathrm{T}\,\overleftrightarrow{\chi} \\ -\dfrac{c}{\omega}\,\overleftrightarrow{\chi}\,\boldsymbol{k} & \overleftrightarrow{\chi} \end{pmatrix}$$

with

$$\boxed{\overleftrightarrow{\chi} = \frac{\delta \boldsymbol{j}_\mathrm{ind}}{\delta \boldsymbol{A}_\mathrm{ext}}}$$

Remaining components form the 3x3 Current Response Tensor $\overleftrightarrow{\chi}(\boldsymbol{k},\omega)$.

UNIVERSAL RESPONSE RELATIONS

Central Claim:
Current Response Tensor $\overleftrightarrow{\chi}$
determines all linear EM materials properties.

$$\boxed{\begin{aligned} \overleftrightarrow{\chi}_{\mathrm{EE}} &= \frac{\mathrm{d}\boldsymbol{E}_{\mathrm{ind}}}{\mathrm{d}\boldsymbol{E}_{\mathrm{ext}}}\,, & \overleftrightarrow{\chi}_{\mathrm{EB}} &= \frac{\mathrm{d}\boldsymbol{E}_{\mathrm{ind}}}{\mathrm{d}\boldsymbol{B}_{\mathrm{ext}}} \\ \overleftrightarrow{\chi}_{\mathrm{BE}} &= \frac{\mathrm{d}\boldsymbol{B}_{\mathrm{ind}}}{\mathrm{d}\boldsymbol{E}_{\mathrm{ext}}}\,, & \overleftrightarrow{\chi}_{\mathrm{BB}} &= \frac{\mathrm{d}\boldsymbol{B}_{\mathrm{ind}}}{\mathrm{d}\boldsymbol{B}_{\mathrm{ext}}} \end{aligned}}$$

$\Rightarrow$ can all be expressed in terms of $\overleftrightarrow{\chi}$ or alternatively in terms of conductivity $\overleftrightarrow{\sigma}$ via

basic relation: $\overleftrightarrow{\chi}(\boldsymbol{k},\omega) = \mathrm{i}\omega\,\overleftrightarrow{\sigma}(\boldsymbol{k},\omega)$

