КИЇВСЬКИЙ АКАДЕМІЧНИЙ УНІВЕРСИТЕТ

Курс:
Фізичні методи дослідження матеріалів

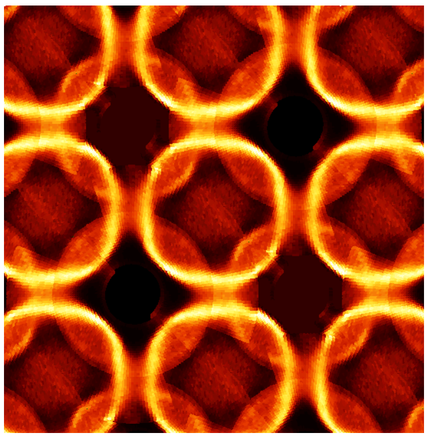
Тема:
Спектральні функції та перетворення Фурьє

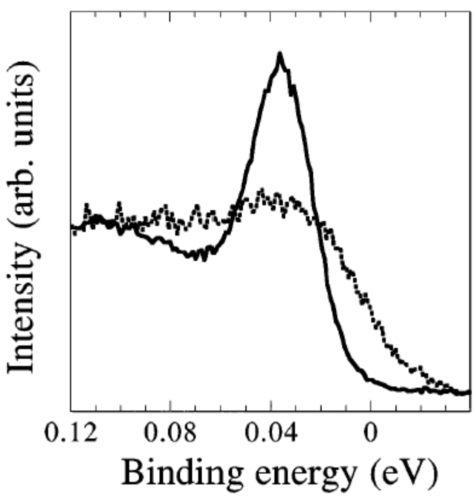
Лектор: О. А. Кордюк

1 particle *vs* 2 particle spectra

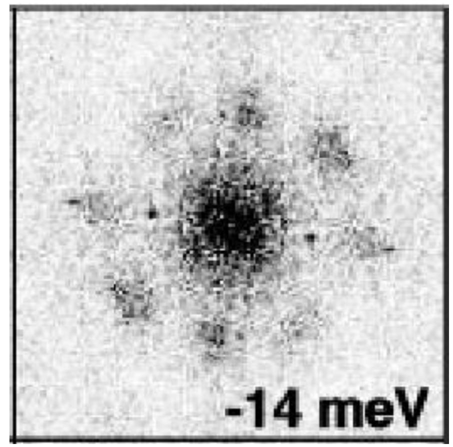
Modern momentum resolving techniques

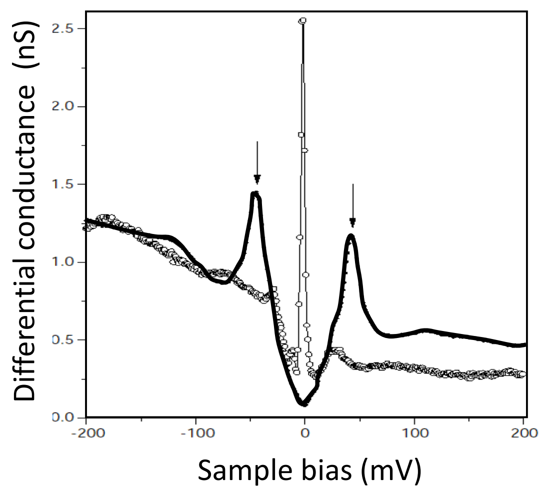
ARPES



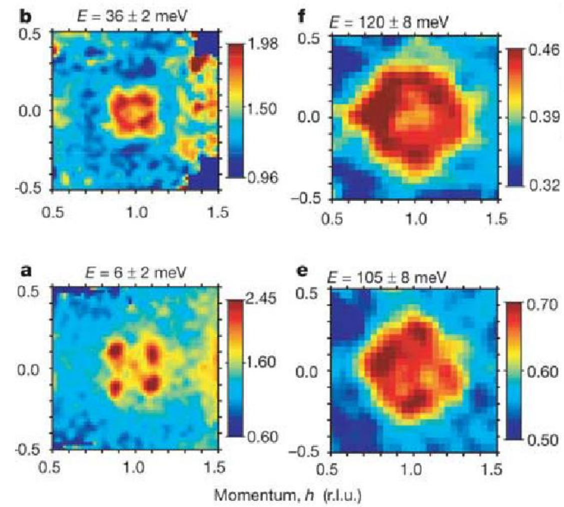


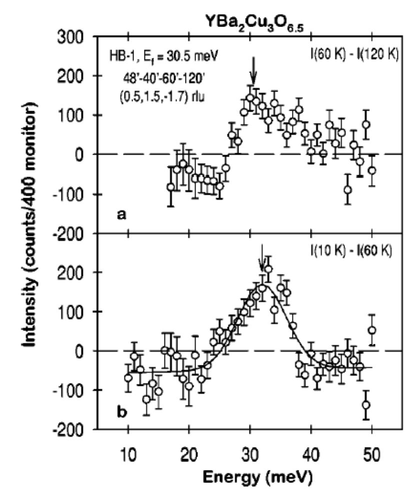
STS





INS





