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# Magnetization of the Metallic Surface States in Topological Insulators

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Journal Club, December 2, 2014

# Topological Insulator

Topological insulator:
Bulk insulator with a metallic spectrum of topologically protected helical surface states

Kane/Mele, PRL (2005)
Qi/Zhang, RMP (2011)

The helical surface states can be described by the Hamiltonian

$$H = \frac{\hbar^2 k^2}{2m} + \hbar v_F (k_x \sigma_y - k_y \sigma_x)$$

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**Schrödinger term**
Describes an electron with effective mass *m*

**Bychkov-Rashba Hamiltonian**
Describes massless Dirac fermions that move with a Fermi velocity $v_F$

***Correction***
*Breaks particle-hole symmetry!*

***Dominant term***
*Dirac-like spectrum*

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Describes massless Dirac fermions that move with a Fermi velocity $v_F$

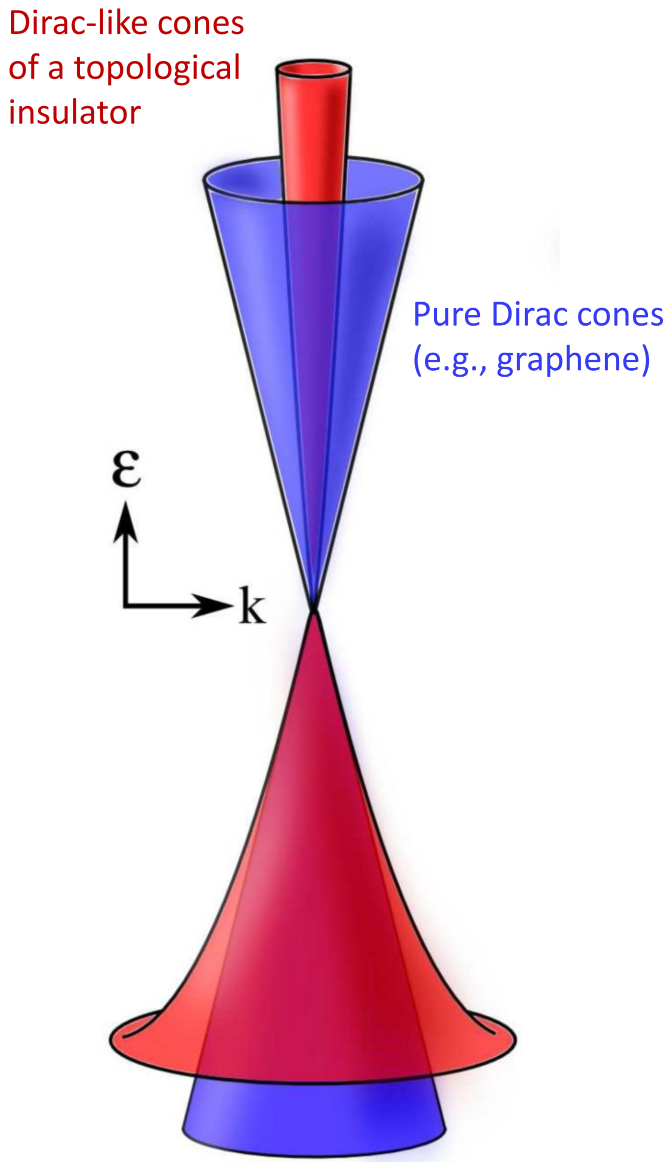
Spectrum and spin arrangement confirmed via angle-resolved photoemission spectroscopy

Chen *et al.*, Science (2009)
Hsieh *et al.*, Nature (2009)

# Spectrum

$$H = \frac{\hbar^2 k^2}{2m} + \hbar v_F (k_x \sigma_y - k_y \sigma_x)$$

$$\rightarrow \quad \varepsilon_\pm(\boldsymbol{k}) = \frac{\hbar^2 k^2}{2m} \pm \hbar v_F k$$



