Orbital polarization and magnetization for independent particles in disordered media

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1. Introduction

Some basic observations:

• Macroscopic polarization in crystalline solids is the sum of two contributions: electronic and nuclear.

• Macroscopic magnetization is a purely electronic phenomenon, but it is the sum of two contributions as well: spin magnetization and orbital magnetization.

While nuclear and the spin contributions are well understood, the microscopic definition and resulting quantitative formulas for the orbital contributions are rather recent.
1. Introduction

Given the intuitive meaning of $P$ and $M$, it is tempting to define them as the dipole moment of a sample, divided by the volume $V$

$$P = \frac{1}{V} \int x \rho(x) \, dx \quad \text{and} \quad M = \frac{1}{V} \int x \wedge j(x) \, dx,$$

where $\rho$ and $j$ are the microscopic charge and current densities.

But these expressions do not define bulk properties.

R. Resta: “The macroscopic polarization (magnetization) of a uniformly polarized (magnetized) crystal has nothing to do with the lattice periodical charge (current) distribution—despite contrary statements in several textbooks.”
1. Introduction

Orbital Polarization:
Experimentally accessible are only polarization differences. 1993 King-Smith, Vanderbilt, Resta observed that

$$\Delta P = \int_0^T j(t) \, dt$$

and derived an explicit formula for $\Delta P$ for perfect crystals in the adiabatic limit. They computed accurately the Piezoelectric polarization in GaAs.

Orbital Magnetization:
The first formula for the orbital magnetization at zero field and zero temperature was given by Gat and Avron in 2003 for the Hofstadter model based on the thermodynamic definition

$$M(\beta, \mu, B) = \frac{\partial}{\partial B} p(\beta, \mu, B).$$

The formula for general periodic solids at zero field and positive temperature was found by Xiao, Shi and Niu and independently by Thonhauser, Ceresoli, Vanderbilt and Resta in 2005.
2. Modeling homogenous media

Our goal is to understand polarization and magnetization for non-interacting electrons or holes in periodic, quasiperiodic or random media under the influence of a constant magnetic field $\mathbf{B}$.

**Tight-binding approximation:**

$$\mathcal{H} = \ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^L$$

For $d = 2$ or $d = 3$ the magnetic field is parametrized as

$$\mathbf{B} = \begin{pmatrix} 0 & B_3 \\ -B_3 & 0 \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} 0 & B_3 & -B_2 \\ -B_3 & 0 & B_1 \\ B_2 & -B_1 & 0 \end{pmatrix}$$

and the magnetic translations on $\ell^2(\mathbb{Z}^d)$ are defined as

$$(U_a \psi)_n = e^{-\frac{i}{2} a \cdot \mathbf{B} n} \psi_{n-a} \quad \text{and} \quad (\tilde{U}_a \psi)_n = e^{\frac{i}{2} a \cdot \mathbf{B} n} \psi_{n-a}.$$ 

As $\mathbf{B}$ enters only through the magnetic translations, we can restrict $\mathbf{B}$ to values in the torus $\Xi = [-\pi, \pi)^{\frac{1}{2}d(d-1)}$. 
Homogeneous families of Hamiltonians:
Let \((H_\omega)_{\omega \in \Omega}\) be a family of bounded self-adjoint operators on \(\mathcal{H}\) depending continuously on a parameter \(\omega\) that varies in the compact space \(\Omega\) of disorder or crystal configurations.

Suppose that there is a continuous action \(T\) of the translation group \(\mathbb{Z}^d\) on \(\Omega\), then \((H_\omega)_{\omega \in \Omega}\) is called **homogeneous** if

\[
U_a H_\omega U_a^{-1} = H_{T_a \omega} \quad \text{for all } a \in \mathbb{Z}^d.
\]