Одно-частинкова спектральна функція = Im *G*

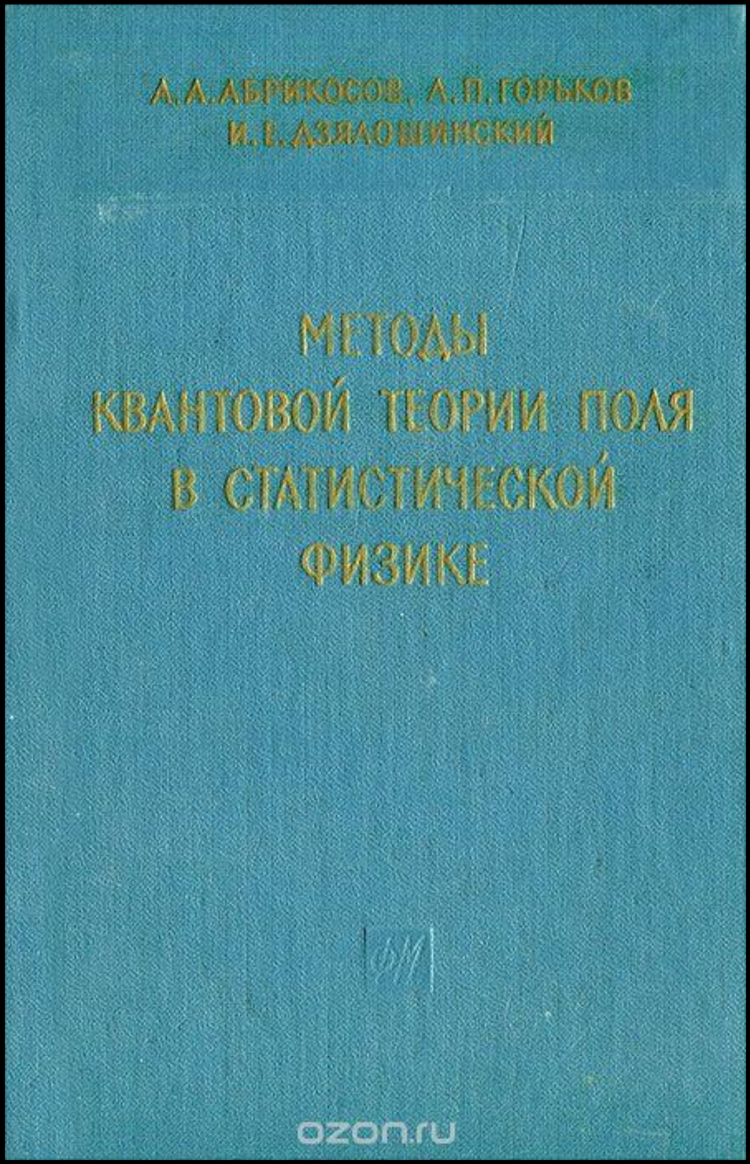
$$G_0(\omega, \mathbf{k}) = \frac{1}{\omega - \varepsilon(\mathbf{k}) + i\delta}$$

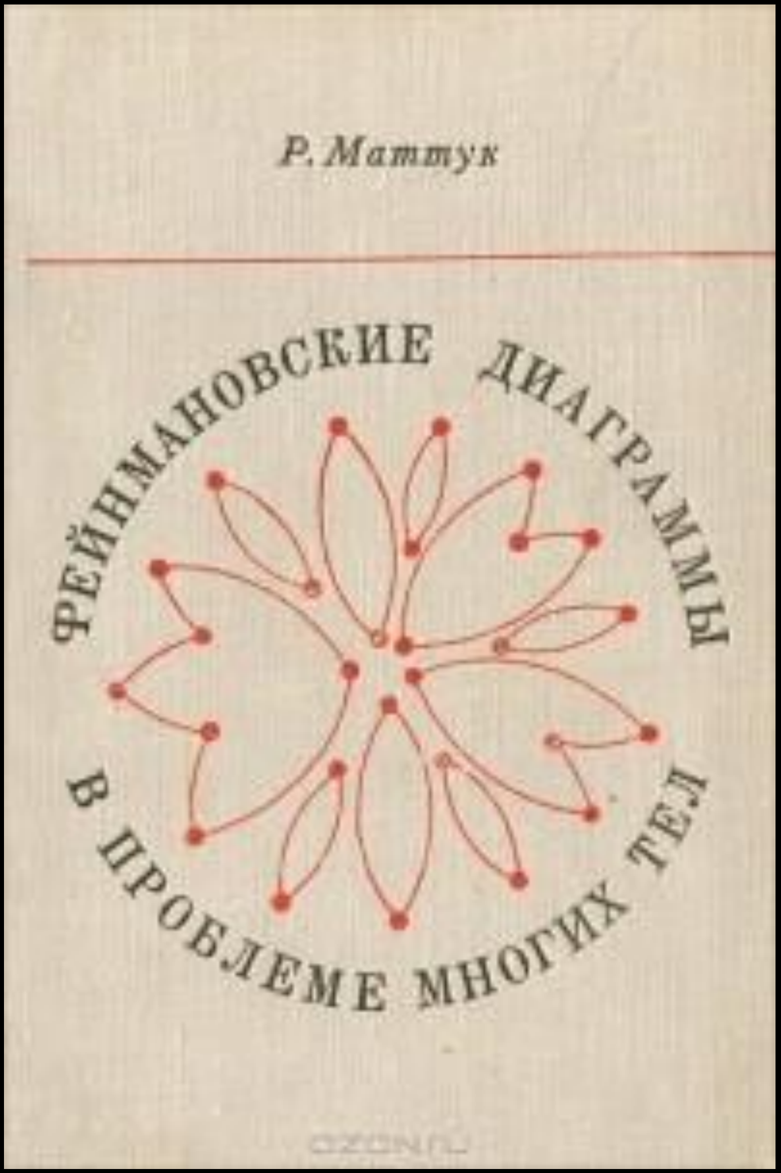
$$G(\omega, \mathbf{k}) = \frac{1}{\omega - \varepsilon(\mathbf{k}) + \Sigma(\omega)}$$

$$A(\omega, \mathbf{k}) = \mathrm{Im}\, G(\omega, \mathbf{k})$$

$$A(\omega, \mathbf{k}) = -\frac{1}{\pi} \frac{\Sigma''(\omega)}{(\omega - \varepsilon(\mathbf{k}) - \Sigma'(\omega))^2 + \Sigma''(\omega)^2}$$

