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Electron polarizability of crystalline solids in quantizing magnetic fields and topological gap numbers

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A theory of the static electron polarizability of crystals whose energy spectrum is modified by quantizing magnetic fields is presented. The polarizability is strongly affected by non-dissipative Hall currents induced by the presence of crossed electric and magnetic fields: these can even change its sign. Results are illustrated in detail for a two dimensional square lattice. The polarizability and the Hall conductivity are respectively linked to the two topological quantum numbers entering the so–called Diophantine equation. These numbers could in principle be detected in actual experiments.

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The polarizability is usually presented as an important property of insulators [1]. An electric field imposed between the plates of a capacitor penetrates into their interior, and charge redistribution is induced within the system. This effect is characterized by the polarizability: the ratio of induced dipole moments per unit volume and the local field. In metals this charge redistribution is non-uniform because of the charge mobility and the local electric field is non-uniform as well. In the particular case that the distribution of the atomic cores is not affected by the applied electric field, it is the electronic charge redistribution only which determines the polarizability of insulators as well as metals.

Crystalline solids have an energy spectrum composed of energy bands. They become insulators whenever the Fermi energy is located within an energy gap between these bands. Additional energy gaps can be opened by applying strong magnetic fields to two-dimensional (2D) as well as to three-dimensional crystals [2, 3, 4]: the energy spectrum of 2D crystals is separated in an integer number of subbands whenever the number of flux quanta contained in the unit cell corresponds to a rational number [2]. The number of electrons per subband is specified by two topological gap numbers, one of which has been linked to the Hall conductance [5]. The present work establishes that for electrons in a "strong" periodic potential subject to a magnetic field, the remaining gap number is directly linked to the polarizability. We thus limit our attention to the static electron polarizability and its dependence on the electron concentration, i.e. on the Fermi energy μ. This limitation allows to exclude dissipative processes from the consideration: no current flow is allowed along the applied electric field. For the sake of simplicity, an ensemble of spinless electrons at zero temperature is considered. We will also limit our treatment to "ideal" crystals with a rectangular unit cell of volume $a_z A_0$, where a_z is the lattice constant along the $\hat{z}$-direction and $A_0 \equiv a_x a_y$ is the area in the $\hat{x}\hat{y}$ plane.

In the considered geometry, the magnetic field is applied along the $\hat{z}$-direction, parallel with capacitor plates as well as with the z-th crystallographic axis. The external field due to the voltage drop between capacitor plates is applied along the $\hat{y}$-direction. The system is assumed to be open along the $\hat{x}$-direction, (i.e. periodic boundary conditions) allowing non-dissipative current flow. This condition allows the direct comparison of the polarizability with the topological gap numbers. Such condition could be realized in a Corbino geometry with cylindrical capacitor plates of large radius.

We start with the case of a vanishing magnetic field. Generally, electrons are not equally distributed over energy bands. The electron occupation $\tilde{s}_i^{(0)}(\mu)$ of the i-th band per volume $a_z A_0$ obeys the sum rule $a_z A_0 N(\mu) = \sum_i \tilde{s}_i^{(0)}(\mu) \equiv \tilde{s}^{(0)}(\mu)$. Here $N(\mu)$ denotes the electron concentration (the integrated density of states). Whenever the Fermi energy is located within an energy gap, $\tilde{s}^{(0)}(\mu) = s$ (s integer). The wave functions of each band are assumed to be of Bloch-like form (i.e. extended) along the $\hat{x}$-direction while along the $\hat{y}$-direction we consider a Wannier-like form (i.e. localized). With this choice the mass-center positions of the electrons along the $\hat{y}$-direction are well defined by the expectation values of the y-coordinate. Averaging over occupied states belonging to the i-th band gives an average value of the mass-center positions $\langle Y_i(\mu)\rangle$. An electric field along the $\hat{y}$-direction, $\mathcal{E}_y$, leads to a redistribution of the electron charge, which can be characterized by the shifts of the mass-center positions $\langle \Delta Y_i(\mu)\rangle$. These shifts are controlled by the balance of the electric force and of the gradient force, due to the background crystalline potential, which acts in opposite direction to bring the electrons back into their equilibrium positions. Within linear response in $\mathcal{E}_y$, the latter is characterized by a force constant $K_i(\mu)$, so that:

$$-\,\tilde{s}_i^{(0)}(\mu)\, e\mathcal{E}_y \,-\, K_i(\mu)\,\langle \Delta Y_i(\mu)\rangle \,=\, 0\,. \qquad (1)$$

