Center for Nanostructured Graphene

DTU

A unified approach to quasiparticle interference in two-dimensional materials

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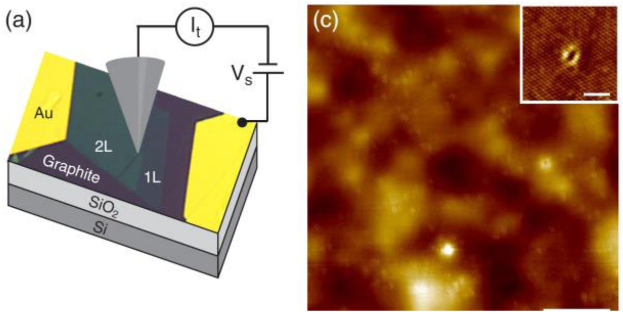
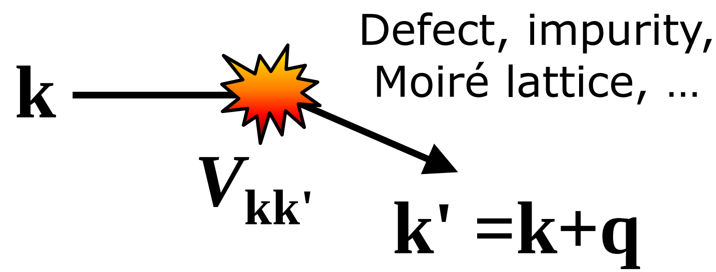
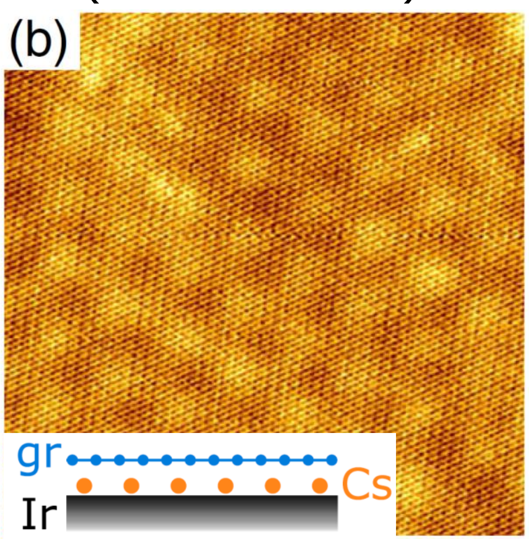
Scanning tunneling spectroscopy

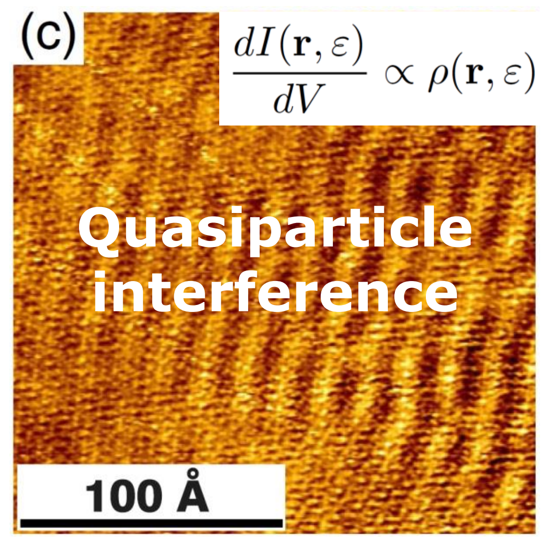




Topography
(const. current)



Spectroscopy



PRL **118**, 116401 (2017)

Fourier transform STS (FT-STS)

$$\rho(\mathbf{q}+\mathbf{G},\varepsilon) = \int d\mathbf{r}\, e^{-i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}\rho(\mathbf{r},\varepsilon)$$

Scattering processes

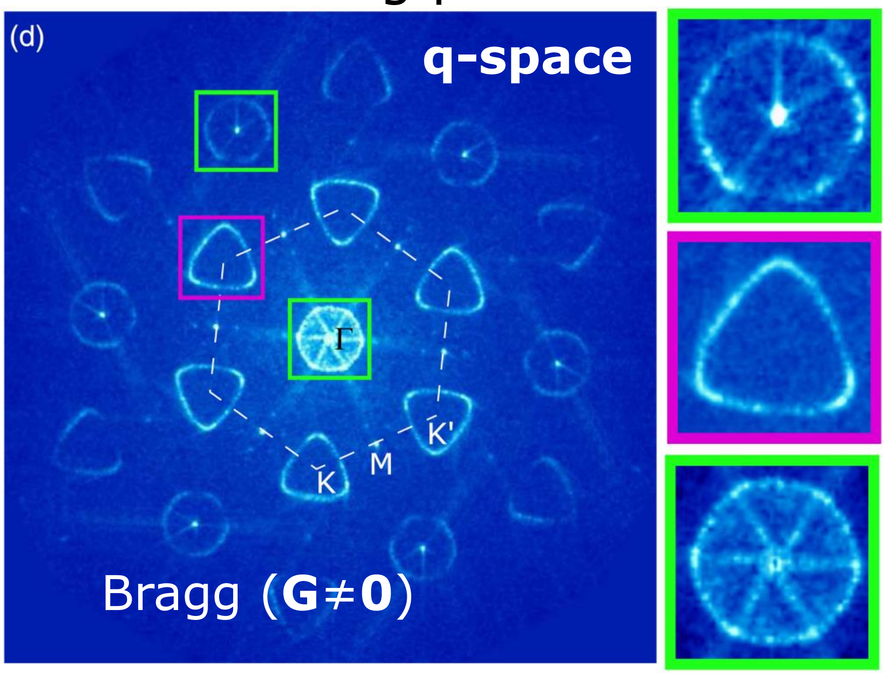
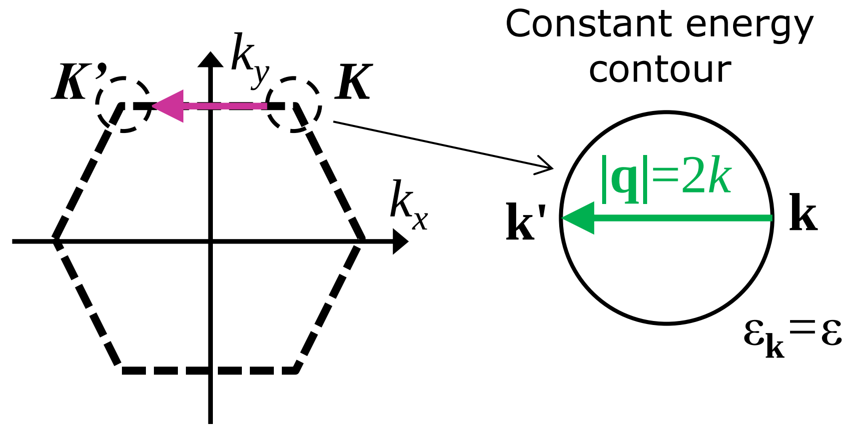