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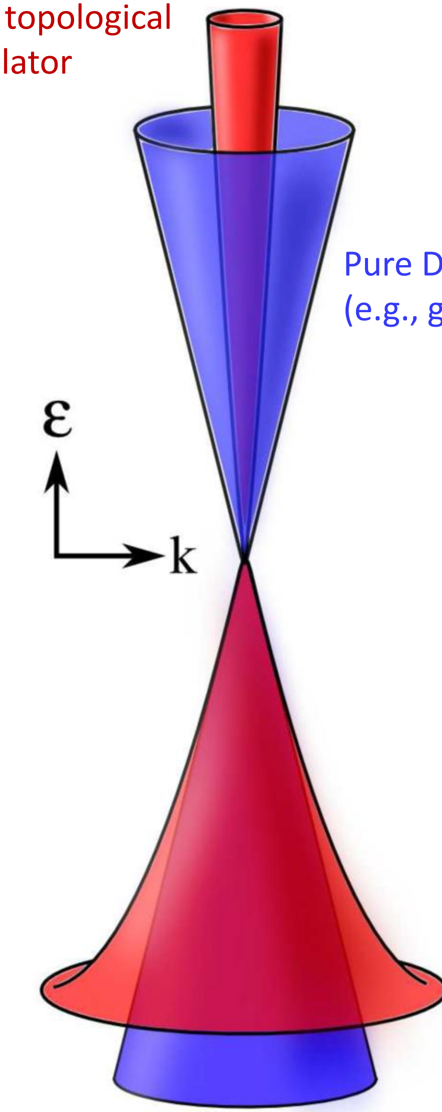
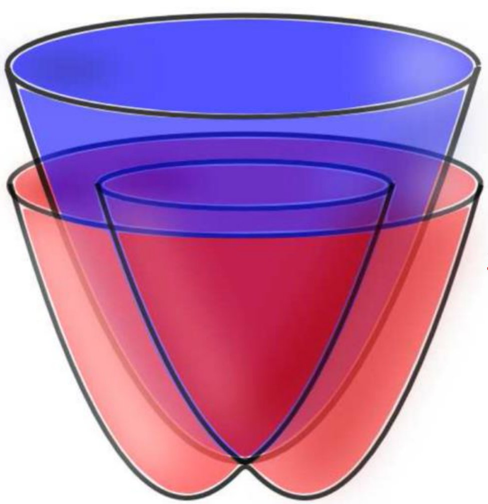
Dirac-like cones of a topological insulator




Pure Dirac cones (e.g., graphene)

Spectrum with dominant Schrödinger term for comparison:

(relevant, e.g., for semiconductors)



Pure Schrödinger dispersion

Spectrum with Rashba spin-orbit interaction

# Spectrum

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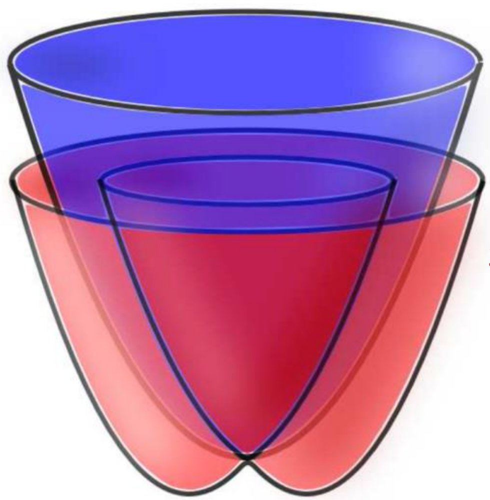
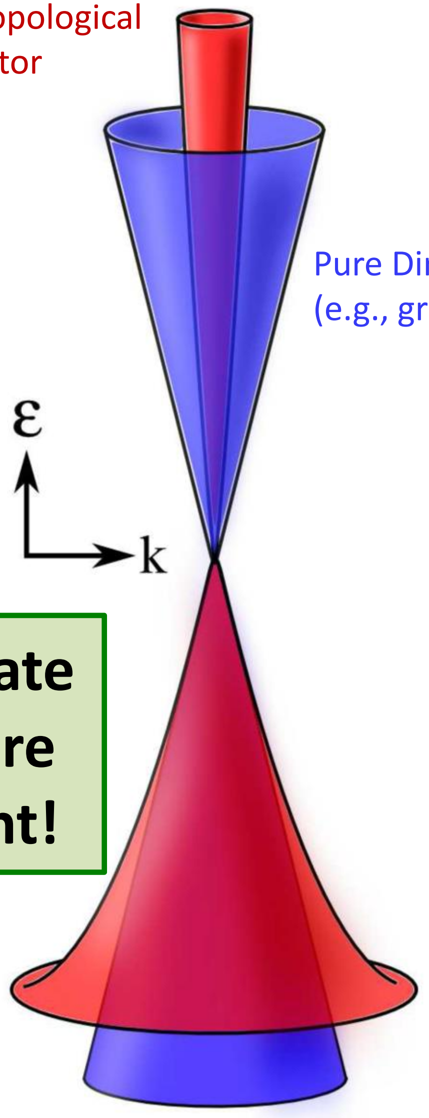
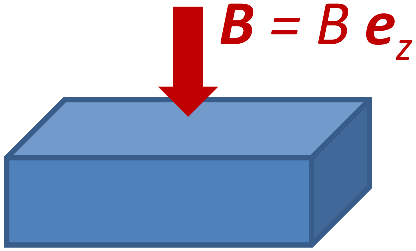