For example

\[
H_\omega = H_0 + V_\omega, \quad H_0 = \sum_{m \in \mathbb{Z}^d} T_m \tilde{U}_m, \quad V_\omega = \sum_{n \in \mathbb{Z}^d} V_{\omega,n} |n\rangle \langle n|,
\]

where \(T_m, V_{\omega,n} \in \text{Mat}(L, \mathbb{C})\) with \(T_m^* = T_{-m}\) and \(V_{\omega,n}^* = V_{\omega,n}\). If \(V_{\omega,n}\) are taken from a compact set \(K \subset \text{Mat}(L, \mathbb{C})\), then \(\Omega = K^{\mathbb{Z}^d}\) and \(T\) the shift.
2. Modeling homogenous media

One can think of the family \((H_\omega)\) as a single element of a suitable \(C^*-\text{Algebra } \mathcal{A}_B\) indexed by the magnetic field \(B\):

The space \(C_0(\Omega \times \mathbb{Z}^d; \text{Mat}(L, \mathbb{C}))\) endowed with the multiplication

\[
AB(\omega, n) = \sum_{l \in \mathbb{Z}^d} A(\omega, l) B(T^{-l} \omega, n - l) e^{i n \cdot B l}
\]

and the involution

\[
A^*(\omega, n) = A(T^{-n} \omega, -n)^*
\]

becomes a \(*\)-algebra.

For \(\omega \in \Omega\), a representation of this \(*\)-algebra on \(\mathcal{H}\) is given by

\[
\left( \pi_{B, \omega}(A) \psi \right)_n = \sum_{l \in \mathbb{Z}^d} A(T^{-n} \omega, l - n) e^{i l \cdot B n} \psi_l
\]

and the representations \(\pi_{B, \omega}\) are related by the covariance relation

\[
U_a \pi_{B, \omega}(A) U_a^{-1} = \pi_{B, T^a \omega}(A).
\]
2. Modeling homogenous media

Now

$$\|A\| := \sup_{\omega \in \Omega} \|\pi_{B,\omega}(A)\|$$

defines a $C^*$-norm on $C_0(\Omega \times \mathbb{Z}^d, \text{Mat}(L, \mathbb{C}))$ and the $C^*$-algebra $A_B$ is defined as its completion under this norm.

Since the norm $\|\pi_{B,\omega}(A)\|$ is independent of $B$, the closures $A_B$ are identical as Banach spaces to a space $\tilde{A}$, even though the algebraic structure and the representations $\pi_{B,\omega}$ do depend on $B$.

Finally let $A$ be the Banach space $C(\Xi, \tilde{A})$ with the sup-norm. By taking products and adjoints pointwise, also $A$ becomes a $C^*$-algebra. It contains the continuous and compactly supported functions on $\Xi \times \Omega \times \mathbb{Z}^d$ with values in $\text{Mat}(L, \mathbb{C})$ as a dense set.

For example $H \in A$ with

$$H(B, \omega, n) = T_n + \delta_{n,0}V_{\omega,0}$$

yields $\pi_{B,\omega}(H) = H_0 + V_{\omega}$. 
2. Modeling homogenous media

As we will be interested in currents, i.e.

\[ \dot{X}_j = i[H_\omega, X_j] \]

we introduce the ∗-derivations \( \nabla_j \) defined on their common dense domain \( C^1_s(A) \) by

\[ \nabla_j A(B, \omega, n) := i n_j A(B, \omega, n) . \]

They satisfy

\[ \pi_{B,\omega}(\nabla_j A) = i[\pi_{B,\omega}(\nabla_j A), X_j] \]

and for \( H \in C^1_s(A) \) we define the corresponding current \( J \) as

\[ J = \nabla H . \]
2. Modeling homogenous media

Given a $T$-invariant probability measure $\mathbb{P}$ on $\Omega$, a positive trace $\mathcal{T}_B$ on $A$ (and each $A_B$) is defined by

$$\mathcal{T}_B(A) = \int_{\Omega} \mathbb{P}(d\omega) \text{Tr}(A(B,\omega,0))$$

and satisfies, in particular,

$$\mathcal{T}_B(\nabla A) = 0 \quad \text{and} \quad \mathcal{T}_B(A\nabla B) = -\mathcal{T}_B(\nabla AB)$$

for all $A, B \in C^1_S(A_B)$.