FIG. 1. Scattering patterns in strongly doped graphene. (a) Inverted LEED pattern of gr/Cs/Ir(111) at $E = 143.5$ eV, the intercalated Cs forms a $(2\times 2)_{gr}$ superstructure. The sketch

PRL **118,** 116401 (2017)



- Scattering (elastic) on constant energy contours in k-space.
- Nesting vectors (backscattering) dominate → Friedel osc.
- Replicas outside 1'st BZ (Bragg).
- JDOS: $\rho_{\mathrm{JDOS}}(\mathbf{q},\varepsilon) \propto \sum_{\mathbf{k}} \rho_{\mathbf{k}}(\varepsilon)\rho_{\mathbf{k}+\mathbf{q}}(\varepsilon)$

A “unified” FT-STS theory

LDOS: $$\rho(\mathbf{r},\varepsilon) = -1/\pi \mathrm{Im} G(\mathbf{r},\mathbf{r};\varepsilon)$$

FT of LDOS:

$$\boxed{\rho(\mathbf{q}+\mathbf{G},\varepsilon) = -\frac{1}{2\pi i}\sum_{mn}\sum_{\mathbf{k}} n^{mn}_{\mathbf{k},\mathbf{q}}(\mathbf{G}) \times \left[G^{nm}_{\mathbf{k}+\mathbf{q},\mathbf{k}}(\varepsilon) - G^{mn}_{\mathbf{k},\mathbf{k}+\mathbf{q}}(\varepsilon)^*\right]}$$

Interference in *q* space

$$n^{mn}_{\mathbf{k},\mathbf{q}}(\mathbf{G}) = \langle\psi_{m\mathbf{k}}|e^{-i(\mathbf{q}+\mathbf{G})\cdot\hat{\mathbf{r}}}|\psi_{n\mathbf{k}+q}\rangle$$

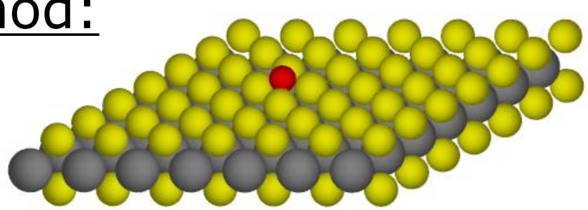
(pristine)

Scattering processes

$$V^{mn}_{\mathbf{k}\mathbf{k}'} = \langle\psi_{m\mathbf{k}}|\hat{V}|\psi_{n\mathbf{k}+q}\rangle$$

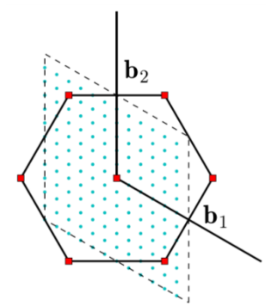
(defect/impurity)

DFT based method:



$$V_i(\mathbf{r}) = V^i_{\mathrm{dis}}(\mathbf{r}) - V_{\mathrm{pris}}(\mathbf{r})$$

- Supercell
- LCAO basis
- Spin-orbit
- *T*-matrix
- *N*x*N* BZ sampling

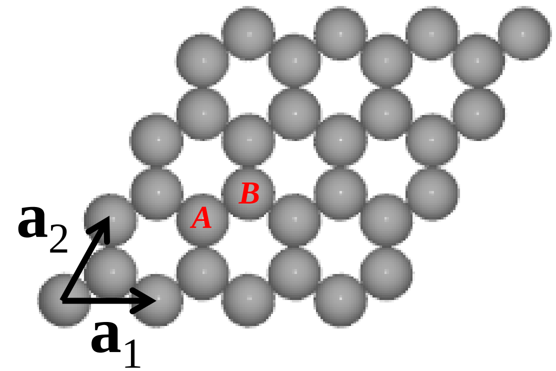


Kaasbjerg *et al.*, PRB **96**, 241411(R) (2017)

Graphene tight-binding

$$H_0 = -t\sum_{\mathbf{k}}[\phi_{\mathbf{k}} c^{\dagger}_{A\mathbf{k}} c_{B\mathbf{k}} + \mathrm{h.c.}]$$

$$\phi_{\mathbf{k}} = 1 + e^{i\mathbf{k}\cdot\mathbf{a}_1} + e^{i\mathbf{k}\cdot\mathbf{a}_2}$$