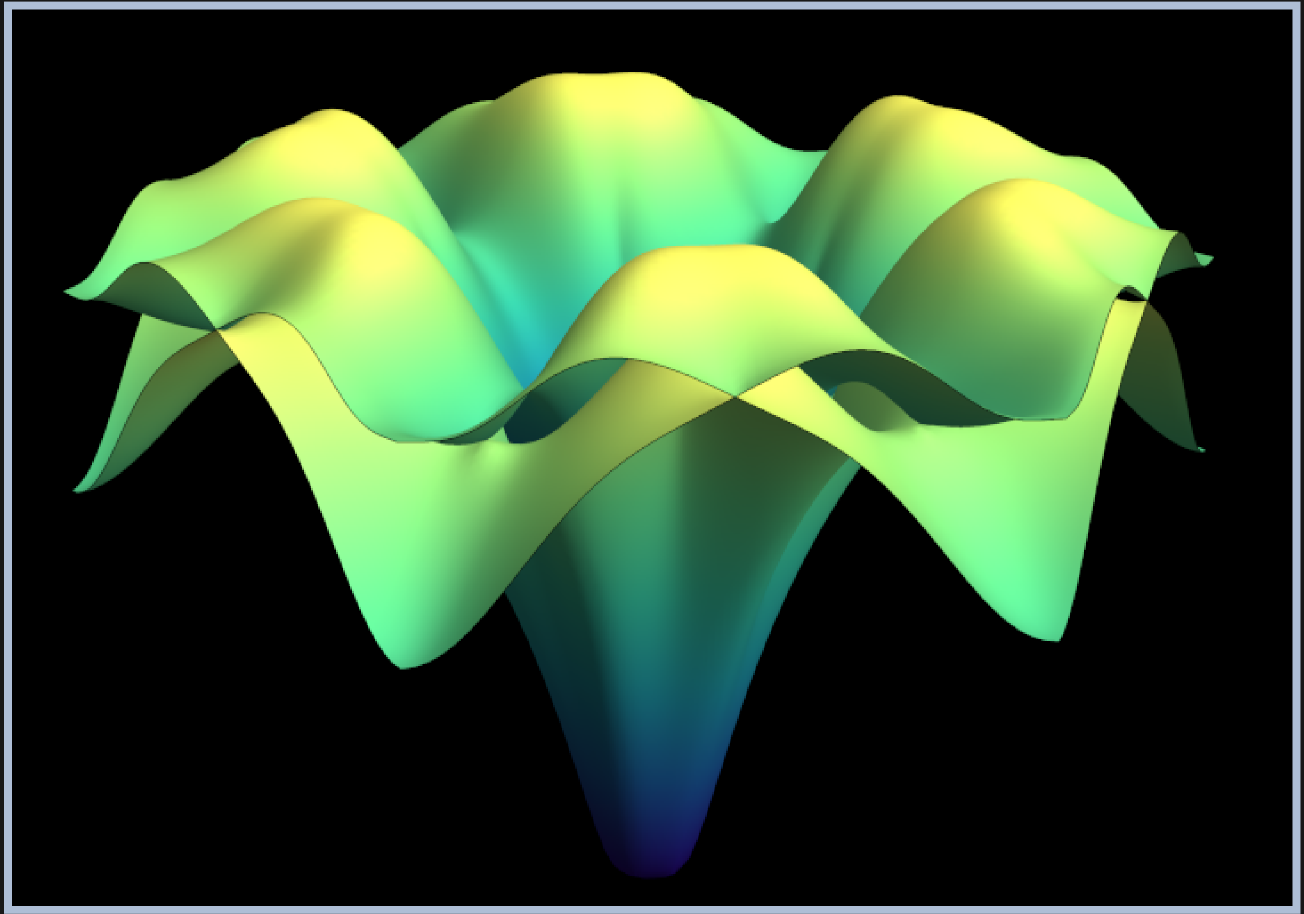
Combined with the power of
Total Functional Derivatives yields
Universal Response Relations (URR)

- model and material-independent relations between EM response functions
- already include all effects of anisotropy, rel. retardation and ME cross-coupling
- all standard relations known in ab initio theory recovered in suitable limiting cases

  e.g. optical limit $\rightarrow$ $\overleftrightarrow{\varepsilon}_{\mathrm{r}}(\omega) = 1 - \dfrac{\overleftrightarrow{\widetilde{\sigma}}(\omega)}{\mathrm{i}\omega\varepsilon_0}$

- conductivity routinely calculated *ab initio*
  $\rightsquigarrow$ URR as post-processing
  $\rightsquigarrow$ see also Elk Optics Analyzer

Quantum Field Theory



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KUBO-GREENWOOD FORMALISM (1)

Q: How to calculate response functions *from first principles*?

A: Employ Kubo Formalism:

$$\chi_{\mathrm{AB}}(t-t') \overset{\text{def}}{=} \boxed{\left.\frac{\delta A(t)}{\delta P(t')}\right|_{P=0}} = -\frac{\mathrm{i}}{\hbar}\,\Theta(t-t')\,\langle\Psi_0|[\hat{A}_{\mathrm{I}}(t),\hat{B}_{\mathrm{I}}(t')]|\Psi_0\rangle$$

Let $P(t)$ be a (weak) time-dependent perturbation which couples to an operator $\hat{B}$ in the Hamiltonian:

$$\hat{\mathcal{H}}(t) = \hat{\mathcal{H}}_0 + P(t)\,\hat{B} \quad \Rightarrow \quad \mathrm{i}\hbar\,\partial_t\,|\Psi(t)\rangle = \hat{\mathcal{H}}(t)\,|\Psi(t)\rangle$$

$$\Rightarrow \quad |\Psi(t)\rangle = \big(|\Psi(t)\rangle\big)[P]$$

Expectation value of some other observable $\hat{A}$ is then given by

$$\boxed{A(t)[P]} = \langle\Psi(t)|\,\hat{A}\,|\Psi(t)\rangle$$

note: $|\Psi\rangle$ is a many-body state!