**Appropriate cutoffs are important!**



# External Magnetic Field



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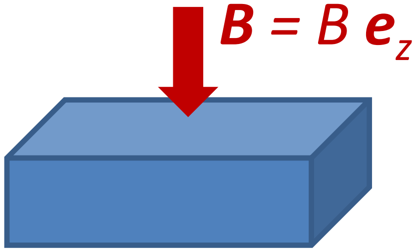


Magnetic vector potential:
(Landau gauge)

$$\boldsymbol{A} = (0, Bx, 0)$$
$$\boldsymbol{B} = \nabla \times \boldsymbol{A}$$

Substitution: $\hat{p}_i \rightarrow \hat{p}_i - q\hat{A}_i$ $\quad q = -e$

*electron charge*

The Zeeman term is omitted because it was found to be negligible for the phenomena of interest in this paper [see Wang *et al.*, PRB (2010)]

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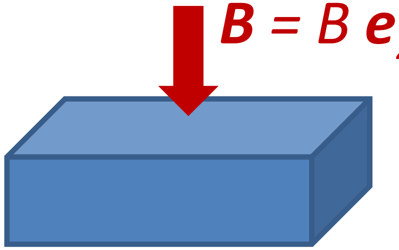


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$$H = \frac{\hbar^2 k^2}{2m} + \hbar v_F (k_x \sigma_y - k_y \sigma_x)$$

$$\longrightarrow \quad H = \frac{\hbar^2}{2m}\left[(-i\partial_x)^2 + (-i\partial_y + eBx/\hbar)^2\right] + \hbar v_F[(-i\partial_x)\sigma_y - (-i\partial_y + eBx/\hbar)\sigma_x]$$

# Landau Levels

$$H = \frac{\hbar^2}{2m}\left[(-i\partial_x)^2 + (-i\partial_y + eBx/\hbar)^2\right]$$
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$$\rightarrow \quad E_{N,s} = \frac{\hbar^2 N}{m l_B^2} + s\sqrt{\left(\frac{\hbar^2}{2ml_B^2}\right)^2 + \frac{2N\hbar^2 v_F^2}{l_B^2}}$$

*s* = +1: conduction band
*s* = -1: valence band

*N* ≥ 0: Landau level index

$$l_B = \sqrt{\hbar/(e|B|)}$$

Magnetic coherence length

# Grand Thermodynamic Potential

Magnetization *M(T, μ)* is given by the derivative of the grand thermodynamic potential Ω*(T, μ)* with respect to B at fixed chemical potential *μ*

$$M(T,\mu) \;=\; -[\partial\Omega(T,\mu)/\partial B]|_{\mu}$$

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For the Dirac-like spectra, the authors use

$$\Omega(T,\mu) = \underbrace{-T\int_{-\infty}^{\infty} N(\omega)\ln\left(1+\mathrm{e}^{(\mu-\omega)/\mathrm{T}}\right)\mathrm{d}\omega}_{\text{Usual non-relativistic grand potential } \Omega_{\mathrm{NR}}(T,\mu)} \;+\; \underbrace{\frac{1}{2}\int_{-\infty}^{\infty}\mu N(\omega)d\omega}_{\text{Chemical potential times total number of states}}$$

Usual non-relativistic grand potential $\Omega_{\mathrm{NR}}(T,\mu)$

Chemical potential times total number of states

*Constant that depends on μ but not on B*

*N(ω)*: Density of states

*Not to be confused with Landau level index N*

# Zero Temperature Limit

$$\Omega(T,\mu) = -T\int_{-\infty}^{\infty} N(\omega)\ln\left(1+\mathrm{e}^{(\mu-\omega)/\mathrm{T}}\right)\mathrm{d}\omega \quad + \frac{1}{2}\int_{-\infty}^{\infty}\mu N(\omega)d\omega$$

$\longrightarrow$ $T = 0$

$$\Omega(T=0,\mu) = \frac{1}{2}\int_{-\infty}^{0^-}(2\omega-\mu)N(\omega)d\omega$$
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Density of states:

$$N(\omega) = \frac{eB}{h}\left[\delta\left(\omega - E_0/2\right) + \sum_{N=1,s=\pm}^{\infty}\delta(\omega - E_{N,s})\right] \qquad E_0 = \hbar e|B|/m$$

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Graphene ($E_0 = 0$):

$\int_{0^+}^{\infty} N(\omega)d\omega = \int_{-\infty}^{0^-} N(\omega)d\omega$

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Topological insulator:

$\int_{0^+}^{\infty} N(\omega)d\omega = \int_{-\infty}^{0^-} N(\omega)d\omega + eB/h$

$$\Omega(0,\mu) = \int_{0^+}^{\mu}(\omega-\mu)N(\omega)d\omega + \int_{-\infty}^{0^-}\omega N(\omega)d\omega + \frac{eB\mu}{2h}$$

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Vacuum contribution

*Depends on B but not on μ*

# Magnetization and Hall Conductivity

Result for a topological insulator when the vacuum contribution is omitted:

$$\tilde{\Omega}(0,\mu) = \frac{eB}{h}\left[\frac{\mu}{2} + (E_0/2-\mu)\,\Theta\left(\mu - E_0/2\right) + \sum_{N=1}^{\infty}\left(E_{N,+}-\mu\right)\Theta\left(\mu - E_{N,+}\right)\right]$$

→ This equation is used by the authors to derive the magnetization *M(μ)*

*Recall:* $M(T,\mu) \;=\; -[\partial\Omega(T,\mu)/\partial B]|_{\mu}$

# Magnetization and Hall Conductivity

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$$\partial M(\mu)/\partial\mu \;=\; (1/e)\sigma_H$$

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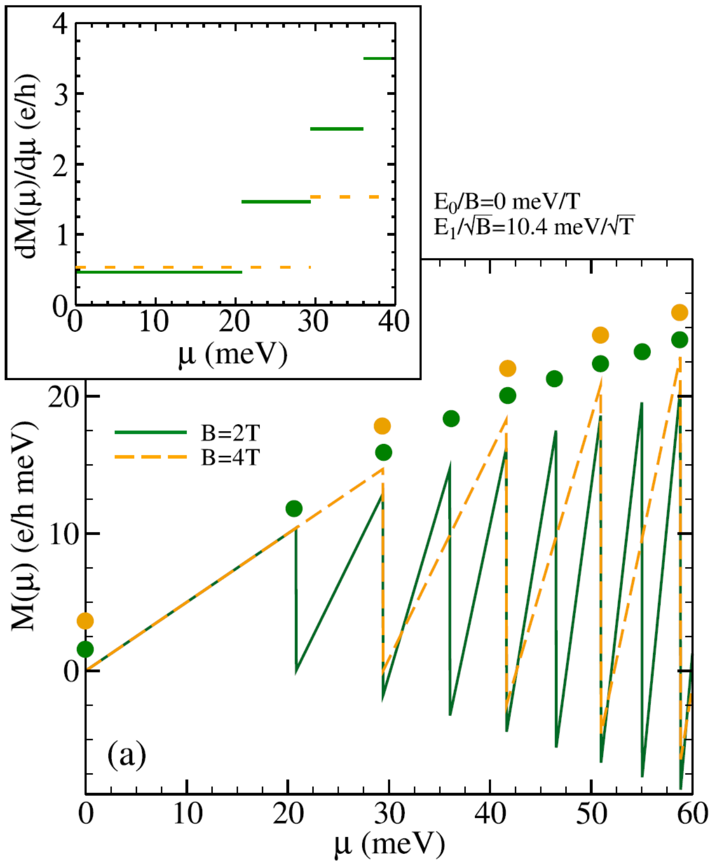
The Hall conductivity $\sigma_H$ is related to the slope of the magnetization via the Streda formula:

$$\partial M(\mu)/\partial\mu = (1/e)\sigma_H$$

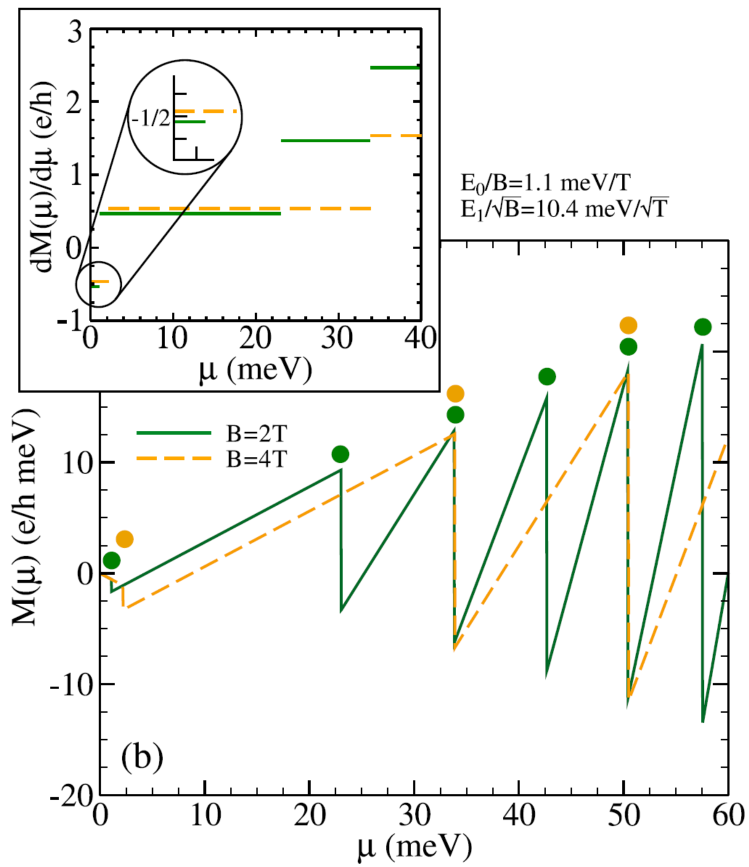
Important result:
Hall conductivity $\sigma_H$ is quantized in half-integer values of $e^2/h$, even in the presence of a Schrödinger term