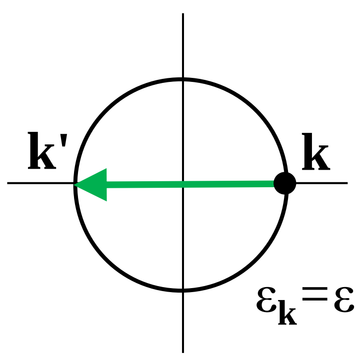


$$\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2$$

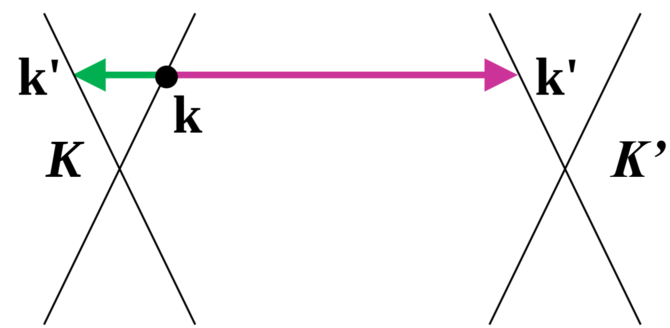
Impurity model:

$$\boldsymbol{V} = V_0\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}$$

Breaks *A*,*B* sublattice symmetry
→ q=2k backscattering allowed

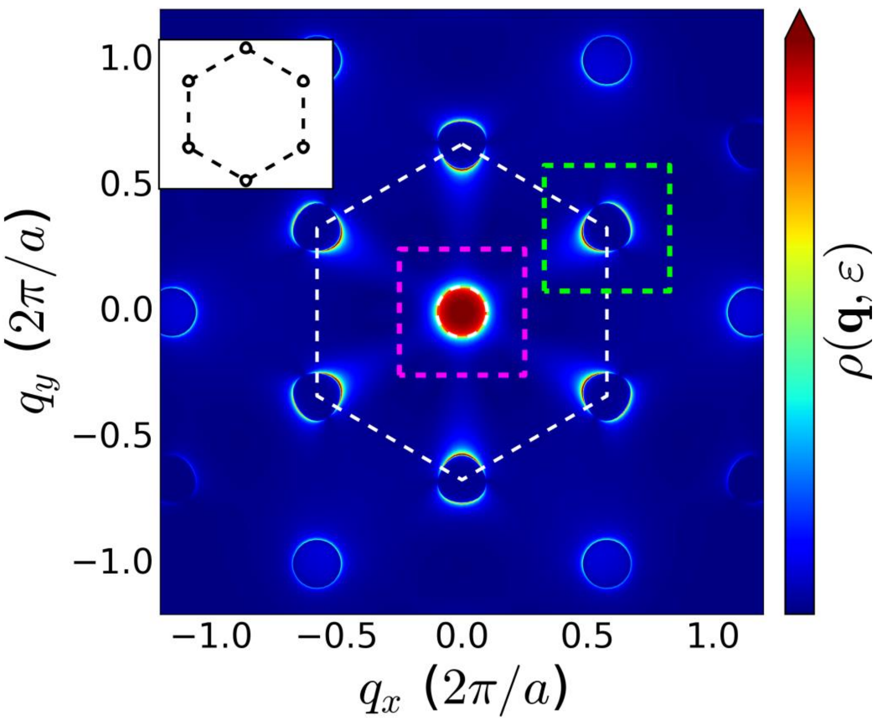


k,**k'** independent → intra +
intervalley scattering

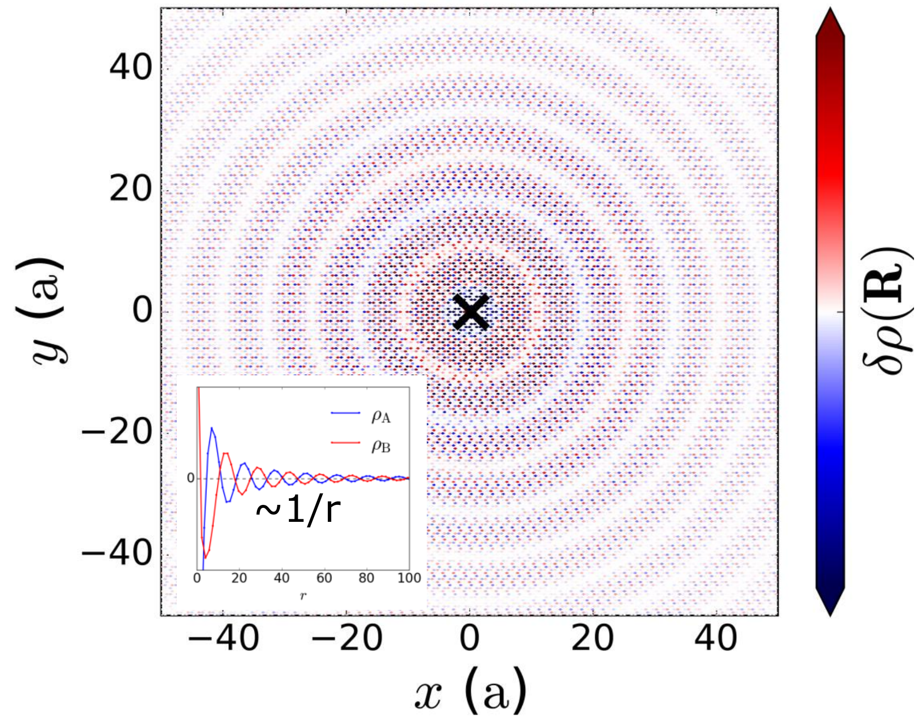


Weak impurity

FT-STS



Friedel oscillations

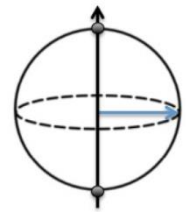


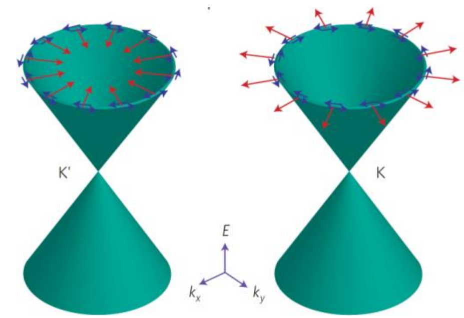
- Filled disc instead of q=2k backscatter ring + strongly anisotropic intervalley features (PRL **100,** 076601 (2008)).
- Backscatter ring at Bragg points (weak intensity).