*Kubo formula allows to express the response χ of the observable w.r.t. the perturbation **solely** in terms of unperturbed quantities !*

KUBO-GREENWOOD FORMALISM (2)

For non-interacting systems, MB-WF can be chosen as Slater determinant

$$|\Psi_0^N\rangle = |\mathrm{SL}(\varphi_1, \ldots, \varphi_N)\rangle$$

Many-body problem decomposes into effective single-particle system

$$\hat{\mathcal{H}}^N = \sum_N \hat{\mathcal{H}}^1 \,, \quad \hat{\mathcal{H}}^1 |\varphi_i\rangle = \epsilon_i |\varphi_i\rangle$$

In Grand Canonical Ensemble, Kubo formula reverts to its Spectral Representation in Fourier space

$$\chi^R_{\mathrm{AB}}(\omega) = \sum_{i,j=0}^{\infty} \frac{\left(f_{\beta,\mu}(\epsilon_i) - f_{\beta,\mu}(\epsilon_j)\right) A_{ij} B_{ji}}{\hbar(\omega + \mathrm{i}\eta) - (\epsilon_j - \epsilon_i)}$$

$$A_{ij} = \langle \varphi_i | \hat{A} | \varphi_j \rangle \,, \qquad f_{\beta,\mu}(\epsilon_i) = \frac{1}{1 + \mathrm{e}^{\beta(\epsilon_i - \mu)}}$$

In plane waves basis …

$$\varphi_{\boldsymbol{k}}(\boldsymbol{x}) = \langle \boldsymbol{x} | \boldsymbol{k} \rangle = \frac{1}{(2\pi)^{3/2}} \, \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}$$

… and for density response

$$\hat{A} \mapsto \hat{\rho}(\boldsymbol{x}) = (-e)\hat{\psi}^\dagger(\boldsymbol{x})\hat{\psi}(\boldsymbol{x})$$
$$\hat{B} \mapsto \hat{\rho}(\boldsymbol{x}') = (-e)\hat{\psi}^\dagger(\boldsymbol{x}')\hat{\psi}(\boldsymbol{x}')$$

$$\hat{\psi}(\boldsymbol{x})|\varphi\rangle = \langle \boldsymbol{x}|\varphi\rangle|0\rangle$$

Kubo formula yields in Thermodynamic Limit

$$\chi_{\rho\rho}(\boldsymbol{q}, \omega) = 2e^2 \int \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3} \frac{f(\epsilon_{\boldsymbol{k}}) - f(\epsilon_{\boldsymbol{k}+\boldsymbol{q}})}{\hbar(\omega + \mathrm{i}\eta) + \epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k}+\boldsymbol{q}}}$$

$$\epsilon_{\boldsymbol{k}} = \hbar\omega_{\boldsymbol{k}}$$

$\Rightarrow$ *famous Lindhard density response*

FULL CURRENT OPERATOR (1)

For current response tensor $\overleftrightarrow{\chi} \equiv \overleftrightarrow{\chi}_{jj}$ *we need* $\hat{\boldsymbol{j}}$ *instead of* $\hat{\rho}$.

1. Start with free Hamiltonian

$$\mathrm{i}\hbar\,\partial_t\,\psi(\boldsymbol{x},t) = \hat{\mathcal{H}}_0\,\psi(\boldsymbol{x},t)\,, \quad \hat{\mathcal{H}}_0 = \frac{|\hat{\boldsymbol{p}}|^2}{2m} \quad \Rightarrow \quad \boxed{\boldsymbol{j} = \underbrace{\frac{(-e)\hbar}{2m\mathrm{i}}\Big(\psi^*(\nabla\psi) - (\nabla\psi)^*\psi\Big)}_{\text{orbital}}}$$