Спектральна функція = Im (функція Гріна)

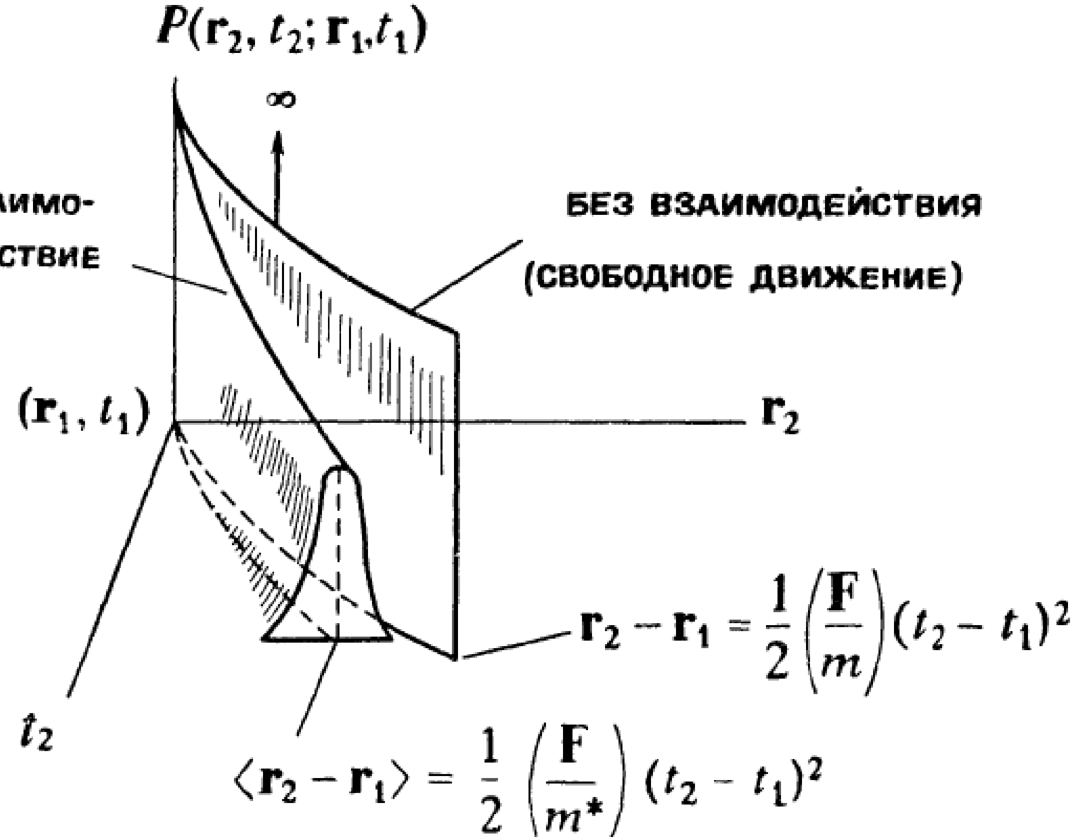




$$\mathbf{r}_2 - \mathbf{r}_1 = \frac{1}{2}\left(\frac{\mathbf{F}}{m}\right)(t_2 - t_1)^2$$

$$P_0(\mathbf{r}_2,\ t_2;\ \mathbf{r}_1,\ t_1) = \delta\left[(\mathbf{r}_2 - \mathbf{r}_1) - \frac{1}{2}\left(\frac{\mathbf{F}}{m}\right)(t_2 - t_1)^2\right]$$