Role of (intrinsic) chirality

$$\mathcal{H}_{\mathbf{k}} = \hbar v_F \mathbf{k}\cdot\boldsymbol{\sigma}$$

$$\boldsymbol{\chi}_{s\mathbf{k}} = (1, se^{i\theta_{\mathbf{k}}})^T =$$





s=+1

s=-1

$$\psi_{s\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{A}} e^{i\mathbf{k}\cdot\mathbf{r}} \boldsymbol{\chi}_{s\mathbf{k}}$$

Phase-factor element:

$$n^{ss'}_{\mathbf{k},\mathbf{q}}(\mathbf{G}) = \langle \psi_{s\mathbf{k}} | e^{-i(\mathbf{q}+\mathbf{G})\cdot\hat{\mathbf{r}}} | \psi_{s'\mathbf{k}+\mathbf{q}} \rangle$$

$$\rightarrow \boldsymbol{\chi}^{\dagger}_{s\mathbf{k}} \boldsymbol{M}(\mathbf{q}+\mathbf{G}) \boldsymbol{\chi}_{s'\mathbf{k}+\mathbf{q}} \quad ; \quad \boldsymbol{M}(\mathbf{q}) = \begin{pmatrix} e^{-i\mathbf{q}\cdot\mathbf{R}_A} & 0 \\ 0 & e^{-i\mathbf{q}\cdot\mathbf{R}_B} \end{pmatrix}$$

<u>Intravalley (q~0)</u>

$$\boldsymbol{M}(\mathbf{q}) \approx \boldsymbol{\sigma}_0$$

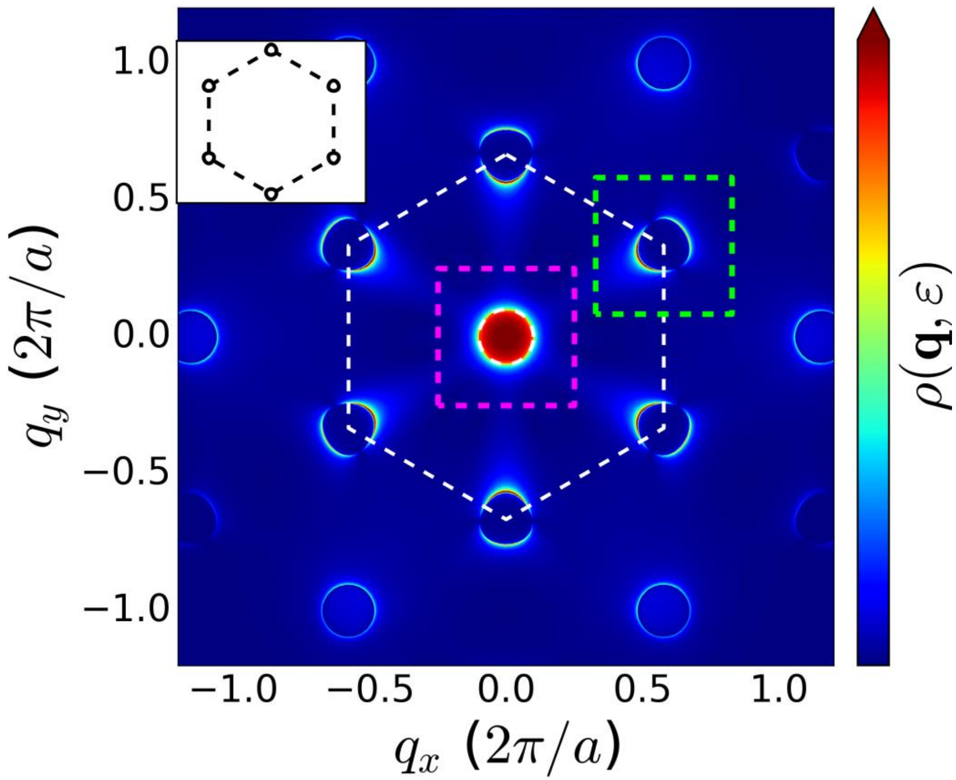
$$n^{ss'}_{\mathbf{k},\mathbf{q}} = \tfrac{1}{2}[1 + ss' \exp(i\theta_{\mathbf{k},\mathbf{k}+\mathbf{q}})]$$

Intervalley (q=K,K')
<u>and Bragg (G≠0)</u>

$$\boldsymbol{M}(\mathbf{q}) \neq \boldsymbol{\sigma}_0$$

$$n^{ss'}_{\mathbf{k},\mathbf{q}} = F(\theta_{\mathbf{k}}, \theta_{\mathbf{k}+\mathbf{q}})$$