2. Extend by U(1) gauge theory → minimal-coupling of EM fields

$$\left.\begin{aligned} \partial_t &\mapsto \partial_t - \tfrac{\mathrm{i}}{\hbar}\,e\varphi \\ \nabla &\mapsto \nabla + \tfrac{\mathrm{i}}{\hbar}\,e\boldsymbol{A} \end{aligned}\right\} \quad \Rightarrow \quad \hat{\mathcal{H}}_{\mathrm{min}} = \frac{|\hat{\boldsymbol{p}} + e\boldsymbol{A}|^2}{2m} - e\varphi \quad \Rightarrow \quad \boxed{\boldsymbol{j} = \boldsymbol{j}_{\mathrm{orb}} + \underbrace{\frac{e}{m}\,\rho\boldsymbol{A}}_{\text{diamagnetic}}}$$

Q: But what about spin-induced magnetism?

A: Commonly not considered for $\boldsymbol{j}$, but: Yes , we can! — By invoking the Pauli Equation …

FULL CURRENT OPERATOR (2)

Institute of Theoretical Physics

The Pauli Equation is of Schrödinger-type and incorporates spin.

$$\hat{\mathcal{H}}_{\text{min}} = \frac{\left|\hat{\boldsymbol{p}} + e\boldsymbol{A}\right|^2}{2m} - e\varphi\,,$$

$$\boldsymbol{\sigma} = (\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3)^{\mathsf{T}}$$

Pauli Matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Leads to a total current operator of the form:

$$\boxed{\hat{\boldsymbol{j}}_{\text{tot}} = \hat{\boldsymbol{j}}_{\text{dia}} + \underbrace{\hat{\boldsymbol{j}}_{\text{orb}} + \hat{\boldsymbol{j}}_{\text{spin}}}_{\text{"paramagnetic"} \to \hat{\boldsymbol{j}}_{\text{p}} = \hat{\boldsymbol{j}}_{\text{tot}}\big|_{A=0}}}$$

with the additional spinorial contribution

$$\hat{\boldsymbol{j}}_{\text{dia}} = \frac{e}{m}\hat{\rho}\boldsymbol{A}\,, \qquad \hat{\boldsymbol{j}}_{\text{orb}} = \frac{(-e)\hbar}{2m\mathrm{i}}\left(\hat{\psi}^\dagger(\nabla\hat{\psi}) - (\nabla\hat{\psi})^\dagger\hat{\psi}\right)$$

$$\boxed{\hat{\boldsymbol{j}}_{\text{spin}} = \frac{(-e)\hbar}{2m}\nabla \times \left(\sum_{s,s'=\uparrow,\downarrow} \hat{\psi}_s^\dagger\,\boldsymbol{\sigma}_{ss'}\,\hat{\psi}_{s'}\right)}$$

This is the most general yet non-relativistic current.

→ can also be derived from Dirac equation in non-relativistic limit

FULL CURRENT RESPONSE TENSOR

Use Generalized Kubo Formula for the current response tensor

$$\overleftrightarrow{\chi}(\boldsymbol{x},t;\boldsymbol{x}',t') = \boxed{\frac{e}{m}\,\rho(\boldsymbol{x})\,\delta^3(\boldsymbol{x}-\boldsymbol{x}')\,\delta(t-t')\,\overleftrightarrow{1}} + \boxed{\frac{\mathrm{i}}{\hbar}\,\Theta(t-t')\left\langle\left[\hat{\boldsymbol{j}}_{\mathrm{p}}(\boldsymbol{x},t),\,\hat{\boldsymbol{j}}_{\mathrm{p}}(\boldsymbol{x}',t')\right]\right\rangle}$$

Because of bilinearity, commutator yields three contributions

$$\overleftrightarrow{\chi} = \overleftrightarrow{\chi}_{\mathrm{dia}} + \left(\overleftrightarrow{\chi}_{\mathrm{orb}} + \overleftrightarrow{\chi}_{\mathrm{spin}} + \overleftrightarrow{\chi}_{\mathrm{cross}}\right)$$

$$[\hat{A},\hat{B}] := \hat{A}\hat{B} - \hat{B}\hat{A}$$

$$\hat{\boldsymbol{j}}_{\mathrm{p}} = \hat{\boldsymbol{j}}_{\mathrm{orb}} + \hat{\boldsymbol{j}}_{\mathrm{spin}}$$