# Magnetization and Hall Conductivity

Dirac term only:




With small Schrödinger term:



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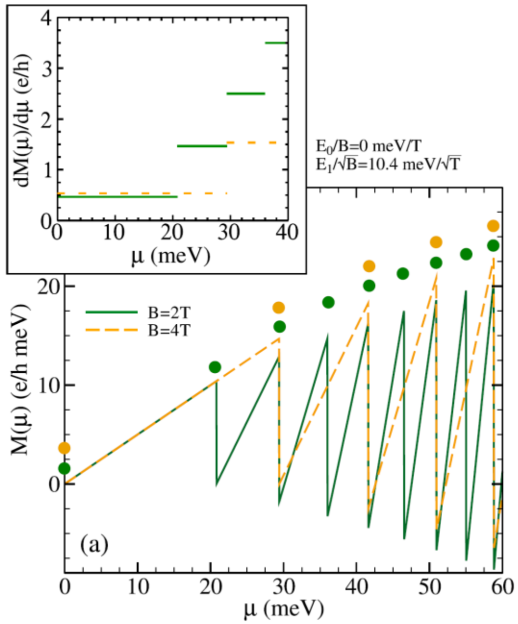


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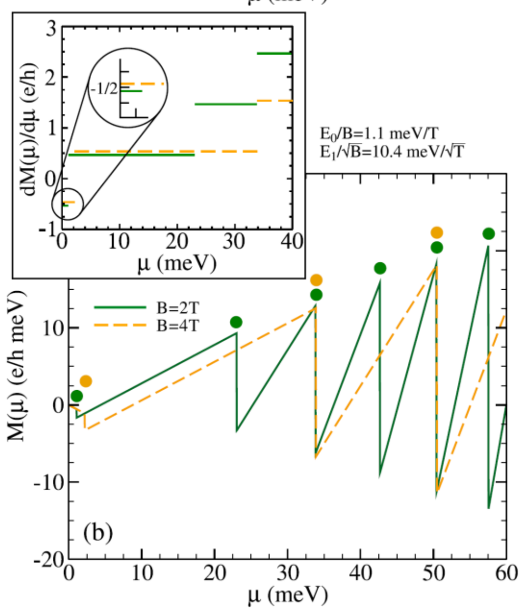

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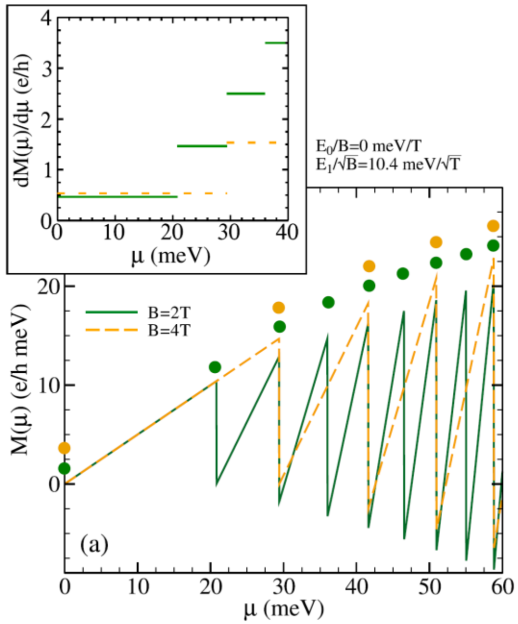