If $\mathbb{P}$ is in addition ergodic, then $\mathcal{T}_B$ is the trace per unit volume, i.e.

$$\mathcal{T}_B(A) = \lim_{l \to \infty} \frac{1}{|\Lambda_l|} \sum_{n \in \Lambda_l} \text{Tr}(\langle n|\pi_B,\omega(A)|n \rangle)$$

for $\mathbb{P}$-almost all $\omega \in \Omega$. 
3. Orbital Polarization

The orbital polarization induced by a time-dependent change of the Hamiltonian at a fixed magnetic field $B$ is defined as

$$\Delta P = \int_0^T dt \, T_B(\rho(t) \nabla H(t)).$$

Here $t \mapsto H(t)$ is a continuous path in $C^1_s(\mathcal{A}_B)$ and $\rho(t) := \eta_{t,0} \rho_0$ is a solution of the Liouville equation

$$\frac{d}{dt} \rho(t) = i[\rho(t), H(t)]$$

with initial data $\rho(0) = \rho_0 \in \mathcal{A}_B$. 
Proposition 1 (The current density for projections)

Let \( P \in C^1_\mathcal{S}(\mathcal{A}) \) be any projection. Then the current associated to the solution \( P(t) = \eta_{t,0}(P) \) of the Liouville equation can be written as

\[
\mathcal{T}_B \left( P(t) \nabla H(t) \right) = i \mathcal{T}_B \left( P(t) \left[ \partial_t P(t), \nabla P(t) \right] \right).
\]

Proof:

\[
i \mathcal{T}_B \left( P \left[ \partial_t P, \nabla P \right] \right) = \mathcal{T}_B \left( P[H, P] \nabla P \right) - \mathcal{T}_B \left( P \left( \nabla P \right)[H, P] \right) \\
= - \mathcal{T}_B \left( (\nabla P) PH \right) - \mathcal{T}_B \left( (\nabla P) HP \right) \\
= \mathcal{T}_B \left( P \nabla (PH) \right) - \mathcal{T}_B \left( P(\nabla P) H \right) \\
= \mathcal{T}_B \left( P \nabla H \right).
\]
3. Orbital Polarization

**Corollary 1 (The general polarization formula)**

Assume that the Fermi level $\mu$ lies in a gap of the spectrum of $H(0)$ and let $\rho_0 = P_\mu(0) := \chi_{(-\infty,\mu]}(H(0))$ be the Fermi projection. Then

$$\Delta P = i \int_0^T dt \ T_B(\rho(t) [\partial_t \rho(t), \nabla \rho(t)]) .$$

**Proof:** For $\mu$ in a gap it holds that $P_\mu(0) \in C^1_S(A)$. 
3. Orbital Polarization

If $H(t)$ changes slowly, then by the adiabatic theorem $\rho(t) \approx P_{\mu(t)}(t)$ and thus

$$\Delta P \approx i \int_0^T dt \ T_B \left( P_{\mu(t)}(t) [\partial_t P_{\mu(t)}(t), \nabla P_{\mu(t)}(t)] \right).$$

In the case of a periodic crystal this formula reduces to the King-Smith and Vanderbilt formula.

Note that inserting the adiabatic approximation into the original formula yields

$$\Delta P = \int_0^T dt \ T_B (\rho(t) \nabla H(t)) \approx \int_0^T dt \ T_B (P_{\mu(t)}(t) \nabla H(t)) = 0,$$

since $T_B (f(H) \nabla H) = 0$ for any $C^2$-function $f$.

To make the adiabatic approximation precise, let $\rho(t)$ be the solution of the adiabatic Liouville equation for $\varepsilon > 0$

$$\varepsilon \frac{d}{dt} \rho(t) = i [\rho(t), H(t)].$$
3. Orbital Polarization

Theorem 1 (The adiabatic polarization formula)

Let

(i) either \( H \in C^{N+2}([0,T], C^1_S(A)) \) with

\[
\partial^n_t H(t)|_{t=0} = \partial^n_t H(t)|_{t=T} = 0, \quad \text{for all } 1 \leq n \leq N,
\]

(ii) or \( H \in C^{N+2}(\mathbb{R}, C^1_S(A)) \) be \( T \)-periodic.