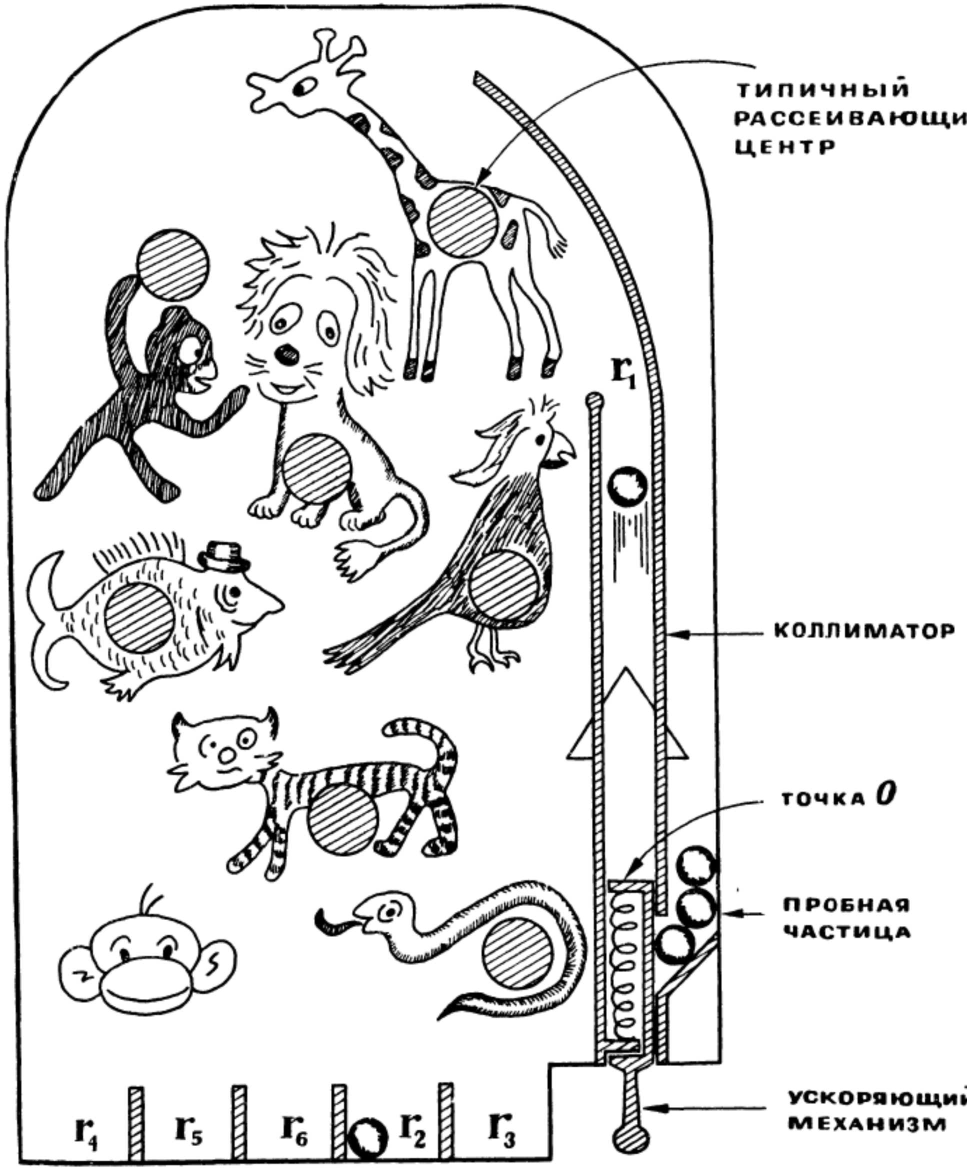
$P(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) =$ Плотность вероятности (вероятность на единицу объема) того, что если частица в момент t_1 помещена в данную систему в точку $\mathbf{r}_1$ то она будет найдена в точке $\mathbf{r}_2$ в более поздний момент времени t_2.



$\langle \mathbf{r}_2 - \mathbf{r}_1 \rangle = \frac{1}{2}\left(\frac{\mathbf{F}}{m^*}\right)(t_2 - t_1)^2$ для максимального значения P

$$P_{\text{макс}}(\mathbf{r}_2,\ t_2;\ \mathbf{r}_1,\ t_1) \sim e^{-(t_2 - t_1)/\tau}$$