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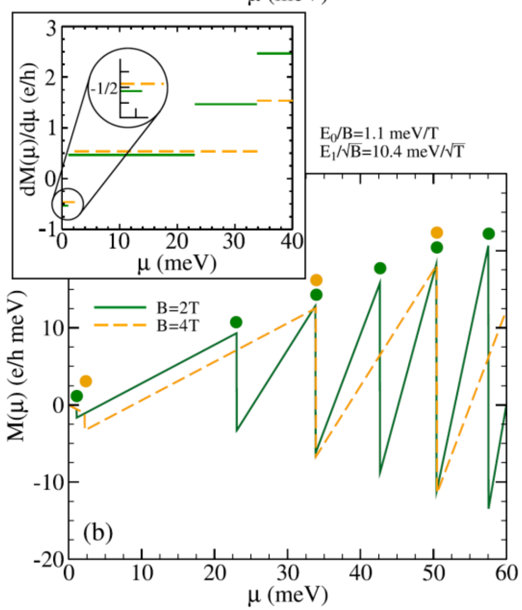
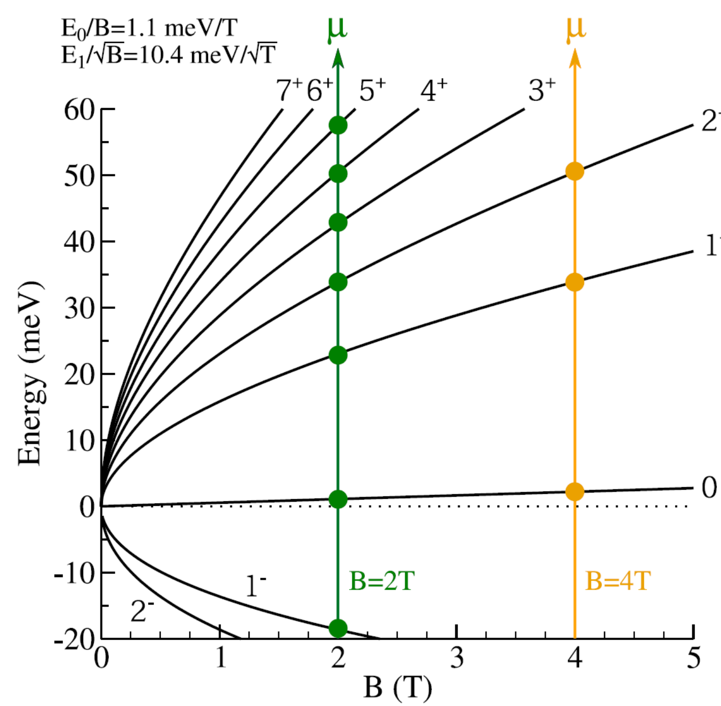



Landau levels with index *N*:

$$E_{N,s} = \frac{\hbar^2 N}{m l_B^2} + s\sqrt{\left(\frac{\hbar^2}{2 m l_B^2}\right)^2 + \frac{2N\hbar^2 v_F^2}{l_B^2}}$$

The circles mark the positions of the Landau levels



# Comparison with Schrödinger Limit

$$\Omega_{\mathrm{NR}}(T,\mu) = -T\int_{-\infty}^{\infty} N(\omega)\ln\left(1+\mathrm{e}^{(\mu-\omega)/\mathrm{T}}\right)\mathrm{d}\omega$$

$$N(\omega) = \frac{eB}{h}\left[\delta\left(\omega - E_0/2\right) + \sum_{N=1,s=\pm}^{\infty}\delta(\omega - E_{N,s})\right]$$

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$$M = -\partial\Omega_{\mathrm{NR}}/\partial B$$

$$\partial M(\mu)/\partial\mu \;=\; (1/e)\sigma_H$$

Landau levels with index *N*:

$$E_{N,s} = \frac{\hbar^2 N}{ml_B^2} + s\sqrt{\left(\frac{\hbar^2}{2ml_B^2}\right)^2 + \frac{2N\hbar^2 v_F^2}{l_B^2}}$$

# Comparison with Schrödinger Limit

When the relativistic term is absent, the Landau levels evolve linearly with *B.* Furthermore, there are degeneracies and the Hall plateaus have even-integer values of $e^2/h$ only.