$\overleftrightarrow{\chi}_{\mathrm{dia}} =$ local contribution (left box above)

$$\overleftrightarrow{\chi}_{\mathrm{orb}} \propto \left\langle[\hat{\boldsymbol{j}}_{\mathrm{orb}},\,\hat{\boldsymbol{j}}'_{\mathrm{orb}}]\right\rangle$$

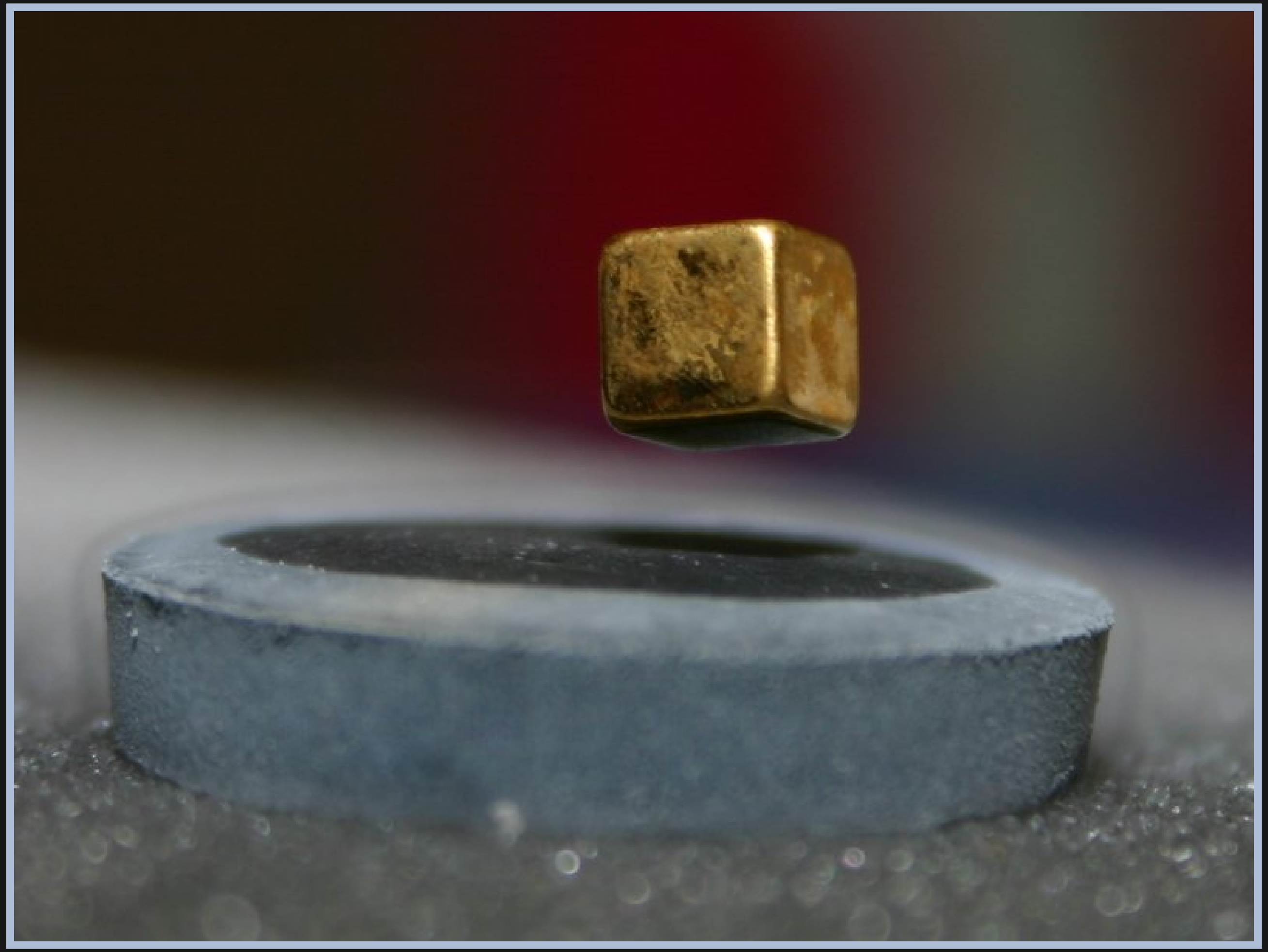
$$\overleftrightarrow{\chi}_{\mathrm{spin}} \propto \left\langle[\hat{\boldsymbol{j}}_{\mathrm{spin}},\,\hat{\boldsymbol{j}}'_{\mathrm{spin}}]\right\rangle$$