Р. Маттук
Фейнмановские диаграммы в проблеме многих тел

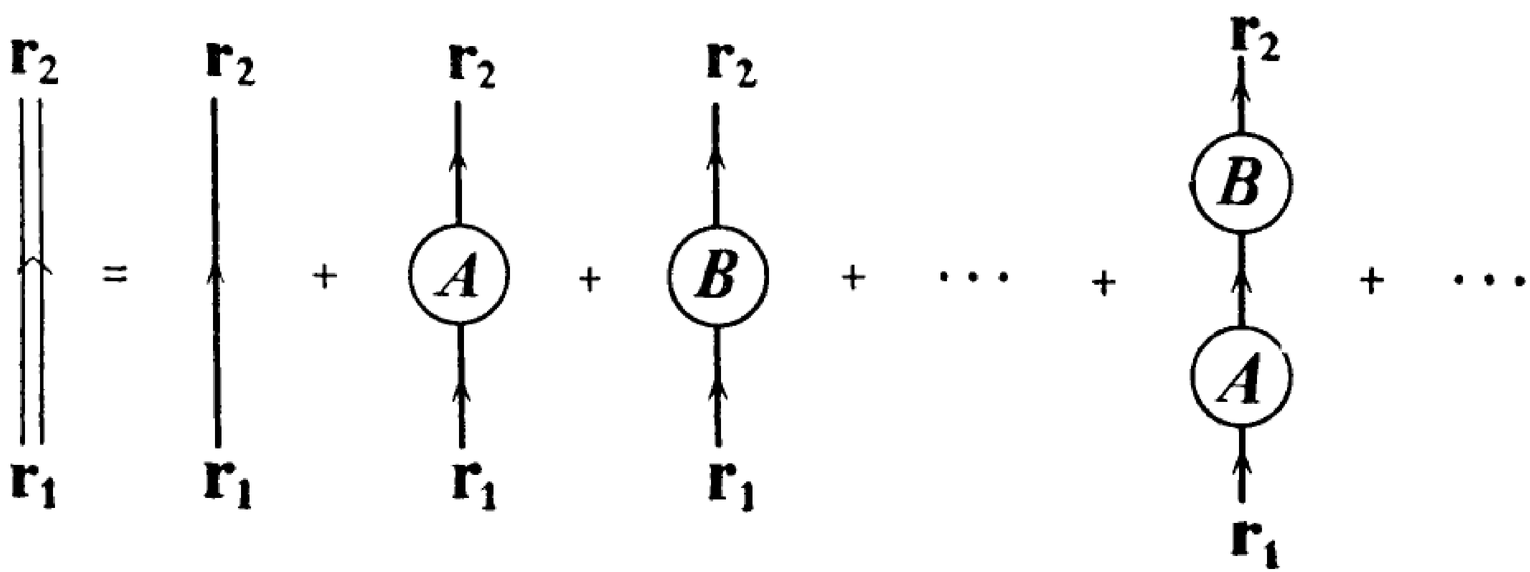


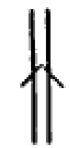
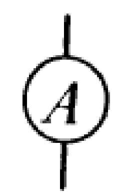
ТИПИЧНЫЙ РАССЕИВАЮЩИЙ ЦЕНТР
КОЛЛИМАТОР
ТОЧКА 0
ПРОБНАЯ ЧАСТИЦА
УСКОРЯЮЩИЙ МЕХАНИЗМ
r_1
r_4
r_5
r_6
r_2
r_3

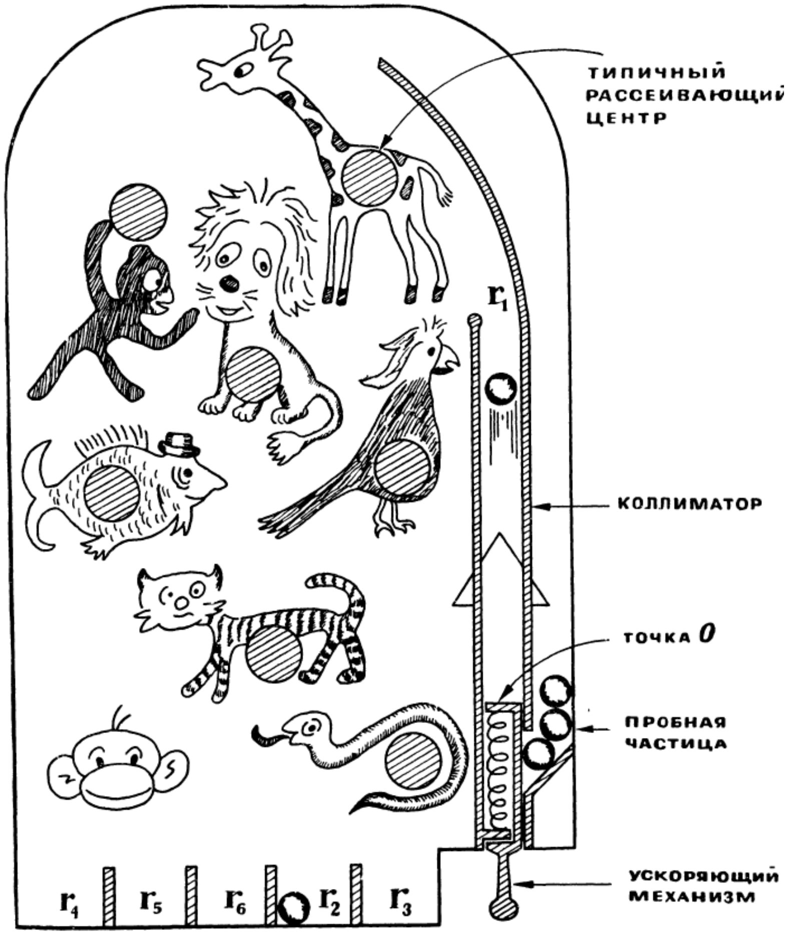
$$P(\mathbf{r}_2, \mathbf{r}_1) = P_0(\mathbf{r}_2, \mathbf{r}_1) + P_0(\mathbf{r}_A, \mathbf{r}_1)\, P(A)\, P_0(\mathbf{r}_2, \mathbf{r}_A) +$$

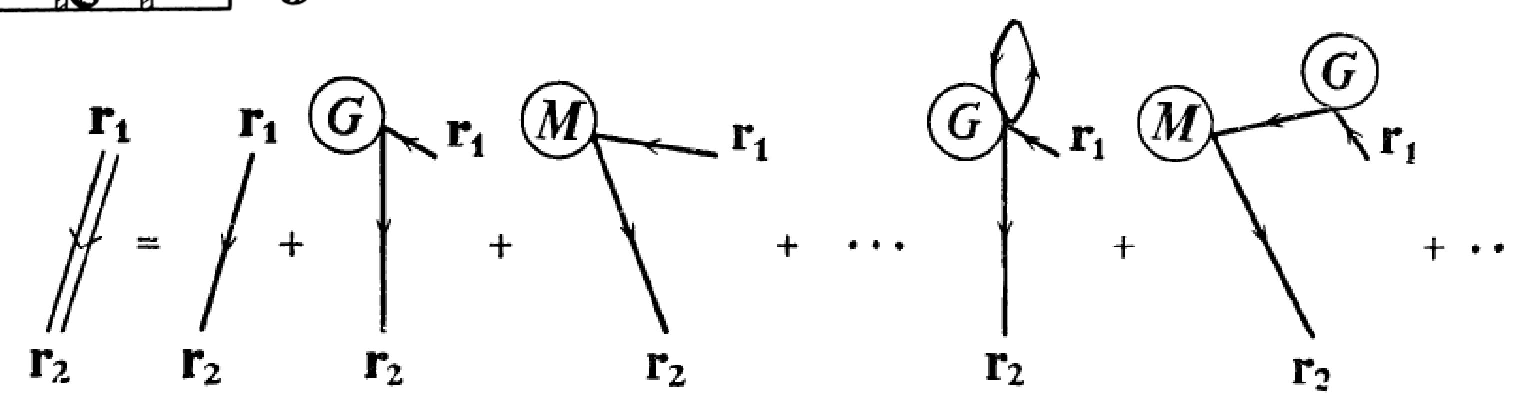
$$+ P_0(\mathbf{r}_B, \mathbf{r}_1)\, P(B)\, P_0(\mathbf{r}_2, \mathbf{r}_B) + \ \ldots$$