In the presence of a relativistic term, the degeneracies are lifted due to corrections of type $\sqrt{B}$

$$E_{N,s} = \frac{\hbar^2 N}{m l_B^2} + s\sqrt{\left(\frac{\hbar^2}{2m l_B^2}\right)^2 + \frac{2N\hbar^2 v_F^2}{l_B^2}} \qquad l_B = \sqrt{\hbar/(e|B|)}$$

Lifting of the Landau level degeneracy results in Hall plateaus at integer values of $e^2/h$

# Comparison with Schrödinger Limit

Landau levels with index *N*:

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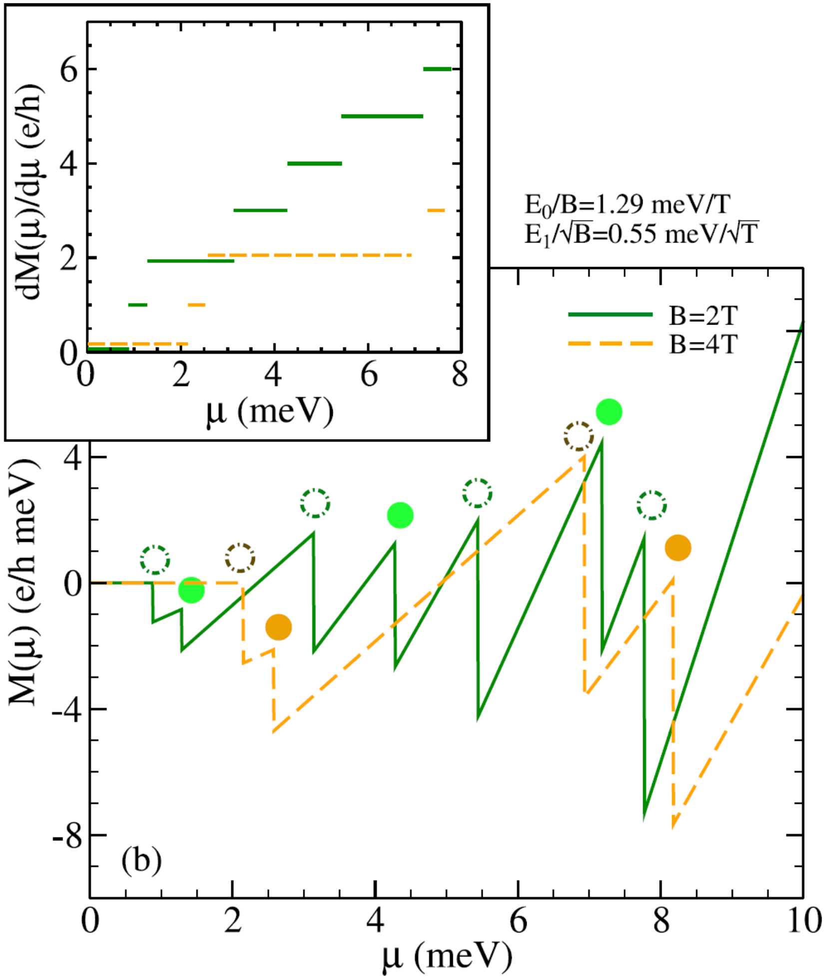


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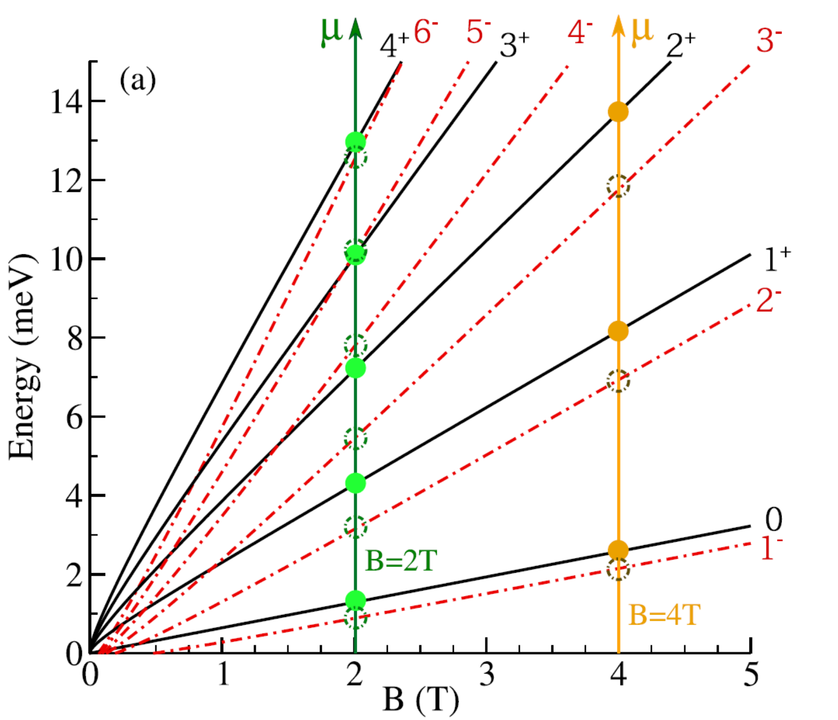