The resulting static electron polarizability $\alpha^{(0)}(\mu)$ is

given as follows

$$\alpha^{(0)}(\mu) \equiv -\frac{e\sum_i \langle \Delta Y_i(\mu)\rangle}{a_z A_0\, \mathcal{E}_y} = \frac{e^2}{a_z A_0} \sum_i \frac{\tilde{s}_i^{(0)}(\mu)}{K_i(\mu)} \,. \quad (2)$$

The above expressions are applicable even in the case of a non-uniform electric field along the $\hat{y}$-direction if the charge redistribution does not affect the values of the force constants K_i. Strictly speaking, for real metallic systems it might be a crude approximation.

Next, an external magnetic field splits the bands into subbands [2, 3, 4]. Because the geometry allows electrons to flow along the $\hat{x}$-direction, the crossed electric $\mathcal{E}_y$ and magnetic B fields give rise to a Hall current density j_H. Consequently, an additional force – the Lorentz force – acts on the electron ensemble. The new balance condition along the $\hat{y}$-direction becomes:

$$-eN(\mu)\,\mathcal{E}_y - \frac{B}{c}\, j_H - \frac{1}{a_z A_0} \sum_i K_i(\mu)\, \langle \Delta Y_i(\mu)\rangle = 0 \,, \quad (3)$$

where the index i now counts available sub-bands. The Hall current density has the standard form

$$j_H = -\frac{e^2}{h}\, \frac{\tilde{\sigma}(\mu)}{a_z}\, \mathcal{E}_y \,, \quad (4)$$

where $\tilde{\sigma}(\mu)$ is dimensionless. Introducing $\tilde{s}(\mu)$ to express the mass-center shifts $\langle \Delta Y_i(\mu)\rangle$ in the form given by Eq. (1), the force balance Eq. (3) becomes:

$$N(\mu) = \frac{\tilde{s}(\mu)}{a_z A_0} + \frac{\tilde{\sigma}(\mu)}{a_z\, 2\pi l_B^2} \,, \quad (5)$$

where $l_B = \sqrt{\hbar c/(eB)}$ is the magnetic length.

The effect of a strong magnetic field on Bloch electrons is more pronounced in 2D systems, which motivates our choice of a crystal formed by 2D planes, perpendicular to the magnetic field, which are separated along the $\hat{z}$-direction by a_z. The lattice constant a_z is large enough that electron transitions between planes are ruled out. We thus consider a single layer only: a 2D crystal with electron concentration $a_z N(\mu)$. As was first noticed by Wannier [6] and recently proved by Kellendonk [7], the necessary condition for the appearance of an energy gap in such systems reads $N(\mu) = s/(a_z A_0) + \sigma/(a_z 2\pi l_B^2)$, where s and σ are integers, often called topological gap numbers, and σ determines the value of the quantum Hall conductance [5]. The comparison of this so-called Diophantine equation with its general form Eq. (5) leads to the conclusion that s is related to the system polarizability.

The relation between polarizability and Hall current is now illustrated with a tight-binding model on a square lattice, $A_0 = a^2$, assuming non-zero overlap between the nearest neighbor sites only. At zero magnetic field it gives a single energy band with cosine dispersion. The effect of the magnetic field is included with the Peierls substitution [2, 8]. This model was first used to obtain the "Hofstadter butterfly" energy spectrum [2]. For rational magnetic fields, satisfying:

$$\frac{A_0}{2\pi l_B^2} = \frac{p}{q} \,, \qquad q = 2i+1 \quad (6)$$

(where p and i are integers), the energy spectrum is composed of q sub-bands well separated by energy gaps for which topological gap numbers are uniquely defined [5, 9].