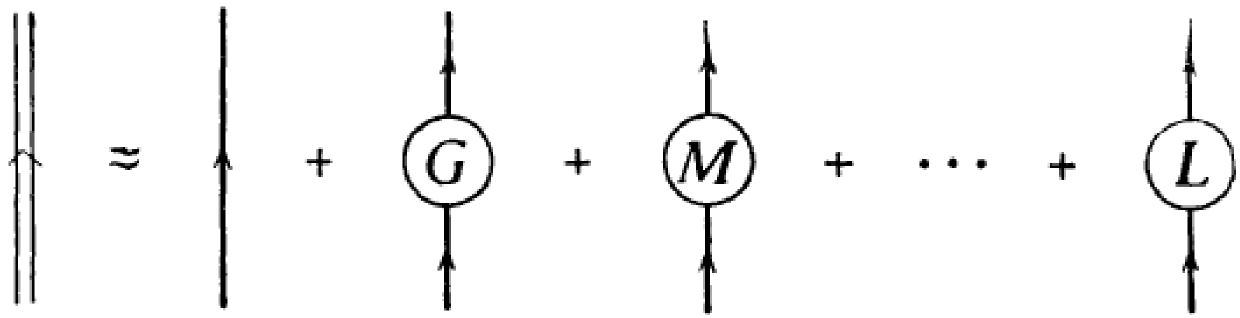
$$+ P_0(\mathbf{r}_A, \mathbf{r}_1)\, P(A)\, P_0(\mathbf{r}_B, \mathbf{r}_A)\, P(B)\, P_0(\mathbf{r}_2, \mathbf{r}_B) + \ \ldots .$$