Role of (intrinsic) chirality



<u>Intravalley ($\mathbf{q}$~$\mathbf{0}$)</u>

$$\boldsymbol{M}(\mathbf{q}) \approx \boldsymbol{\sigma}_0$$

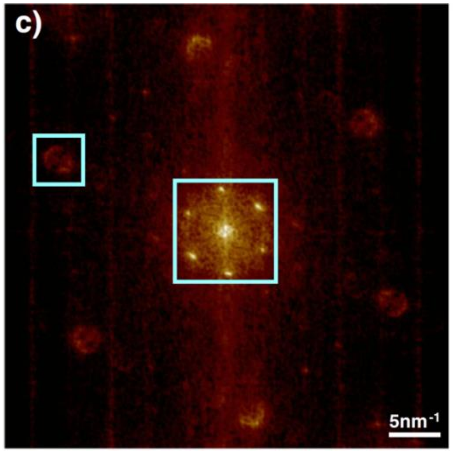
$$n^{ss'}_{\mathbf{k},\mathbf{q}} = \frac{1}{2}[1 + ss' \exp(i\theta_{\mathbf{k},\mathbf{k}+\mathbf{q}})]$$

Intervalley ($\mathbf{q}$=$\mathbf{K}$,$\mathbf{K'}$)
<u>and Bragg ($\mathbf{G}\neq\mathbf{0}$)</u>

$$\boldsymbol{M}(\mathbf{q}) \neq \boldsymbol{\sigma}_0$$

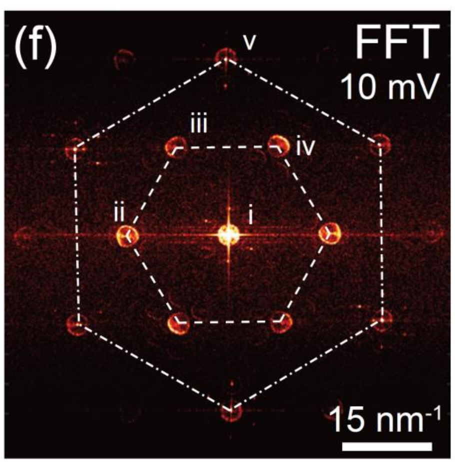
$$n^{ss'}_{\mathbf{k},\mathbf{q}} = F(\theta_{\mathbf{k}}, \theta_{\mathbf{k}+\mathbf{q}})$$

QPI/FT-STS in graphene



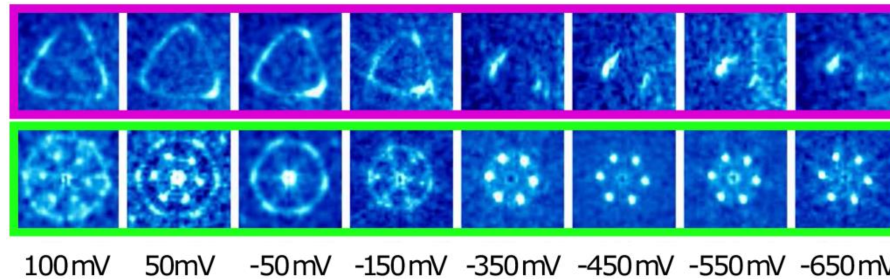
PRL **101**, 206802 (2008)

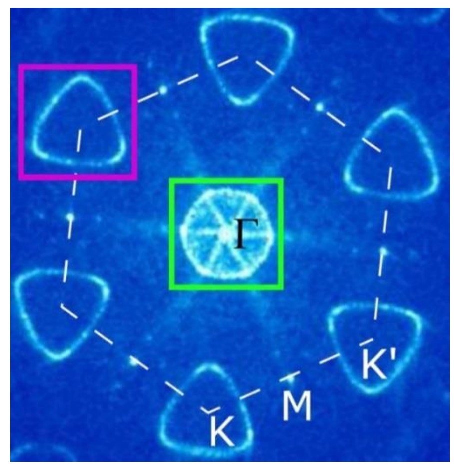
PHYSICAL REVIEW B **86**, 045444 (2012)



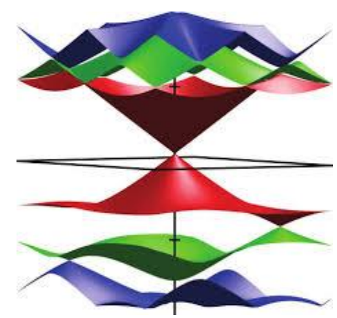
PHYSICAL REVIEW B **95**, 075429 (2017)

PRL **118**, 116401 (2017)





Moiré minibands



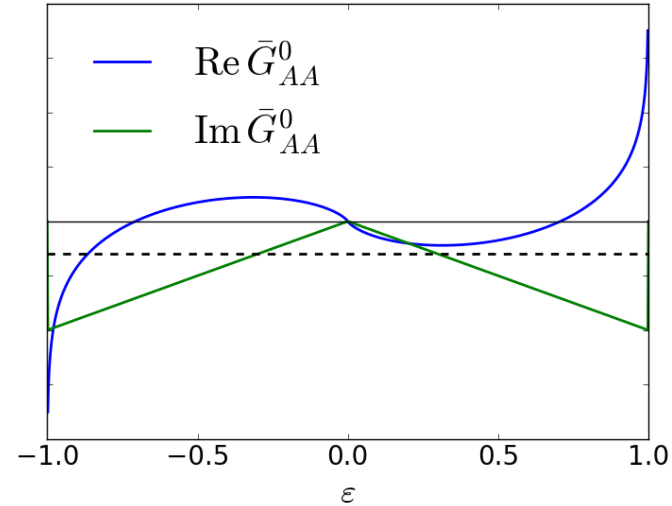
Resonant impurity

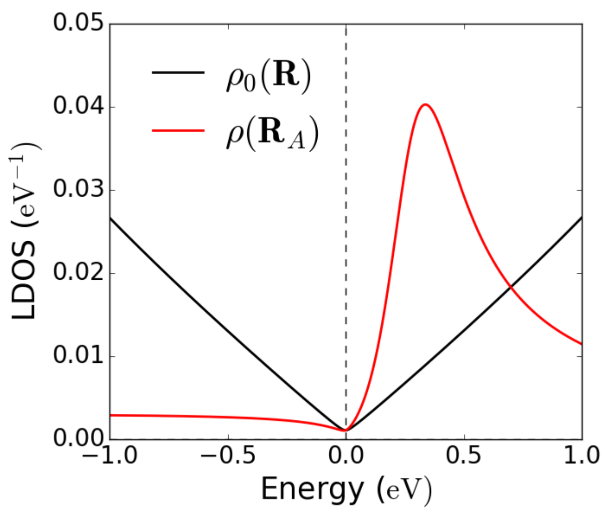
Impurity T-matrix:

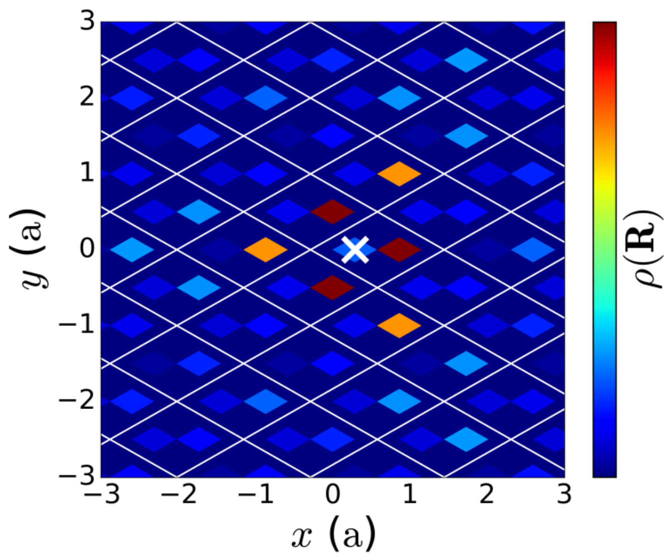
$$T_{AA}(\varepsilon) = V_0/[1 - V_0 \bar{G}^0_{AA}(\varepsilon)]$$

$$\bar{G}^0_{ij}(\varepsilon) = \frac{1}{N}\sum_{\mathbf{k}} G^{0,ij}_{\mathbf{k}}(\varepsilon)$$

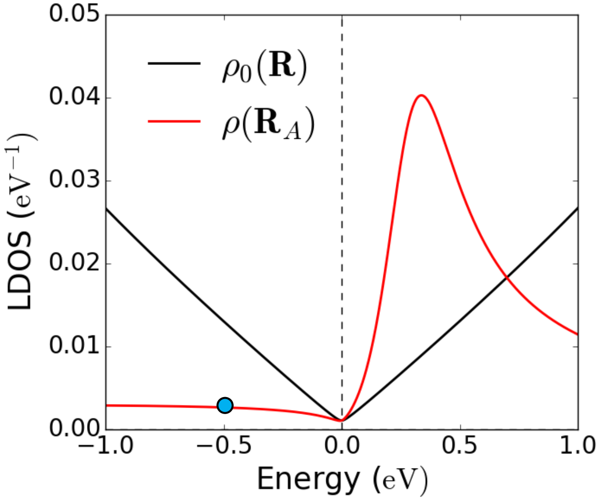
Strong impurity: $V_0 = -16\,\mathrm{eV}$