$$\overleftrightarrow{\chi}_{\mathrm{cross}} \propto \left\langle[\hat{\boldsymbol{j}}_{\mathrm{orb}},\,\hat{\boldsymbol{j}}'_{\mathrm{spin}}] + [\hat{\boldsymbol{j}}'_{\mathrm{spin}},\,\hat{\boldsymbol{j}}_{\mathrm{orb}}]\right\rangle$$

known: diamagnetic + orbital
novel: spin + cross-correlation

but: cross-correlation vanishes for non spin-polarized systems like FEG

Impact on Materials Models



FROM COVARIANT WAVE EQUATION TO LONDON MODEL

Inserting $\boldsymbol{E} = -\nabla\varphi - \partial_t \boldsymbol{A}$ and $\boldsymbol{B} = \nabla \times \boldsymbol{A}$ into the Maxwell equations leads to the fundamental Lorentz-covariant Wave Equation

$$(\eta^\mu{}_\nu \Box + \partial^\mu \partial_\nu)\, A^\nu_{\mathrm{tot}} = \mu_0\, (\boldsymbol{j}_{\mathrm{ind}} + \boldsymbol{j}_{\mathrm{ext}})$$

Eliminating the induced current in the spirit of response theory and setting $\boldsymbol{j}_{\mathrm{ext}} \equiv 0$ produces

$$(\eta^\mu{}_\nu \Box + \partial^\mu \partial_\nu - \mu_0\, \widetilde{\chi}^\mu{}_\nu)\, A^\nu_{\mathrm{tot}} = 0$$

$\widetilde{\chi}^\mu{}_\nu = \dfrac{\delta j^\mu_{\mathrm{ind}}}{\delta A^\nu_{\mathrm{tot}}}$ $\qquad$ $\widetilde{\chi}^\mu{}_\nu \equiv 0$ → vacuum case

Q: What happens for the most simple assumption of a constant $\widetilde{\chi}^\mu{}_\nu$?

A: We obtain the London model with purely diamagnetic current $\boldsymbol{j} = \boldsymbol{j}_{\mathrm{dia}}$.

The London Model of Superconductivity is the simplest possible materials model from a response theoretical point of view.

$$\boxed{\text{London:} \quad \boldsymbol{j} = -\frac{ne^2}{m}\boldsymbol{A}} \quad \text{with} \quad \overleftrightarrow{\chi} = \overleftrightarrow{\chi}_{\mathrm{dia}}$$

- completely isotropic, local and instantaneous (proper) response
- Meißner Effect, zero electrical "DC resistance" and plasma frequency via URR
- highly related to Drude Model and with some cheating also Lorentz Oscillator Model

→ Spin-correction has no considerable effect.

LONDON MODEL VS. FREE ELECTRON GAS

Based on QM, the Free Electron Gas describes free charge carriers in a solid and is surprisingly successful in reproducing many exp. phenomena.

Q: What changes when we replace the London Model with the Free Electron Gas and explicitly include spinorial current contributions ?