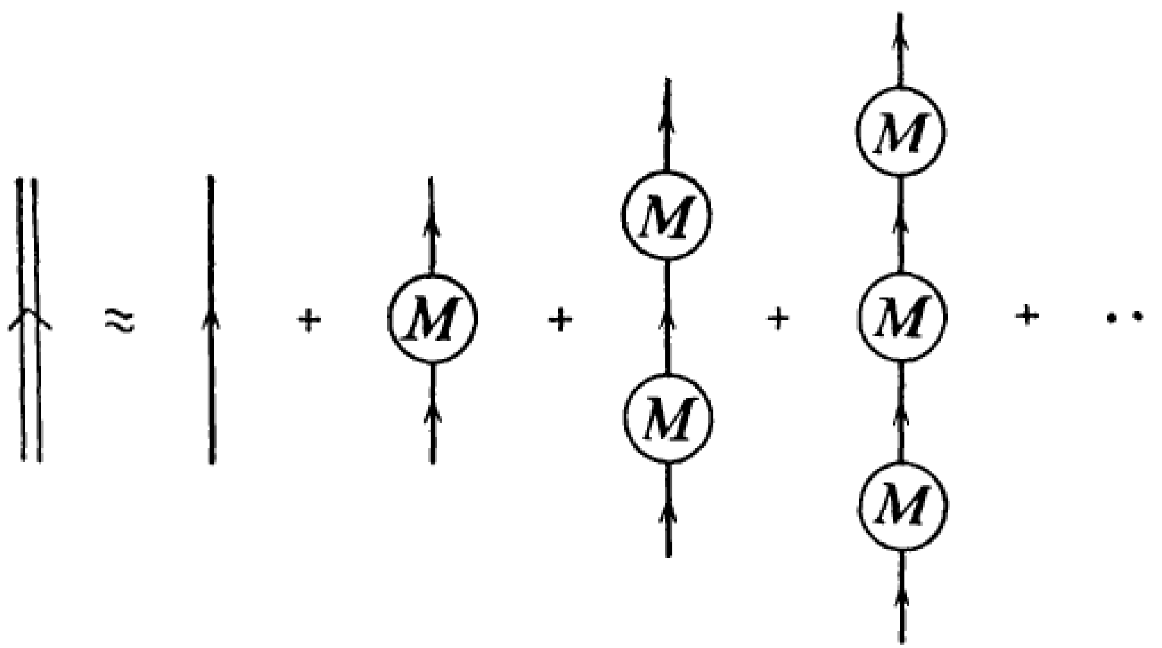


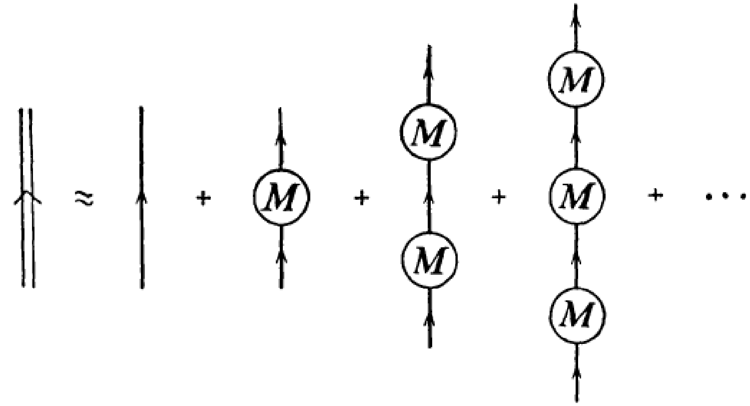
Слово	Диаграмма
$P(\mathbf{r}_j, \mathbf{r}_i, t_j - t_i)$	 $\mathbf{r}_j, t_j$; $\mathbf{r}_i, t_i$
$P_0(\mathbf{r}_j, \mathbf{r}_i, t_j - t_i)$	 $\mathbf{r}_j, t_j$; $\mathbf{r}_i, t_i$
$P(A)$	


ТИПИЧНЫЙ
РАССЕИВАЮЩИЙ
ЦЕНТР
$\mathbf{r}_1$
КОЛЛИМАТОР
ТОЧКА O
ПРОБНАЯ
ЧАСТИЦА
УСКОРЯЮЩИЙ
МЕХАНИЗМ
$\mathbf{r}_4$ $\mathbf{r}_5$ $\mathbf{r}_6$ $\mathbf{r}_2$ $\mathbf{r}_3$


$\mathbf{r}_1$
$\mathbf{r}_2$
G
M
$= \; + \; + \; + \cdots \; + \; + \cdots$

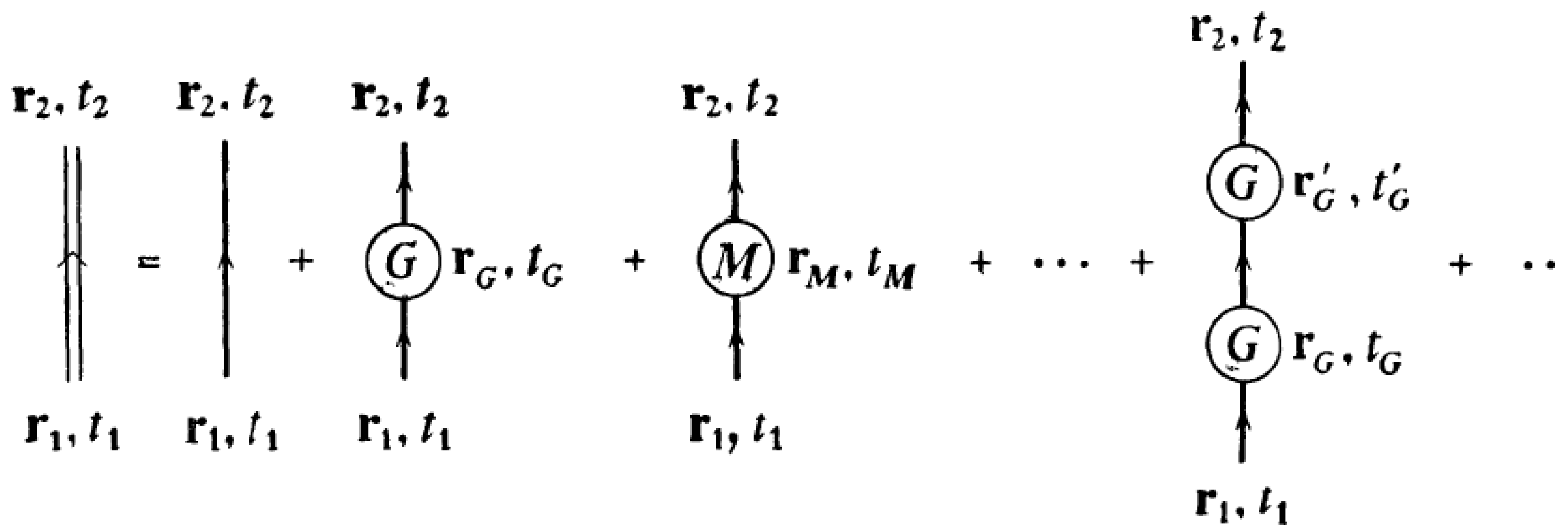

G
M
L


M
M
M
M
M
M



$$P(\mathbf{r}_2, \mathbf{r}_1) \approx P_0(\mathbf{r}_2, \mathbf{r}_1) + P_0(\mathbf{r}_M, \mathbf{r}_1)\, P(M)\, P_0(\mathbf{r}_2, \mathbf{r}_M) + \\ + P_0(\mathbf{r}_M, \mathbf{r}_1)\, P(M)\, P_0(\mathbf{r}_M, \mathbf{r}_M)\, P(M)\, P_0(\mathbf{r}_2, \mathbf{r}_M) + \; \ldots .$$

$$P(\mathbf{r}_2, \mathbf{r}_1) \approx P_0(\mathbf{r}_2, \mathbf{r}_1) + P_0(\mathbf{r}_M, \mathbf{r}_1)\, P(M)\, P_0(\mathbf{r}_2, \mathbf{r}_M) \times \\ \times [1 + P(M)\, P_0(\mathbf{r}_M, \mathbf{r}_M) + P(M)^2 P_0(\mathbf{r}_M, \mathbf{r}_M)^2 + \; \ldots] = \\ = P_0(\mathbf{r}_2, \mathbf{r}_1) + \frac{P_0(\mathbf{r}_M, \mathbf{r}_1)\, P(M)\, P_0(\mathbf{r}_2, \mathbf{r}_M)}{1 - P(M)\, P_0(\mathbf{r}_M, \mathbf{r}_M)}$$



