Single-particle propagator

① Electron propagator in a non-interacting system

- definition of an electron propagator

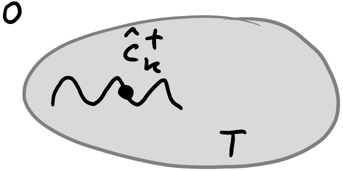
$$G_R(t) = -\frac{i}{\hbar}\langle[\hat{A}(t),\hat{B}(0)]_\varepsilon\rangle\,\vartheta(t) \quad\rightarrow\quad G_R(k,t) = -\frac{i}{\hbar}\langle\{\hat{c}_k(t),\hat{c}_k^+(0)\}\rangle\,\vartheta(t)$$

(momentum conserved)

$\hat{B}$ ... creation of particle via $\hat{c}^+_{k\sigma}$

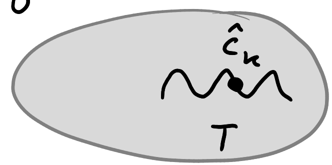
$\hat{A}$ ... annihilation of particle via $\hat{c}_{k\sigma}$

$t=0$



$\xrightarrow{\text{time evolution}}$

$t>0$



- interpretation:
  - amplitude of "survivel" in the initiel Bloch state (reflecting quasiparticle decay)
  - phase oscillations corresponding to particle energy $\quad G \sim e^{-\frac{i}{\hbar}\varepsilon_k t}$

- non-interacting electrons in a single band captured by $\hat{H} = \sum_{k\sigma} \varepsilon_k \hat{c}^{+}_{k\sigma} \hat{c}_{k\sigma}$

typically includes chemical potential

- direct evaluation of G_R

$$\hat{c}_{k\sigma}(t) = e^{\frac{i}{\hbar}\hat{H}t}\, \hat{c}_{k\sigma}\, e^{-\frac{i}{\hbar}\hat{H}t}$$

$|\psi\rangle$ any configuration of electrons with $k\sigma$ occupied

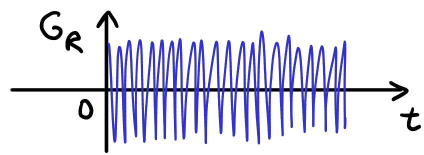
$$\begin{array}{cccccc} k_1\uparrow & k_1\downarrow & k_2\uparrow & k_2\downarrow & \dots & \\ |\,1 & 0 & 0 & 1 & \dots & \rangle \end{array}$$

$$e^{\frac{i}{\hbar}\hat{H}t}\, \hat{c}_{k\sigma}\, e^{-\frac{i}{\hbar}\hat{H}t} \underbrace{|\psi\rangle}_{\hat{H}\text{ eigenstate with energy } E} = e^{-\frac{i}{\hbar}Et}\, e^{\frac{i}{\hbar}\hat{H}t} \underbrace{\hat{c}_{k\sigma}|\psi\rangle}_{\hat{H}\text{ eigenstate with energy } E-\varepsilon_k} = e^{-\frac{i}{\hbar}\varepsilon_k t}\, \hat{c}_k |\psi\rangle$$

$\hat{c}_{k\sigma}(t) = e^{-\frac{i}{\hbar}\varepsilon_k t}\, \hat{c}_{k\sigma}$ inserted into $G_R(k,t) = -\frac{i}{\hbar}\langle\{\hat{c}_{k\sigma}(t), \hat{c}^{+}_{k\sigma}\}\rangle\, \vartheta(t)$

$$G_R(k,t) = -\frac{i}{\hbar}\, e^{-\frac{i}{\hbar}\varepsilon_k t} \langle \hat{c}_{k\sigma}\hat{c}^{+}_{k\sigma} + \hat{c}^{+}_{k\sigma} c_{k\sigma} \rangle\, \vartheta(t) = -\frac{i}{\hbar}\, e^{-\frac{i}{\hbar}\varepsilon_k t}\, \vartheta(t)$$

$\rightarrow$ infinite lifetime, oscillations with frequency $\frac{\varepsilon_k}{\hbar}$



- in energy domain

$$G_R(k,E) = \int_{-\infty}^{\infty} dt\; e^{\frac{i}{\hbar}(E+i0^+)t}\, G_R(k,t) = -\frac{i}{\hbar}\int_0^{\infty} dt\; e^{\frac{i}{\hbar}(E+i0^+-\varepsilon_k)t} = \frac{1}{E+i0^+-\varepsilon_k}$$

Spectral function $A(k,E) = -\frac{1}{\pi}\,\mathrm{Im}\, G_R(k,E) = \delta(E-\varepsilon_k)$