# Magnetic Oscillations

The authors also investigate the oscillating part of the magnetization

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The density of states

$$N(\omega) = \frac{eB}{h}\left[\delta\left(\omega - E_0/2\right) + \sum_{N=1, s=\pm}^{\infty} \delta(\omega - E_{N,s})\right]$$

can be rewritten as

$$\begin{aligned} N(\omega) = \frac{eB}{h}\frac{d}{d\omega}\Bigg\{ & \frac{1}{2}\Theta(\omega - E_0/2) - \frac{1}{2}\Theta(\omega + E_0/2) \\ & + [\Theta(\omega + E_0/2) + \Theta(\omega - E_0/2) - \Theta(\omega - \omega_{\min})] \\ & \times \left[x_1 + \sum_{k=1}^{\infty} \frac{1}{\pi k}\sin(2\pi \mathrm{kx}_1)\right] \\ & + \Theta(\omega - \omega_{\min})\left[x_2 + \sum_{k=1}^{\infty} \frac{1}{\pi k}\sin(2\pi \mathrm{kx}_2)\right]\Bigg\} \end{aligned}$$

... (long calculation) ...

# Magnetic Oscillations

The authors also investigate the oscillating part of the magnetization

In the regime of small *B* they find

$$M_{\text{osc}}(0,\mu) \approx -\frac{e}{h}\frac{\mu}{2}\sum_{k=1}^{\infty}\left[1+\frac{\mu}{2mv_F^2}\right]\frac{\sin(2\pi k x_1)}{\pi k}$$

$$x_1 = \frac{\hbar A(\mu)}{2\pi e B} - \gamma$$

$$A(\mu) \approx \frac{\pi\mu^2}{\hbar^2 v_F^2}\left(1-\frac{\mu}{mv_F^2}\right)$$

*Area of cyclotron orbit*

$$\gamma = \frac{\hbar e B}{8m^2 v_F^2}$$

*Phase shift linear in B*

*but very small for typical values*

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Results consistent with the pure Dirac limit ($m \to \infty$)

$$A(\mu) \approx \frac{\pi\mu^2}{\hbar^2 v_F^2}\left(1 - \frac{\mu}{m v_F^2}\right)$$

*Area of cyclotron orbit*

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# Line Broadening due to Impurities

Landau level broadening due to impurities is taken into account via convolution with a scattering function

$$M_{\mathrm{osc}}(\mu, \Gamma) = \int_{-\infty}^{\infty} d\omega \frac{\Gamma}{\pi\left[(\omega-\mu)^2+\Gamma^2\right]} M_{\mathrm{osc}}(\omega)$$

*Scattering function:*

$$P_{\Gamma}(\varepsilon) = \frac{\Gamma}{\pi\left(\varepsilon^2+\Gamma^2\right)}$$

*Previous result with $\mu = \omega$*

# Line Broadening due to Impurities

Landau level broadening due to impurities is taken into account via convolution with a scattering function

$$\Rightarrow \quad M(\mu,\Gamma) \approx -\frac{e}{h}\frac{\mu^2-\Gamma^2}{2\mu}\left(1+\frac{\mu}{2mv_F^2}\right)\sum_{k=1}^{\infty}\frac{\sin(2\pi k\tilde{x}_1)}{\pi k}R_D$$

$$\tilde{x}_1 \approx \frac{\mu^2-\Gamma^2}{2\hbar v_F^2 eB}\left(1-\frac{\mu}{mv_F^2}\right)-\frac{\hbar eB}{8m^2v_F^2}$$

$$R_D = e^{-2\pi\Gamma k\frac{\mu}{\hbar v_F^2 eB}\left(1-\frac{\mu}{mv_F^2}\right)}$$

*Dingle factor*

# Line Broadening due to Temperature

An analogous calculation can be carried out for the line broadening due to nonzero temperature

$$P_T(\varepsilon) = \frac{1}{4T\cosh^2\left(\frac{\varepsilon}{2\mathrm{T}}\right)}$$

$$\Rightarrow \quad M(\mu, T) \approx -\frac{e}{h}\frac{\mu}{2}\left(1 + \frac{\mu}{2mv_F^2}\right)\sum_{k=1}^{\infty}\frac{\sin(2\pi k x_1)}{\pi k}R_T$$

$$R_T = \frac{k\lambda}{\sinh(k\lambda)} \qquad \lambda = \frac{2\pi^2 T\mu}{\hbar v_F^2 eB}\left(1 - \frac{\mu}{mv_F^2}\right)$$

*Temperature factor*

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