Optical Properties:

→ FEG adds q^2 term

$$\operatorname{Im}\sigma_{\mathrm{T}}^{\mathrm{ns}} = \frac{ne^2}{\omega m}\left(1 + \frac{1}{5}\,\frac{\boldsymbol{q}^2 v_{\mathrm{F}}^2}{\omega^2} + \frac{3}{35}\,\frac{q^4 v_{\mathrm{F}}^4}{\omega^4} + \mathcal{O}\left(q^6\right)\right)$$

→ spin-correction adds order q^4 contributions

$$\operatorname{Im}\sigma_{\mathrm{T}}^{\mathrm{spin}} = \frac{ne^2}{\omega m}\left(\frac{1}{4}\,\frac{v_{\mathrm{F}}^2}{k_{\mathrm{F}}^2}\,\frac{\boldsymbol{q}^4}{\omega^2} + \mathcal{O}(q^6)\right)$$

⇒ no significant impact on dispersion relation!

Magnetic Properties:

→ (dia + orb) parts lead to Landau Diamagnetism

$$\chi_{\mathrm{m}}^{\mathrm{ns}} \stackrel{\omega\to 0}{=} \mu_0\mu_B^2\, g(E_{\mathrm{F}})\left(-\frac{1}{3} + \frac{1}{60}\,\frac{q^2}{k_{\mathrm{F}}^2} + \mathcal{O}(q^4)\right)$$

→ spin-correction adds `Pauli Paramagnetism`

$$\chi_{\mathrm{m}}^{\mathrm{spin}} \stackrel{\omega\to 0}{=} \mu_0\mu_B^2\, g(E_{\mathrm{F}})\left(1 - \frac{1}{12}\,\frac{q^2}{k_{\mathrm{F}}^2} + \mathcal{O}(q^4)\right)$$

⇒ reproduces Landau and Pauli mag. via URR

LINDHARD INTEGRAL THEOREM

Central Result: Current response of FEG can be reduced to 3 dimensionless parameter integrals. Complete response is then determined by these integrals, Lindhard density response and constant charge density.

$$(\overleftrightarrow{\chi})_{ij}(\boldsymbol{q},\omega) = -\left(\frac{e^2 n}{m} + \frac{\hbar^2 |\boldsymbol{q}|^2}{4m^2}\,\chi_{nn}(\boldsymbol{q},\omega)\right)\delta_{ij} + \alpha_{ij}(\boldsymbol{q},\omega) + q_i\,\beta_j(\boldsymbol{q},\omega) + \beta_i(\boldsymbol{q},\omega)\,q_j$$

$$\alpha_{ij}(\boldsymbol{q},\omega) = -\frac{\hbar^2}{4m^2}\left(2e^2\int\frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3}\,4k_i k_j\,\frac{f_{\boldsymbol{k}} - f_{\boldsymbol{k}+\boldsymbol{q}}}{\hbar\omega^+ + \varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}+\boldsymbol{q}}}\right)$$

$$\beta_i(\boldsymbol{q},\omega) = -\frac{\hbar^2}{4m^2}\left(2e^2\int\frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3}\,2k_i\,\frac{f_{\boldsymbol{k}} - f_{\boldsymbol{k}+\boldsymbol{q}}}{\hbar\omega^+ + \varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}+\boldsymbol{q}}}\right)$$

⇒ can be reduced from 12 to 3

⇒ can be solved analytically for Zero Temperature Case

⇒ can be expressed by Lindhard Int.

$$n = 2\int\frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3}\,f_{\boldsymbol{k}} = \int \mathrm{d}\omega\, g(\omega)\, f(\omega)\,, \qquad \chi_{nn}(\boldsymbol{q},\omega) = 2e^2\int\frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3}\;1\;\frac{f_{\boldsymbol{k}} - f_{\boldsymbol{k}+\boldsymbol{q}}}{\hbar\omega^+ + \varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}+\boldsymbol{q}}}$$

SUMMARY & CONCLUSION

Based on exclusively microscopic field theory it is shown that via URR that all relevant linear optical and magnetic materials properties of the FEG follow from the full current response tensor. (Central Claim)

In particular:

- By Ampères Law, every magnetization is generated by a microscopic current
- As a matter of principle, this also includes spin-induced magnetism

Implication

- All contributions to the current should be treated equally in Linear Response Theory

Derived in this Thesis

- Full current operator based on the Pauli Equation
- General form of $\overleftrightarrow{\chi}$ for the FEG
- Analytic expressions in Zero Temperatur Case
- Postulation & proof of Lindhard Integral Theorem

Further Work

- Algorithm for n_{e} and n_{o} from given σ
- 2^{nd}-order non-linear analogon of $\chi^{\mu}{}_{\nu}$

THANKS FOR THE ATTENTION!