- evaluation via universal spectral representation

$$G(k,z) = \frac{1}{Z}\sum_{mn} |\langle n|\hat{c}^{+}_{k\sigma}|m\rangle|^2\, \frac{e^{-\beta E_m}+e^{-\beta E_n}}{z+E_m-E_n}$$

$\hat{c}^{+}_{k\sigma}$ brings ε_k

$\rightarrow E_n - E_m = \varepsilon_k$

$$= \frac{1}{z-\varepsilon_k}\;\frac{1}{Z}\sum_m \langle m|\hat{c}_{k\sigma}\sum_n |n\rangle\langle n|\hat{c}^{+}_{k\sigma}|m\rangle\; e^{-\beta E_m}\left(1+e^{-\beta\varepsilon_k}\right)$$

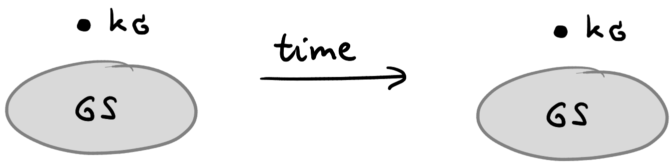
$$= \frac{1}{z-\varepsilon_k}\left(1+e^{-\beta\varepsilon_k}\right)\underbrace{\frac{1}{Z}\sum_m e^{-\beta E_m}\langle m|\hat{c}_{k\sigma}\hat{c}^{+}_{k\sigma}|m\rangle}_{1-\langle n_{k\sigma}\rangle = 1-n_F(\varepsilon_k) = 1-\frac{1}{e^{\beta\varepsilon_k}+1}} \rightarrow \langle m|1-\hat{c}^{+}_{k\sigma}\hat{c}_{k\sigma}|m\rangle$$

$$= \frac{1}{z-\varepsilon_k}$$

② Quasiparticle renormalization

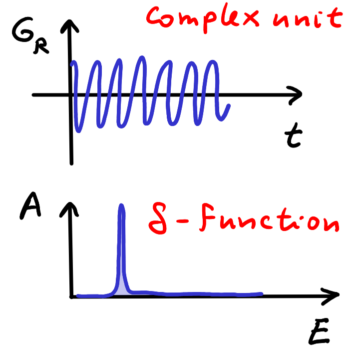
$$G_R(k,t) = -\frac{i}{\hbar}\langle\{\hat{c}_{k\sigma}(t), \hat{c}^\dagger_{k\sigma}\}\rangle\,\vartheta(t) \;\longrightarrow\; G_R(k,E) \;\longrightarrow\; A(k,E) = -\frac{1}{\pi}\,\mathrm{Im}\,G_R(k,E)$$

- non-interacting system



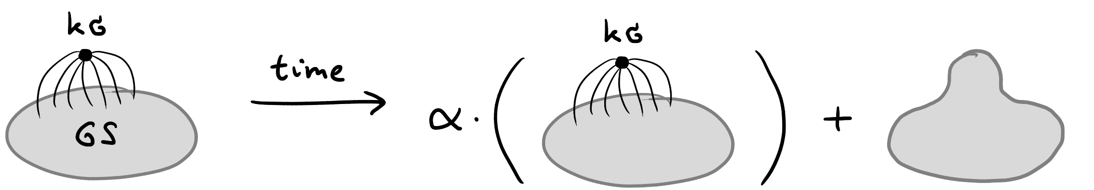
$$G_R(t) \sim e^{-\frac{i}{\hbar}\varepsilon_k t}$$

$$A(k,E) = \delta(E-\varepsilon_k)$$

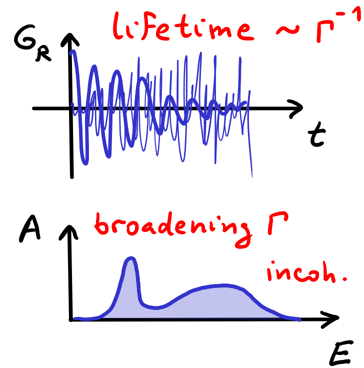


- interacting system

$$G_R \sim e^{-\frac{\Gamma_k}{\hbar}t}\, e^{-\frac{i}{\hbar}\tilde{\varepsilon}_k t} \qquad A \sim \frac{1}{(E-\tilde{\varepsilon}_k)^2 + \Gamma_k^2}$$



quasiparticle part   incoherent part



- components of the electron spectral function

$$A(k,E) = \frac{1}{Z}\sum_{mn} e^{-\beta E_m}\left\{ |\langle n|\hat{c}^+_{kG}|m\rangle|^2 \delta[E-(E_n-E_m)] + |\langle n|\hat{c}_{kG}|m\rangle|^2 \delta[E+(E_n-E_m)]\right\}$$