Choosing the Landau gauge $\vec{A} \equiv (-By, 0, 0)$, the Hamiltonian of the system remains periodic in the $\hat{x}$-direction. Zero-order wavefunctions of each row of atomic orbitals $\phi_a(x-am, y-an)$ along the $\hat{x}$-direction are thus of the following standard form:

$$\Psi^{(0)}_{n,k_x}(\vec{r}) = \sum_m e^{ik_x am} \phi_a(x-am, y-an) \,, \quad (7)$$

where k_x is the wave number. The vector potential between atomic sites belonging to different rows differs by $\Delta A_x = -Ba\Delta n$, and the Peierls substitution suggests to shift k_x entering the zero-field eigenenergies as follows:

$$k_x \to k_x - 2\pi \frac{p}{q}\frac{n}{a} \,, \quad (8)$$

so that phase factors in the overlap integrals arise between orbitals of the neighboring rows. Assuming zero-order eigenfunctions in the form of a linear combination of row-eigenfunctions, Eq. (7), the coefficients $c_n(k_x)$ have to satisfy the following Harper's equation [8, 10]:

$$c_n(k_x)\left[2\cos\left(k_x a - 2\pi\frac{np}{q}\right) + \frac{E-E_a}{\Delta V}\right] + c_{n-1}(k_x) + c_{n+1}(k_x) = 0 \,, \quad (9)$$

where E_a is the energy of the atomic orbitals (chosen to be zero) and ΔV is the overlap strength (the zero field band width is $8\Delta V$). The modulus of the c_n coefficients are periodic with a period q, but their amplitude differs by a phase β: $c_{n+q} = e^{i\beta} c_n$ [11]. For a given $\beta \in [0, 2\pi]$, Eq. (9) gives a system of q equations, and the $c_n(k_x, \beta)$ are eigenvectors of a $q \times q$ matrix. The eigenvalues $E_\beta(k_x)$ give the q sub-bands, each of them composed of energy branches determined by the phase β, which are periodic in k_x with period $2\pi/a$. Because of the periodicity of the $|c_n(k_x, \beta)|$, it is natural to define Wannier-like functions, which are extended (localized) along the $\hat{x}$ ($\hat{y}$) direction:

$$w_{n,k_x,\beta}(\vec{r}) = \sum_{\lambda=-i}^{+i} c_{n+\lambda}(k_x, \beta)\, \Psi^{(0)}_{n+\lambda,k_x}(\vec{r}) \,. \quad (10)$$

The average mass-center position in the $\hat{y}$-direction reads:

$$Y_{n,\beta}(k_x) \equiv \int y |w_{n,\beta,k_x}(\vec{r})|^2 d\mathbf{r} = an + Y^{(B)}_\beta(k_x) \,, \quad (11)$$

where

$$Y_\beta^{(B)}(k_x) \;=\; a \sum_{\lambda=-i}^{+i} \lambda |c_\lambda(k_x,\beta)|^2 \;, \qquad (12)$$

which vanishes at zero magnetic field.

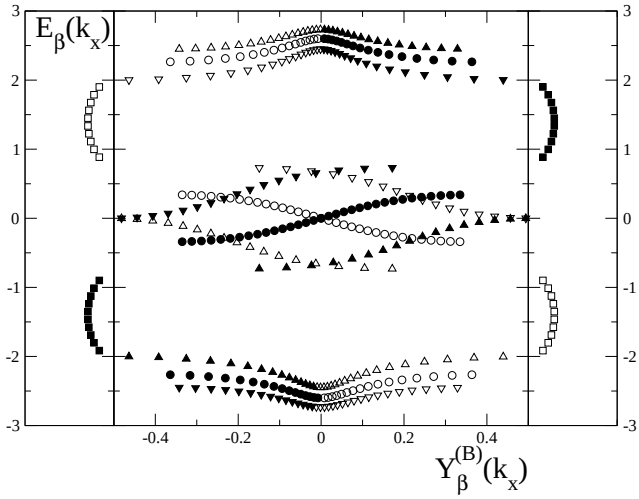

FIG. 1: Energy spectrum $E_\beta(k_x)$ (in units of the overlap strength ΔV) as a function of the center of mass coordinate $Y_\beta^{(B)}(k_x)$ (in units of the lattice constant) for the fraction $p/q = 1/3$, shown for $\beta = 0$ (down triangles), $\beta = \pi/2$ (circles) and $\beta = \pi$ (up triangles). Empty (filled) symbols correspond to positive (negative) velocity along the x axis. The left and right sides show the magnetic edge states inside the energy gaps.

