GDR Physique Quantique Mésoscopique - Session Plénière 2016, Aussois

Imaging the Berry Phase from Friedel Oscillations in 2D Semimetals

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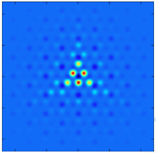
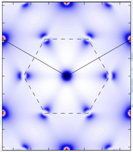




Content

Friedel Oscillations

Jacques Friedel: static ($\omega \to 0$) response of conduction electrons to a localized charge in metals [*Friedel, Philos. Mag. (1952)*]

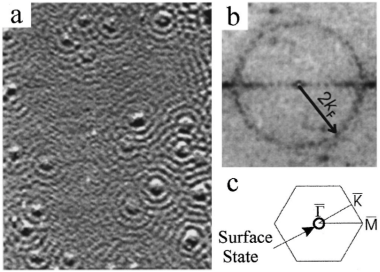
$$\Pi_0(\mathbf{q}, \omega) \sim \int d^3k \frac{f(\epsilon_\mathbf{k}) - f(\epsilon_{\mathbf{k}+\mathbf{q}})}{\omega - (\epsilon_\mathbf{k} - \epsilon_{\mathbf{k}+\mathbf{q}}) + i\delta}$$

- Thomas-Fermi ($\mathbf{q} \to 0$): Debye screening (exponential)
- Nesting ($\epsilon_\mathbf{k} = \epsilon_{\mathbf{k}+\mathbf{q}}$): long-range oscillations $\rho(\mathbf{r}) \sim \frac{\cos(2q_F r)}{r^2}$ in 2D

FO arise from the existence of a Fermi surface and thus also appear in the context of magnetic interactions (RKKY), or non-interacting electron gas [*Adhikari, Am. J. Phys. (1986)*]

Friedel Oscillations

Scanning Tunneling Microscopy: imaging the LDOS $\rho(\mathbf{r}, \omega)$ of metallic surfaces with atomic-scale resolution [*Binnig and Rohrer at IBM Zürich (1981)*]



[*Petersen et al., PRB (1998)*]

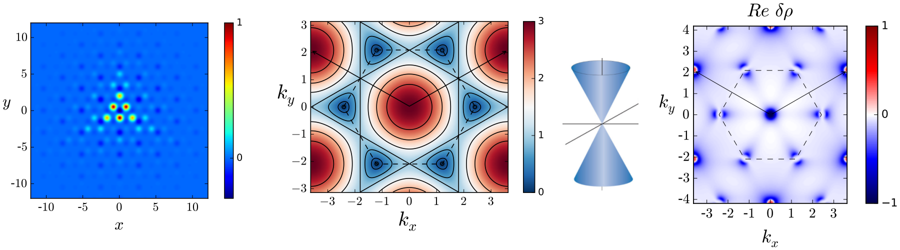
(a) $\rho(\mathbf{r}, \omega) \sim \frac{\cos(2q_F r)}{r}$

(b) $\rho(\mathbf{q}, \omega) \sim \frac{\Theta(q - 2q_F)}{\sqrt{q^2 - (2q_F)^2}}$

Backscattering is the most efficient process
STM can be thought of as a technique to probe Fermi contours

Friedel Oscillations

Elastic scattering between circular Fermi contours in graphene:



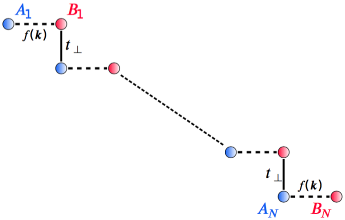
$$\delta\rho(\mathbf{q},\omega) \sim \frac{\pi}{2}\Theta\left(2q_F - q\right) + \mathrm{asin}\left(\frac{2q_F}{q}\right)\Theta\left(q - 2q_F\right)$$ [*Bena, PRL (2008)*]

$$\delta\rho\left(\mathbf{r},\omega\right) = \delta\rho_A + \delta\rho_B \sim \frac{\cos\left(2q_F r\right)}{r^2}$$ [*Cheianov and Fal'ko, PRL (2006)*]

STM is able to probe the absence of backscattering, i.e. a property of Dirac electron wavefunctions [*Brihuega et al., PRL (2008)*]

Rhombohedral *N*-layer graphene

Momentum space representation:



Bipartite lattice with two zero-energy edge states exponentially localized on A_1 and B_N when $|f(\mathbf{k})| < t_\perp$ [*Tamm (1932), Shockley (1939)*]

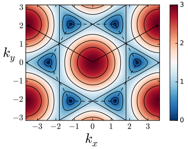
Low-energy ($\mathcal{E}(\mathbf{k}) \ll t_\perp$) Bloch band structure in basis $\{A_1, B_N\}$:

$$\mathcal{H}_N(\mathbf{K}^\xi + \mathbf{q}) \simeq \begin{pmatrix} 0 & q^N\, \xi^N e^{i\xi N\theta_{\mathbf{q}} + iN\Phi^\xi} \\ q^N\, \xi^N e^{-i\xi N\theta_{\mathbf{q}} - iN\Phi^\xi} & 0 \end{pmatrix}$$

The two orbitals involved at low-energy belong to opposite surfaces

Rhombohedral N-layer graphene

Dispersion relation: $\mathcal{E}(\mathbf{K}^\xi + \mathbf{q}) = \pm|\mathbf{q}|^N$

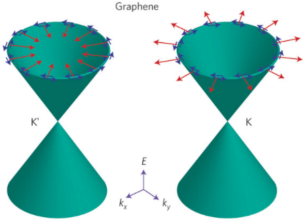


Bloch spinors: $\Psi_\pm(\mathbf{K}^\xi+\mathbf{q}) \simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \mp\xi^N e^{-iN\Phi^\xi} e^{-i\xi N\theta_\mathbf{q}} \end{pmatrix}$ $\begin{matrix} A_1 \\ B_N \end{matrix}$

This defines the low-energy Bloch band structure of a two-band 2D semimetal with two nonequivalent valleys (time reversal symmetry)

π-quantized Berry phase:

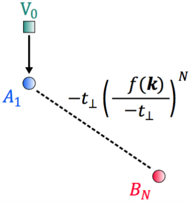
$$\begin{aligned} \gamma_\xi &= i \oint_{\mathcal{C}^\xi} d\mathbf{q} \cdot \langle \Psi_\pm(\mathbf{K}^\xi + \mathbf{q}) | \nabla_\mathbf{q} | \Psi_\pm(\mathbf{K}^\xi + \mathbf{q}) \rangle \\ &= \frac{1}{2} \oint_{\mathcal{C}^\xi} d\mathbf{q} \cdot \nabla_\mathbf{q}\, \xi N \theta_\mathbf{q} \\ &= \xi N \pi \end{aligned}$$

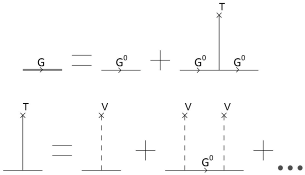


[*Rotenberg, Nat. Phys. 7, 8 (2011)*]

Localized impurity scattering

Localized impurity $V_0\delta(\mathbf{r})$ on sublattice A_1:





For a given scattering defined by $\Delta\mathbf{K} = \mathbf{K}^{\xi} - \mathbf{K}^{\xi'}$:

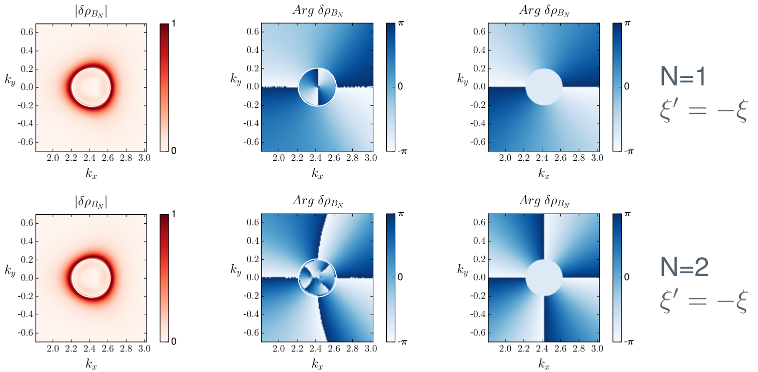
$$\begin{cases} \delta\rho_{A_1}(\mathbf{r},\omega) \propto \dfrac{\cos(2q_F r)}{r} \cos\left(\Delta\mathbf{K}\cdot\mathbf{r}\right) \\ \delta\rho_{B_N}(\mathbf{r},\omega) \propto \dfrac{\cos(2q_F r)}{r} \cos\left(\Delta\mathbf{K}\cdot\mathbf{r} - N(\phi^{\xi}-\phi^{\xi'}) - N(\xi-\xi')\theta_{\mathbf{r}} + N\xi'\pi\right)\left(\xi\xi'\right)^N \end{cases}$$