$\rightarrow A_+(k,E)$ electron addition, iPES

$\rightarrow A_-(k,-E)$ electron removal, PES

$$= A_+(k,E) + A_-(k,-E)$$

$$A_+(k,E) = \frac{1}{Z}\sum_{mn} e^{-\beta E_m} |\langle n|\hat{c}^+_{kG}|m\rangle|^2 \delta[E-(E_n-E_m)]$$

relabel $m \leftrightarrow n$ and use $\langle m|c^+|n\rangle = \langle n|c|m\rangle^*$

$$= \frac{1}{Z}\sum_{mn} e^{-\beta E_n} |\langle n|\hat{c}_{kG}|m\rangle|^2 \delta[E+(E_n-E_m)] = e^{\beta E} A_-(k,-E)$$

$E_n \leftarrow E_m - E$

$$A(k,E) = (e^{\beta E}+1)A_-(k,-E) = (1+e^{-\beta E})A_+(k,E)$$

$\rightarrow A_+(k,E) = [1-n_F(E)]A(k,E)$

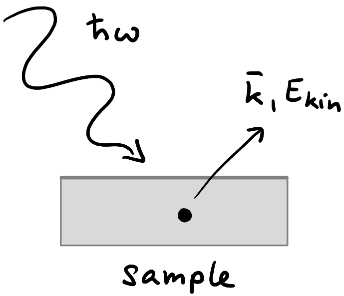
$\rightarrow A_-(k,-E) = n_F(E)A(k,E)$

- sum rules

$$\int_{-\infty}^{\infty} dE\, A(k,E) = \langle\{\hat{c}_{kG}, \hat{c}^+_{kG}\}\rangle = 1$$

$$\int_{-\infty}^{\infty} dE\, A(k,E)\, n_F(E) = \langle n_{kG}\rangle$$

③ Angle-resolved photoemission spectroscopy (ARPES)



sudden approximation: photoelectron removed instantaneously

intensity $\sim n_F(E)\, A(k,E) = A_-(k,-E)$

energy loss $E = \hbar\omega - E_{kin}$

scientaomicron

Damascelli, Hussain, and Shen: Photoemission studies of the cuprate superconductors

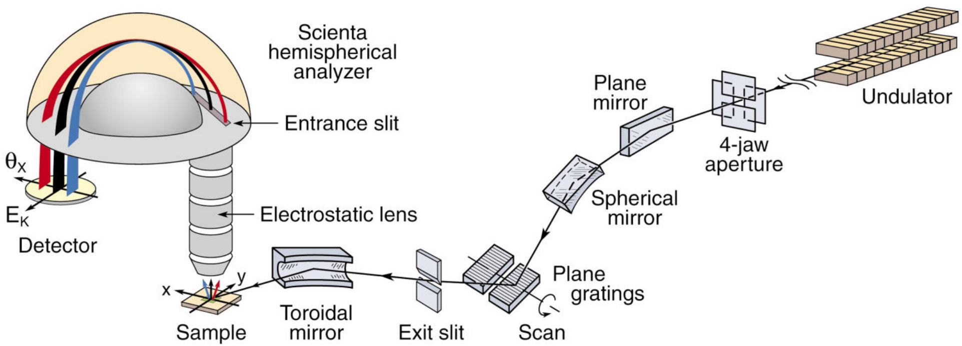


FIG. 6. Generic beamline equipped with a plane grating monochromator and a Scienta electron spectrometer (Color).

Rev. Mod. Phys. 75, 473 (2003)