— Acknowledgements —

Prof. Jens Kortus
(supervisor)

Prof. Caterina Cocchi
(2nd referee)

Haushalt
(funding)

Institute for Theoretical Physics
(hospitality)

ANY QUESTIONS?

— Special Thanks —

Dr. Ronald Starke
(person in charge)

Dr. Giulio Schober
(2nd person in charge)

My Wife
(not in charge but calls the tune anyways)

Friends & Family
(always helpful...
...most of the time)

LINDHARD INTEGRAL THEOREM (2)

For zero temperature case:

$$\alpha_{xx} = E_\mathrm{F}\, g(E_\mathrm{F})\, \frac{e^2}{m}\, \frac{(-2)}{4\hat{q}} \left(I_{\alpha xx}(\nu_-) - I_{\alpha xx}(\nu_+)\right)$$

$$\alpha_{zz} = E_\mathrm{F}\, g(E_\mathrm{F})\, \frac{e^2}{m}\, \frac{(-4)}{4\hat{q}} \left(I_{\alpha zz}(\nu_-) - I_{\alpha zz}(\nu_+)\right)$$

$$\beta_{z} = \frac{E_\mathrm{F}\, g(E_\mathrm{F})}{k_\mathrm{F}}\, \frac{e^2}{m}\, \frac{(-2)}{4\hat{q}} \left(I_{\beta z}(\nu_-) + I_{\beta z}(\nu_+)\right)$$

$$\frac{\hbar^2}{4m^2}\chi_{nn} = \frac{E_\mathrm{F}\, g(E_\mathrm{F})}{k_\mathrm{F}^2}\, \frac{e^2}{m}\, \frac{(+1)}{4\hat{q}} \left(I_{\chi}(\nu_-) - I_{\chi}(\nu_+)\right)$$

Master Formula

$$\hat{\gamma}(\hat{q},\hat{\omega}) = \frac{\gamma_0}{4\hat{q}} \left(I_\gamma(\nu_-) + I_\gamma(-\nu_+)\right)$$

γ	χ_{nn}	α_{xx}	α_{zz}	β_z
γ_0	$+1$	-2	-4	-2

$$I_{\alpha xx}(z) \stackrel{\mathrm{def}}{=} \int_0^1 \mathrm{d}x\, x^4 \int_0^\pi \mathrm{d}\theta\, \frac{\sin^3\theta}{z - x\cos\theta} = \frac{1}{3}z + \frac{1-z^2}{2} I_\chi(z)$$

$$I_{\alpha zz}(z) \stackrel{\mathrm{def}}{=} \int_0^1 \mathrm{d}x\, x^4 \int_0^\pi \mathrm{d}\theta\, \frac{\sin\theta\cos^2\theta}{z - x\cos\theta} = -\frac{2}{3}z + z^2 I_\chi(z)$$

$$I_{\beta z}(z) \stackrel{\mathrm{def}}{=} \int_0^1 \mathrm{d}x\, x^3 \int_0^\pi \mathrm{d}\theta\, \frac{\sin\theta\cos\theta}{z - x\cos\theta} = -\frac{2}{3} + z I_\chi(z)$$

$$\nu_\pm = \frac{\omega}{q v_\mathrm{F}} \pm \frac{q}{2k_\mathrm{F}}$$

$$I_\chi(z) = z + \frac{1-z^2}{2}\,\mathrm{Ln}\left(\frac{z+1}{z-1}\right)$$

All characteristic integrals can be expressed in terms of the Lindhard integral!