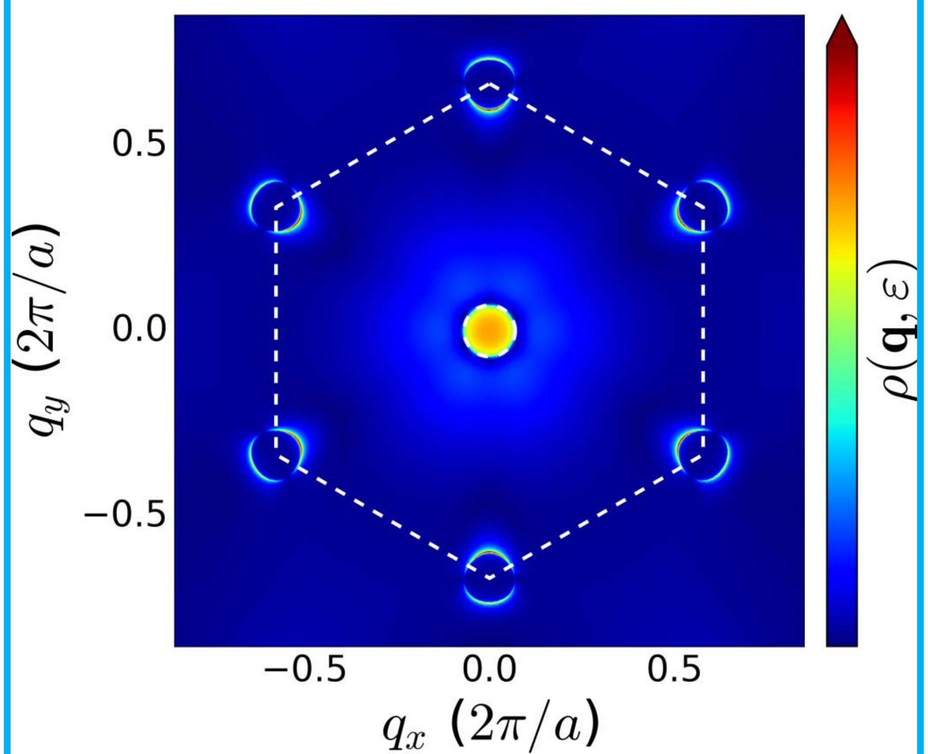




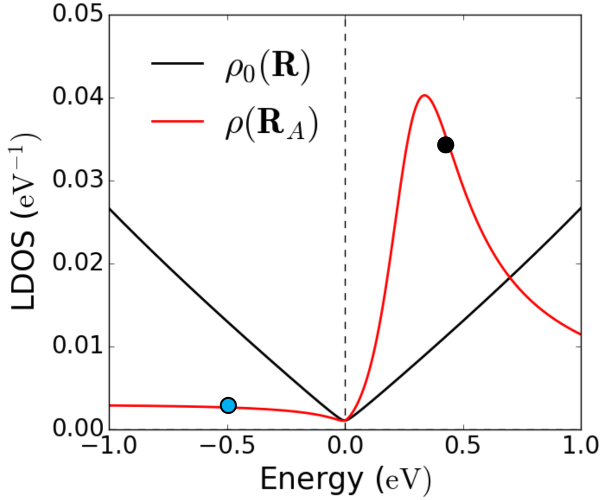


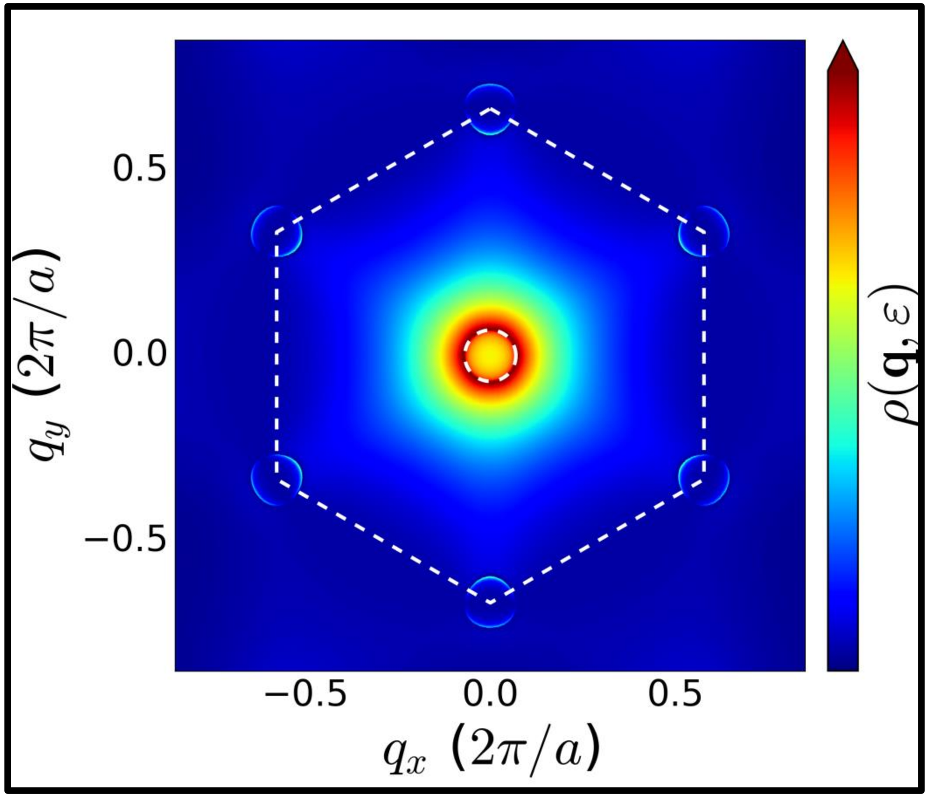
FT-STS for resonant scattering



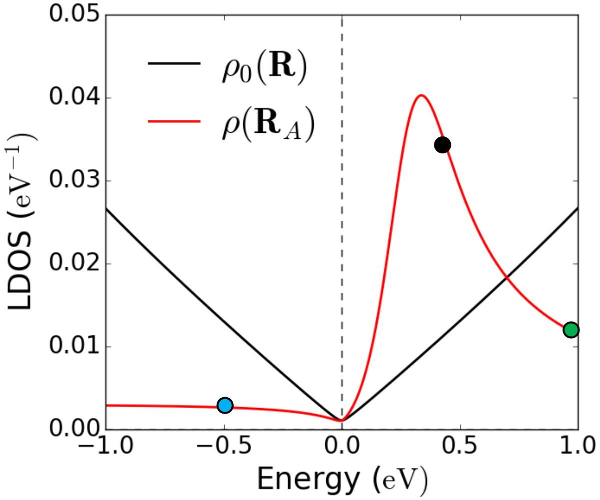


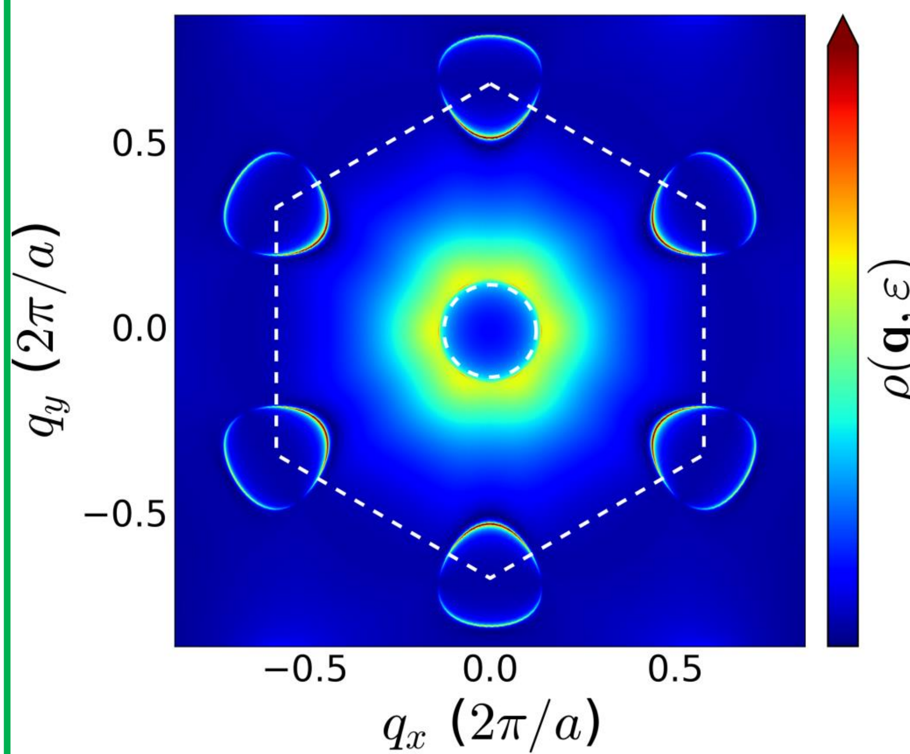
FT-STS for resonant scattering



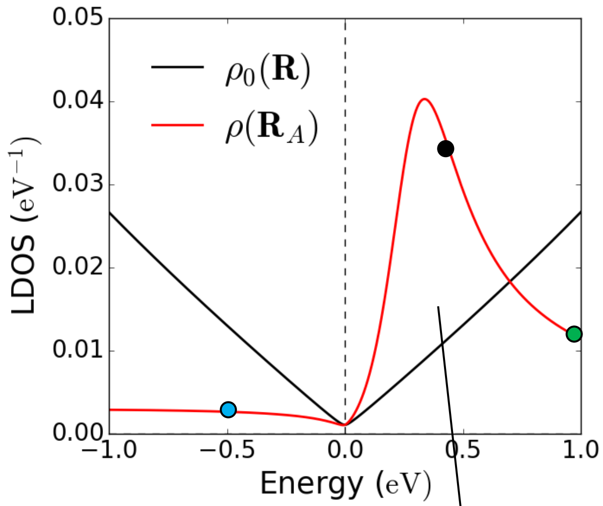


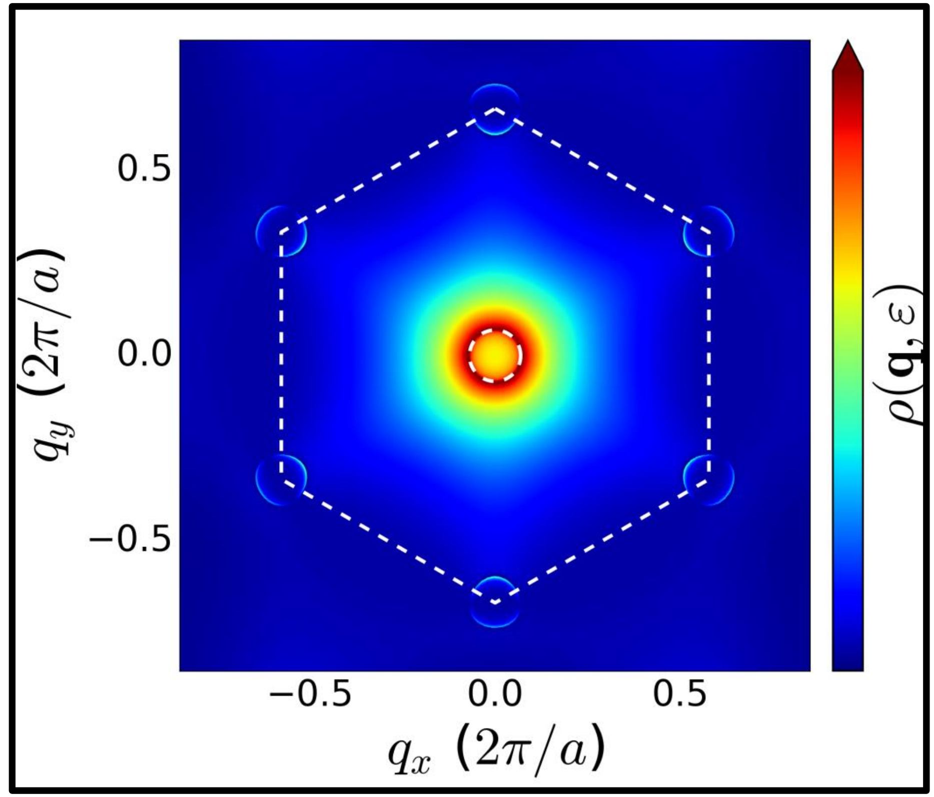
FT-STS for resonant scattering





FT-STS for resonant scattering





$$|\Psi_{s\mathbf{k}}(\varepsilon)\rangle = |\psi_{s\mathbf{k}}\rangle + \sum_{\mathbf{k}'} |\psi_{s\mathbf{k}'}\rangle \hat{G}^0_{\mathbf{k}'}(\varepsilon)\hat{T}_{\mathbf{k}'\mathbf{k}}(\varepsilon)$$

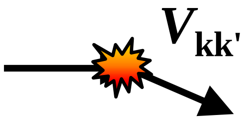
- Reappearance of broad backscatter ring at resonance
  → standard “scattering picture” breaks down.

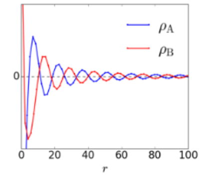
Kaasbjerg *et al.*, in preparation (2018)

Summary

1. QPI/FT-STS unique method for probing QP states and the scattering properties of defects → direct fingerprint.

2. Unified theoretical framework for calculating FT-STS/QPI spectra in two-dimensional materials:
   - Impurity matrix element (scattering processes).
   - Phase-factor matrix element (interference).





3. The latter can mask scattering processes in FT-STS:
   - intravalley backscattering in graphene (spinor overlap).

4. Uncovered a hitherto unexplored variant of the backscatter ring for resonant scattering in graphene.

5. Relevant for QPI in Moiré lattices, other 2D materials (e.g., silicene), as well as surfaces of TIs and Weyl semimetals.

Acknowledgments

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