Sr_2RuO_4

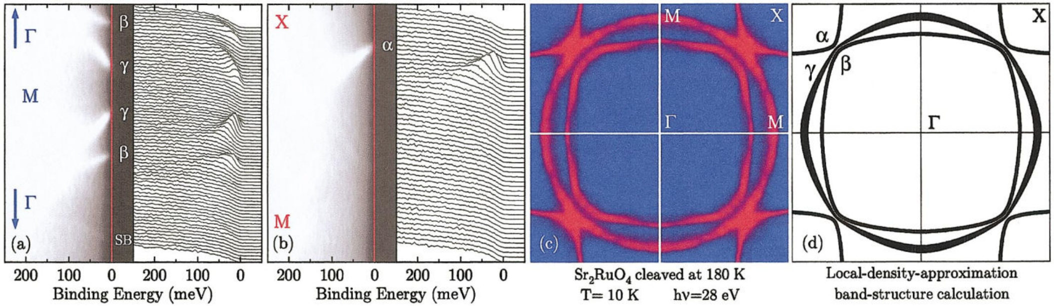
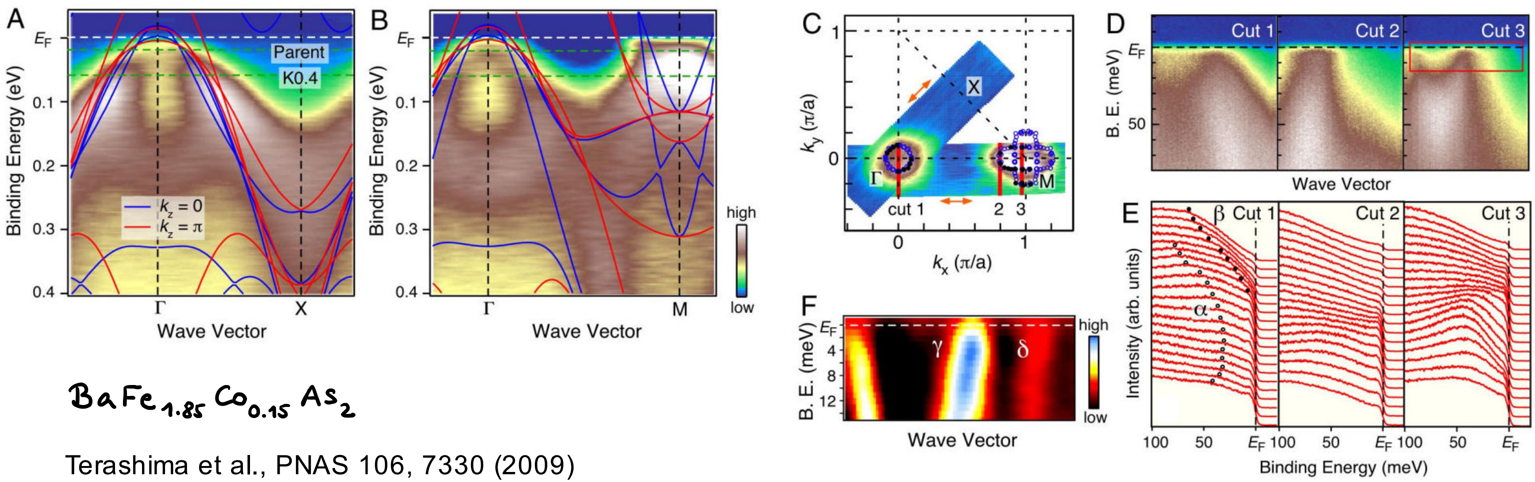


FIG. 9. Photoemission results from Sr_2RuO_4: ARPES spectra and corresponding intensity plot along (a) Γ-*M* and (b) *M*-*X*; (c) measured Fermi surface; (d) calculated Fermi surface (Mazin and Singh, 1997). From Damascelli *et al.*, 2000 (Color).



$BaFe_{1.85}Co_{0.15}As_2$

Terashima et al., PNAS 106, 7330 (2009)

Spin-orbit splitting of the Shockley surface state on Cu(111)

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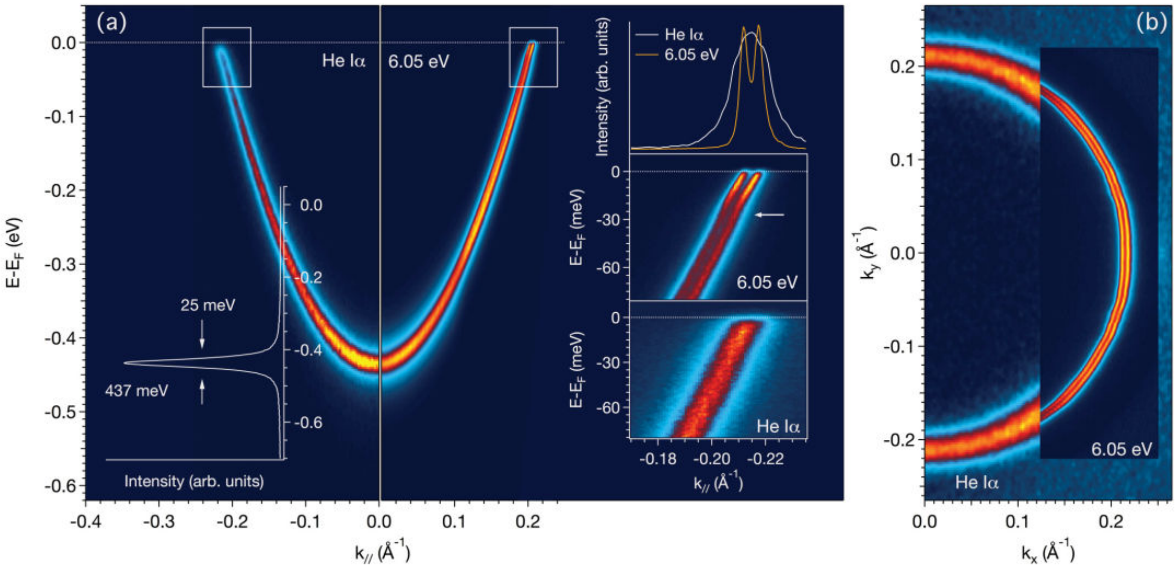