Monolayer graphene is the only material of the rhombohedral class that exhibits $1/r^2$-decaying oscillations

Localized impurity scattering

Fourier transform of the interference pattern:

$$\begin{cases} \delta\rho_{A_1}(\Delta\mathbf{K}+\mathbf{q},\omega) \simeq -\dfrac{\Theta(q-2q_F)}{\sqrt{q^2-(2q_F)^2}} \\ \delta\rho_{B_N}(\Delta\mathbf{K}+\mathbf{q},\omega) \simeq -\dfrac{\Theta(q-2q_F)}{\sqrt{q^2-(2q_F)^2}}(-\xi\xi')^N\, e^{-iN(\phi^{\xi}-\phi^{\xi'})}\, e^{-iN(\xi-\xi')\theta_{\mathbf{q}}} \end{cases}$$

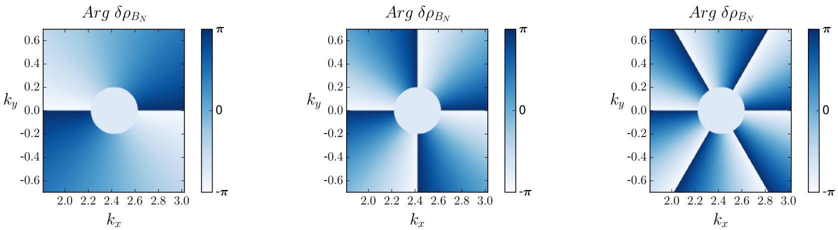


Localized impurity scattering

Bloch eigenstates from nonequivalent-valley scattering ($\xi' = -\xi$):

$$\text{Arg}\,\delta\rho_{B_N} = -2\xi N\theta_{\mathbf{q}} + \Phi^{\xi}$$

N=1 N=2 N=3



Berry phase of the valley ξ:

$$\frac{1}{4}\oint_{\mathcal{C}_{2\mathbf{q_F}}} d\mathbf{q}\cdot\nabla_{\mathbf{q}}[\text{Arg}\,\delta\rho_{A_1} - \text{Arg}\,\delta\rho_{B_N}] = \xi N\pi$$

Localized impurity scattering

Fourier transform of Friedel oscillations:

$$\begin{cases} \delta\rho_{A_1}(\Delta\mathbf{K}+\mathbf{q},\omega) \simeq -\dfrac{\Theta(q-2q_F)}{\sqrt{q^2-(2q_F)^2}}\, e^{i\Phi_{A_1}+i(N_0-1)(\xi-\xi')\theta_{\mathbf{q}}} \\ \delta\rho_{B_N}(\Delta\mathbf{K}+\mathbf{q},\omega) \simeq -\dfrac{\Theta(q-2q_F)}{\sqrt{q^2-(2q_F)^2}}\, e^{i\Phi_{B_N}-i(N-N_0+1)(\xi-\xi')\theta_{\mathbf{q}}} \end{cases}$$

Berry phase of the valley ξ:

$$\frac{1}{4}\oint_{\mathcal{C}_{2\mathbf{q_F}}} d\mathbf{q}\cdot\nabla_{\mathbf{q}}[\mathrm{Arg}\,\delta\rho_{A_1} - \mathrm{Arg}\,\delta\rho_{B_N}] = \xi N\pi$$

Summary

Localized-impurity scattering in rhombohedral N-layer graphene:

- low-energy physics takes place on external layers
- $1/r^2$-decaying oscillations in monolayer graphene
- $1/r$ -decaying oscillations in multilayer graphene

Bloch band structure from LDOS Fourier analysis:

- probing Fermi contours and absence of backscattering
- probing Bloch spinors via nonequivalent valley scattering
- probing Berry phases (topological feature)

[Phys. Rev. B 93, 035413 (2016)] in collaboration with M. I. Katsnelson

Thank you for your attention