Further suppose that there is a continuous function \( \mu(t) \) with \( \mu(t) \notin \sigma(H(t)) \) for all \( t \in [0,T] \). Let \( \rho_0 = P_\mu(0) \) in case (i) and \( \rho_0 = P^\varepsilon_N(0) \) in case (ii), where \( P^\varepsilon_N(0) \) is a superadiabatic projection constructed in the proof. Then

\[
\Delta P = i \int_0^T dt \, \mathcal{T}_B \left( P_\mu(t) [\partial_t P_\mu(t), \nabla P_\mu(t)] \right) + \mathcal{O}(\varepsilon^N).
\]
3. Orbital Polarization

**Proof:** A suitable version of the super-adiabatic construction of Nenciu for $C^*$-dynamical systems yields the superadiabatic projections $P^\varepsilon_N(t)$ with

$$P^\varepsilon_N(t) - \rho(t) = \mathcal{O}(\varepsilon^N) \quad \text{and} \quad P^\varepsilon_N(t) - P_\mu(t) = \mathcal{O}(\varepsilon)$$

and thus

$$\Delta P = i \int_0^T dt \, \mathcal{T}_B\left(P^\varepsilon_N(t) [\partial_t P^\varepsilon_N(t), \nabla P^\varepsilon_N(t)]\right) + \mathcal{O}(\varepsilon^N).$$

But with

$$\partial_\varepsilon \int_0^T dt \, \mathcal{T}_B\left(P^\varepsilon_N[\dot{P}^\varepsilon_N, \nabla P^\varepsilon_N]\right) = \int_0^T dt \, \mathcal{T}_B\left(P^\varepsilon_N[\partial_\varepsilon \dot{P}^\varepsilon_N, \nabla P^\varepsilon_N] + P^\varepsilon_N[\dot{P}^\varepsilon_N, \partial_\varepsilon \nabla P^\varepsilon_N]\right)$$

$$= \mathcal{T}_B\left(P^\varepsilon_N[\partial_\varepsilon P^\varepsilon_N, \nabla P^\varepsilon_N]\right) \bigg|_0^T$$

$$- \int_0^T dt \, \mathcal{T}_B\left(P^\varepsilon_N[\partial_\varepsilon P^\varepsilon_N, \nabla \dot{P}^\varepsilon_N]\right) + \int_0^T dt \, \mathcal{T}_B\left(P^\varepsilon_N[\dot{P}^\varepsilon_N, \nabla \partial_\varepsilon P^\varepsilon_N]\right) = 0.$$

the expression does not depend on $\varepsilon$ for cases (i) and (ii) and thus we can go to the limit $\varepsilon \to 0$ without changing the value of the integral.
3. Orbital Polarization

Remarks

• By the same argument one can show that $\Delta P$ is invariant under diffeotopic changes of the path $H(t)$.

• For a periodic change the charge transported in one cycle is quantized,

$$\Delta P = \hat{\mathcal{T}}_B(\hat{P}_\mu \lbrack \partial_t \hat{P}_\mu, \nabla \hat{P}_\mu \rbrack) = 2\pi \text{Ch}(\hat{P}_\mu) + \mathcal{O}(\varepsilon^N)$$

where $\hat{P}_\mu = (P_\mu(t)) \in C(S^1_T) \otimes \mathcal{A}$ and by the first item independent of any disorder that does not close the gap.

• For periodic systems and $\mathbf{B} = 0$ this formula was proved in [Panati-Sparber-T., 2007] also without the tight-binding approximation.
4. Orbital Magnetization

The magnetization at inverse temperature $\beta$ and chemical potential $\mu$ is defined as the derivative of the free energy per volume with respect to the magnetic field,

$$M_j(\beta, \mu, B) = \partial_{B_j} \frac{1}{\beta} \mathcal{T}_B \left( \ln(1 + e^{-\beta(H-\mu)}) \right).$$