FIG. 1. (Color online) Conventional and laser-ARPES data from the Cu(111) surface state. (a) The full parabolic dispersion measured with He Iα (left) and laser excitation (right). The insets show momentum distribution curves at the Fermi level (E_F) and expand the most crucial region of the dispersion near E_F, revealing the momentum-independent splitting of the dispersion, which is characteristic of Rashba systems with small wave vectors. (b) A section of the Fermi surface measured with He Iα and laser excitation, respectively.

Substrate-induced bandgap opening in epitaxial graphene

Zhou et al., Nature Materials 6, 770 (2007)

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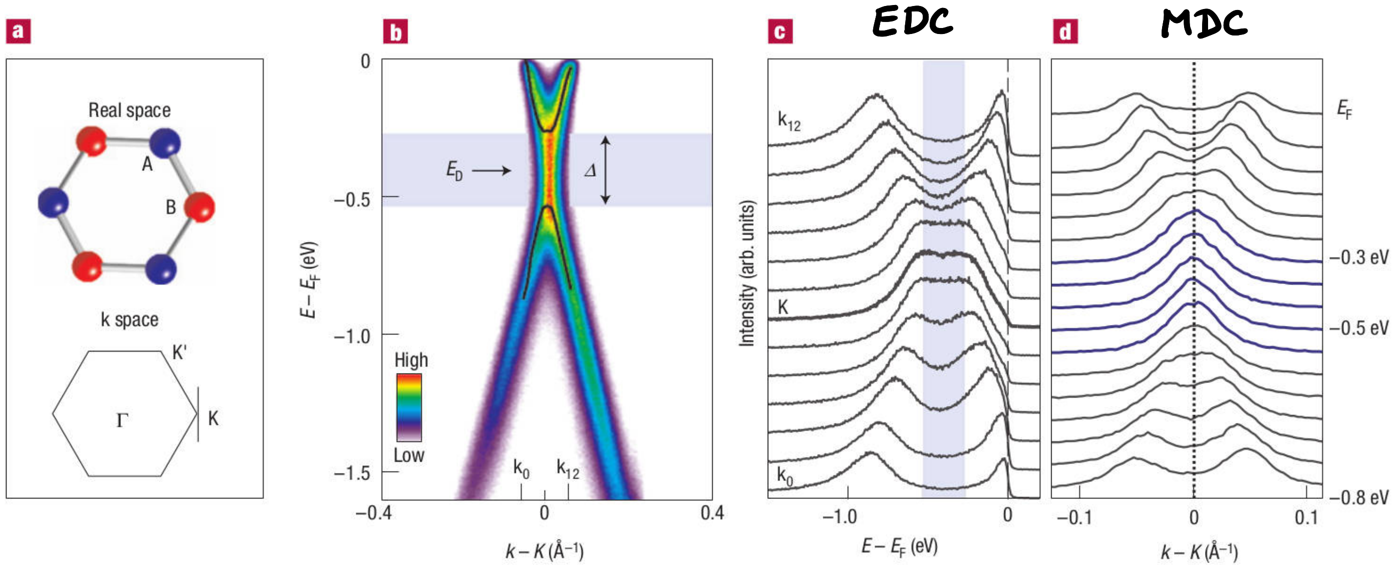

Figure 1 Observation of the gap opening in single-layer graphene at the K point. a, Structure of graphene in the real and momentum space. **b**, ARPES intensity map taken along the black line in the inset of **a**. The dispersions (black lines) are extracted from the EDC peak positions shown in **c**. **c**, EDCs taken near the K point from k_0 to k_{12} as indicated at the bottom of **b**. **d**, MDCs from E_F to −0.8 eV. The blue lines are inside the gap region, where the peaks are non-dispersive.