The eigenvalue problem is mathematically equivalent to the one found for a weak periodic potential in a strong magnetic field [12], and leads to the same spectrum as a function of k_x, except that the values of p and q are interchanged. However, the spectrum presented as a function of the mass center position differs substantially from that of the weak periodic potential. For the ratio $p/q = 1/3$, the energy spectrum is composed of three subbands, each of them formed by the branches obtained for all values of β. The spectrum is symmetric with respect to zero energy because of electron-hole symmetry. This is illustrated in Fig. 1, where only three values $\beta = 0, \pi/2$ and π are shown. The branches $\beta = 0,\ \pi$ correspond to the subband edges, while $\beta = \pi/2$ characterizes the central branch. At the crystal edges, determined by the values n_L and n_R of the row index n, the natural condition that $c_{n_L-1} = c_{n_R+1} = 0$ leads to the appearance of edge states formed by contributions from each of the energy branches β. Two types of edge states appear, non-magnetic edge states and magnetic ones [8, 13] which are responsible for the quantum Hall effect. The latter have opposite velocities at opposite edges, and are shown in Fig. 1 for $p/q = 1/3$. Note that in the thermodynamic limit, the mass-center positions of edge states can be identified with the edges of the physical system.

Next, we switch on $\mathcal{E}_y$, which shifts the position of the atomic orbitals. The force trying to return electrons back to their original positions is assumed to be linear in this shift, with a proportionality ("force") constant $K \equiv m_0\Omega_0^2$, with a confinement frequency Ω_0 (m_0 is the free electron mass). Within linear response with respect to $\mathcal{E}_y$ the mass-center positions of atomic orbitals are shifted along the $\hat{y}$-direction by the distance $-e\mathcal{E}_y/(m_0\Omega_0^2)$ from their equilibrium positions na. This shift enters the Peierls substitution, Eq. (8), giving rise to an additional shift of $k_x \to k_x + \Delta k_x$:

$$\Delta k_x \equiv \frac{\omega_c^2}{\Omega_0^2}\,\frac{e\mathcal{E}_y}{\hbar\omega_c}\,, \qquad (13)$$

where $\omega_c = eB/m_0c$ is the cyclotron frequency. The resulting shift of the mass-center position reads:

$$\Delta Y_\beta(k_x) \;=\; -\frac{e\mathcal{E}_y}{m_0\Omega_0^2}\left(1 - l_B^{-2}\,\frac{dY_\beta^{(B)}(k_x)}{dk_x}\right). \qquad (14)$$

The electric field $\mathcal{E}_y$ also gives rise to a potential energy, and up to the lowest order the eigenenergies are modified simply by an additive contribution $e\mathcal{E}_y Y_{n,\beta}(k_x)$. As a result the expectation value of the velocity along the $\hat{x}$-direction changes as:

$$\Delta v_x(\beta,k_x) \;=\; \frac{e\mathcal{E}_y}{\hbar}\,\frac{dY_\beta^{(B)}(k_x)}{dk_x}\,. \qquad (15)$$

Consequently, a non-zero current density along $\hat{x}$-direction (the Hall current) is induced by $\mathcal{E}_y$. It can be expressed in the form of Eq. (4) with $\tilde{\sigma}(\mu)$ given as:

$$\tilde{\sigma}(\mu) = N_\beta^{-1}\sum_{\beta=1}^{N_\beta}\int dk_x\; f_0\left(E_\beta(k_x)-\mu\right)\,\frac{dY_\beta(k_x)}{dk_x}, \quad (16)$$

where $f_0(E-\mu)$ denotes Fermi-Dirac distribution function and N_β denotes number of branches. When the Fermi energy μ lies within the energy gaps, $\tilde{\sigma}$ approaches an integer value σ, which can differ from zero due to the presence of magnetic edge states.

Using the Eq. (14) defining the average shift of the mass-center positions and the identity Eq. (5), the electron polarizability can be written as:

$$\alpha(\mu) = \frac{e^2}{m_0\Omega_0^2}\left(N(\mu) - \frac{\tilde{\sigma}(\mu)}{a_z 2\pi l_B^2}\right) = \frac{e^2}{m_0\Omega_0^2}\,\frac{\tilde{s}(\mu)}{a_z A_0}\,. \quad (17)$$

For the tight-binding model considered here, the dependence of $\alpha(\mu)$ is fully specified by the effective topological number $\tilde{s}(\mu)$. The latter is plotted as a function of the filling factor of the tight-binding band, $\nu_b \equiv a_z A_0 N(\mu)$ in Fig. 2 for several values of the ratio p/q. The case $p/q = 0$ corresponds to the zero magnetic field, for which $\tilde{s} \to \tilde{s}^{(0)} = \nu_b$ as follows from Eq. (5). For non-zero ratios a rich behavior is induced by the applied magnetic field.