Our main result is

**Theorem 2 (Magnetization at zero temperature)**

Suppose that the chemical potential $\mu$ lies in an interval $\Delta$ with finite localization length $\ell^2(\Delta)$ and that the density of states has no atom at $\mu$. Let $P_\mu = f_{\infty, \mu}(H)$ denote the Fermi projection and suppose that $\delta H = 0$. Then, with $j$ taken cyclically,

$$M_j(\infty, \mu, B) = -\frac{i}{2} \mathcal{T}_B \left( |\mu - H| [\nabla_{j+1} P_\mu, \nabla_{j+2} P_\mu] \right).$$
4. Orbital Magnetization

On \( C^1(\Xi, \tilde{A}) \), the set of all continuously differentiable elements in \( \mathcal{A} = C(\Xi, \tilde{A}) \), let us set for each \( j = 1, 2, 3 \),

\[
(\delta_j A)(B) = \partial_{B_j} A(B).
\]

\( \delta \) is not a derivation but satisfies instead

\[
\delta_j(AB) = (\delta_j A)B + A(\delta_j B) + \frac{i}{2}(\nabla_{j+1} A \nabla_{j+2} B - \nabla_{j+2} A \nabla_{j+1} B),
\]

\[
\delta_j(A^*) = \delta_j(A)^*, \quad \delta_j \nabla_k A = \nabla_k \delta_j A \quad \text{and} \quad \partial_{B_j} \mathcal{T}_B(A) = \mathcal{T}_B(\delta_j A).
\]

As a consequence, for \( H = H(\omega, n) \in \mathcal{A} \) independent of \( B \), we have

\[
\delta_j H = 0 \quad \text{but} \quad \delta_j H^2 = \frac{i}{2}[\nabla_{j+1} H, \nabla_{j+2} H].
\]

Hence

\[
M_j(\beta, \mu, B) = \partial_{B_j} \frac{1}{\beta} \mathcal{T}_B \left( \ln(1 + e^{-\beta(H-\mu)}) \right)
\]

is nontrivial even when \( \delta H = 0 \).
4. Orbital Magnetization

For \( z \in \mathbb{C} \) we prove a generalized Duhamel formula

\[
\delta_j e^{zA} = z \int_0^1 ds \ e^{(1-s)zA} \delta_j A e^{szA} \\
+ \frac{i}{2} z^2 \int_0^1 ds \int_0^s dr \ e^{(1-s)zA} \left( \nabla_{j+1} A e^{rzA} \nabla_{j+2} A e^{(s-r)zA} - \nabla_{j+2} A e^{rzA} \nabla_{j+1} A e^{(s-r)zA} \right)
\]

that together with the identity

\[
\ln(1 + e^{-\beta E}) = \ln(2) + \int_0^\beta d\beta' \frac{-E}{1 + e^{\beta' E}}
\]

allows us to compute

\[
M_j(\beta, \mu, B) = \partial_{B_j} \frac{1}{\beta} \mathcal{T}_B \left( \ln(1 + e^{-\beta(H-\mu)}) \right)
\]
4. Orbital Magnetization

The resulting expression can be written in terms of the current-current correlation measure $m_{i,j}$ which is a positive-matrix-valued measure on $\mathbb{R}^2$ defined through

$$\mathcal{T}_B \left( f(H) \nabla_i H g(H) \nabla_j H \right) = \int_{\mathbb{R} \times \mathbb{R}} m_{i,j}(dE, dE') f(E) g(E') \quad \text{for all } f, g \in C_0(\mathbb{R}).$$

**Theorem 3 (Magnetization at finite temperature)**

Let $\delta H = 0$. Then

$$M_j(\beta, \mu) = i \int_{\mathbb{R}^2} m_{j+1,j+2}(dE, dE') g_{\beta,\mu}(E, E') ,$$

where $g_{\beta,\mu}$ is the following smooth function

$$g_{\beta,\mu}(E, E') = \frac{1}{2} \frac{1}{E' - E} \left( f_{\beta,\mu}(E) + \frac{1}{\beta} \frac{\ln(1 + e^{-\beta(E'-\mu)}) - \ln(1 + e^{-\beta(E-\mu)})}{E' - E} \right)$$

$$- (E \leftrightarrow E').$$
4. Orbital Magnetization

The current-current correlation measure is related to the localization length (Bellissard, Elst, Schulz-Baldes 1994)

\[ \ell^2(\Delta) = \sup_{T>0} \int_0^T \frac{dt}{T} \mathbb{E} \langle 0 | \chi_{\Delta}(\pi_B, \omega(H)) \left( e^{i\pi_B, \omega(H)t} X e^{-i\pi_B, \omega(H)t} - X \right)^2 \chi_{\Delta}(\pi_B, \omega(H)) | 0 \rangle \]

through

\[ \ell^2(\Delta) = 2 \int_{\Delta \times \mathbb{R}} m(dE, dE') \frac{1}{|E - E'|^2}. \]

To get Theorem 2, we assume \( \ell^2(\Delta) < \infty \) and take the limit \( \beta \to \infty \) on the expression

\[ M_j(\beta, \mu) = i \int_{\mathbb{R}^2} m_{j+1, j+2}(dE, dE') g_{\beta, \mu}(E, E'). \]

In a last step, the limiting expression can be connected again to the Fermi projection, but this time in \( H^1(A, T) \).
Corollary 2 (Magnetization for periodic systems)

Let $H$ be 1-periodic, $\delta H = 0$ and $B = 0$. Suppose that all Bloch-bands are isolated, i.e. $E_1(k) < E_2(k) < \ldots < E_L(k)$ for all $k \in \mathbb{T}^d$. Then the magnetization is given by

$$M_j(\beta, \mu) = \sum_{l=1}^L \int \frac{dk}{(2\pi)^d} \left( f_{\beta, \mu}(E^{(l)}(k)) \left[ R_{j+1,j+2}^{(l)}(k) + \frac{1}{\beta} \ln \left( 1 + e^{-\beta (E^{(l)}(k) - \mu)} \right) \Omega_{j+1,j+2}^{(l)}(k) \right] \right)$$

where

$$R_{ij}^{(l)}(k) = \frac{i}{2} \text{tr} \left( P^{(l)}(k) \left[ \partial_{k_i} P^{(l)}(k) | H(k) - E^{(l)}(k) | \partial_{k_j} P^{(l)}(k) \right] \right)$$

is the Rammal-Wilkinson tensor and

$$\Omega_{ij}^{(l)}(k) = i \text{tr} \left( P^{(l)}(k) \left[ \partial_{k_i} P^{(l)}(k), \partial_{k_j} P^{(l)}(k) \right] \right)$$

the curvature of the Berry connection of the $l$th Bloch band.
4. Orbital Magnetization

Remarks

• The formula for zero temperature with $\mu$ in a gap was first stated by Gat and Avron in 2003 for the Hofstadter Hamiltonian.

• The finite temperature formula for periodic crystals was first found by Niu et al. in 2005 using the modified semiclassical model:

$$p(\beta, \mu, B) = \frac{1}{(2\pi)^2} \sum_{l=1}^{L} \int_{\mathbb{T}^3} d\lambda^{(l)}_B \ln \left( 1 + e^{-\beta (H_B^{(l)}(k) - \mu)} \right) + O(B^2)$$

with Liouville measure

$$d\lambda^{(l)}_B = \left( 1 + \text{tr} \left( \Omega^{(l)}(k) B \right) \right) d^3k$$

and classical Hamiltonian function

$$H_B^{(l)}(k) = E^{(l)}(k) + \text{tr} \left( R^{(l)}(k) B \right).$$

• The same formula was independently derived by Ceresoli, Thonhauser, Vanderbilt and Resta 2005.

• Rigorous derivation of the semiclassical model in Stiepan-T. 2012.
4. Orbital Magnetization

From Ceresoli, Thonhauser, Vanderbilt and Resta:

“The fact that our final formula is identical to the one derived from the semiclassical wavepacket treatment [of Xiao, Shi and Niu] is reassuring, but neither of these approaches can yet be said to constitute a derivation of the formula in the fully quantum context. Nevertheless, we provide strong numerical evidence of their validity, thus posing a theoretical challenge: how to provide an analytic proof of the heuristic formula, beyond the range of the semiclassical approximation, for both the metallic and Chern-insulating cases.”
5. Literature

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Many thanks for your attention!