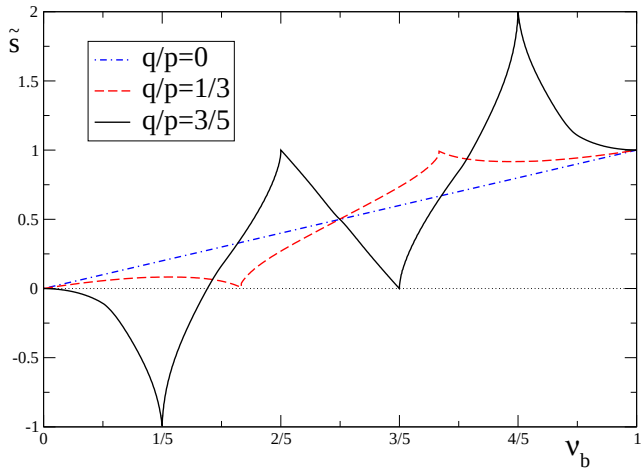

FIG. 2: Dependence of the effective topological number $\tilde{s}$, on the band filling factor ν_b for the ratio $p/q = 0$, $1/3$ and $3/5$.

Whenever the Fermi energy is located within the energy gap between subbands, i.e. if ν_b is given by integer multiples of $1/q$, the effective topological number $\tilde{s}(\mu)$ takes an integer value which is just equal to the topological gap number. As seen in Fig. 2, for $p/q = 1/3$, the total contribution of the lower and the upper sub-bands to the polarizability vanishes. In this particular case the applied electric force acting on carriers belonging to these subbands is fully compensated by the Lorentz force due to the induced non-dissipative edge Hall currents. For the case $p/q = 3/5$ the magnetic field even changes the sign of $\tilde{s}$ and consequently the sign of the polarizability. At half-filling of the band ($\nu_b = 1/2$), the Hall current vanishes and $\tilde{s}$ approaches its zero-field value $1/2$. The central symmetry of all curves around this half-filling point ($\nu_b = 1/2$, $\tilde{s} = 1/2$) is a consequence of the electron-hole symmetry of the single tight-binding band.

In this letter we have analyzed the interplay between the Hall current and the electron polarizability for the tight-binding model of a crystalline solid. This interplay is controlled by the compensation of the external electric force with the two other forces acting on the electrons: the gradient force, due to the periodic background potential, which is related to the polarizability, and on the other hand the Lorentz force, which determines the non-dissipative Hall current. The presence of the quantizing magnetic field induces a rich and complex behavior for the electron polarizability, which can even change sign as a function of the electron concentration.

Most importantly, we provide an answer to the long-standing question: *what measurable quantity is determined by the topological gap number s entering the Diophantine equation*? While it has been understood for a long time that σ determines the quantum Hall effect, a similar interpretation of s has so far remained unclear. We have shown that s is directly linked to the static electron polarizability. Contrary to the quantum Hall effect, the proportionality constant between the polarizability and the topological number s is a material dependent quantity rather than an universal constant, which can even depend on the magnetic field. The independence of the force constant $m_0\Omega_0^2$ on the magnetic field considered here is a mere consequence of the use of the Peierls substitution which is justified when $\Omega_0 \gg \omega_c$. A shrinking of atomic orbitals by the magnetic field, which leads to a suppression of the overlap strength and thus to a decrease of the overall band width, could be included by the substitution $\Omega_0^2 \to \Omega_0^2 + \omega_c^2/4$.

The predicted effect requires that a few flux quanta penetrate the lattice area A_0. Even for solids with a lattice constant of the order of 10Å, this requires exceedingly large fields ($\sim 10^3$ T). If, however, the magnetic field is tilted with respect to the high–symmetry crystallographic directions (here $\hat{z}$), an effective area (which is larger than A_0) can accomodate a few flux quanta, so that the above condition can be reached with experimentally available fields [4]. This condition can also be reached in 2D arrays of quantum dots or antidots with a lattice constant $\sim$ 100 nm. However, such (anti) dots need to be weakly coupled in order to reproduce a tight binding energy spectrum. Their size reduction (which implies a weak overlap and well separated atomic states) is thus a necessary condition for observing the predicted effect, and it still represents an experimental challenge.

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