$$P(\mathbf{r}_2,\ \mathbf{r}_1,\ t_2-t_1)=P_0(\mathbf{r}_2,\ \mathbf{r}_1,\ t_2-t_1)+$$

$$+\int_{t_1}^{t_2} dt_G P_0(\mathbf{r}_G,\ \mathbf{r}_1,\ t_G-t_1)\,P(G)\,P_0(\mathbf{r}_2,\ \mathbf{r}_G,\ t_2-t_G)+$$

$$+\int dt_M \ldots + \int\int + \ldots + \int\int\int + \ldots + \ldots.$$

$$P_0(\mathbf{r}_j, \mathbf{r}_i, t_j - t_i) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega e^{-i\omega(t_j - t_i)} P_0(\mathbf{r}_j, \mathbf{r}_i, \omega)$$

$$P_0(\mathbf{r}_2, \mathbf{r}_1, t_2 - t_1) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega e^{-i\omega(t_2 - t_1)} P_0(\mathbf{r}_2, \mathbf{r}_1, \omega),$$

$$\int_{-\infty}^{+\infty} dt_G P_0(\mathbf{r}_G, \mathbf{r}_1, t_G - t_1) P(G) P_0(\mathbf{r}_2, \mathbf{r}_G, t_2 - t_G) =$$

$$= \int_{-\infty}^{+\infty} dt_G \left[\frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega' e^{-i\omega'(t_G - t_1)} P_0(\mathbf{r}_G, \mathbf{r}_1, \omega') \right] \times$$

$$\times P(G) \left[\frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega e^{-i\omega(t_2 - t_G)} P_0(\mathbf{r}_2, \mathbf{r}_G, \omega) \right] =$$

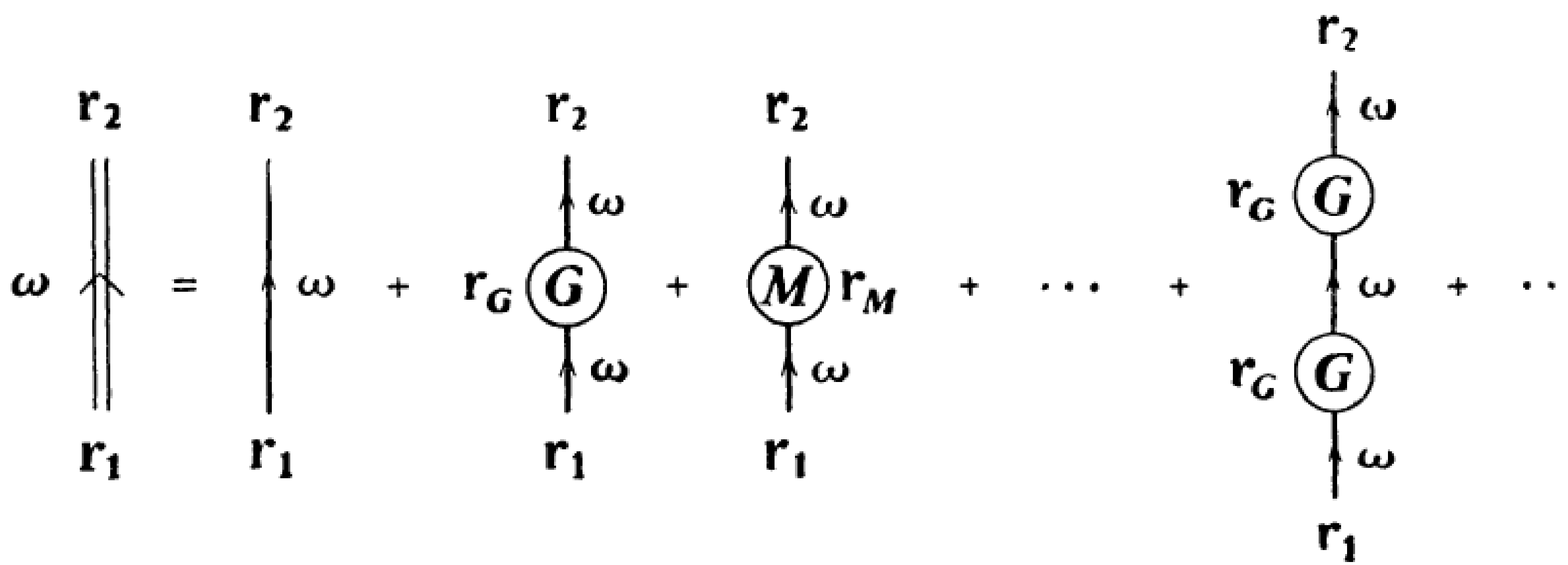
$$= \frac{1}{(2\pi)^2} \int_{-\infty}^{+\infty} d\omega \int_{-\infty}^{+\infty} d\omega' P_0(\mathbf{r}_G, \mathbf{r}_1, \omega') \times$$

$$\times P(G) P_0(\mathbf{r}_2, \mathbf{r}_G, \omega) e^{+i(\omega' t_1 - \omega t_2)} \underbrace{\int_{-\infty}^{+\infty} dt_G e^{-it_G(\omega' - \omega)}}_{2\pi\delta(\omega' - \omega)} =$$

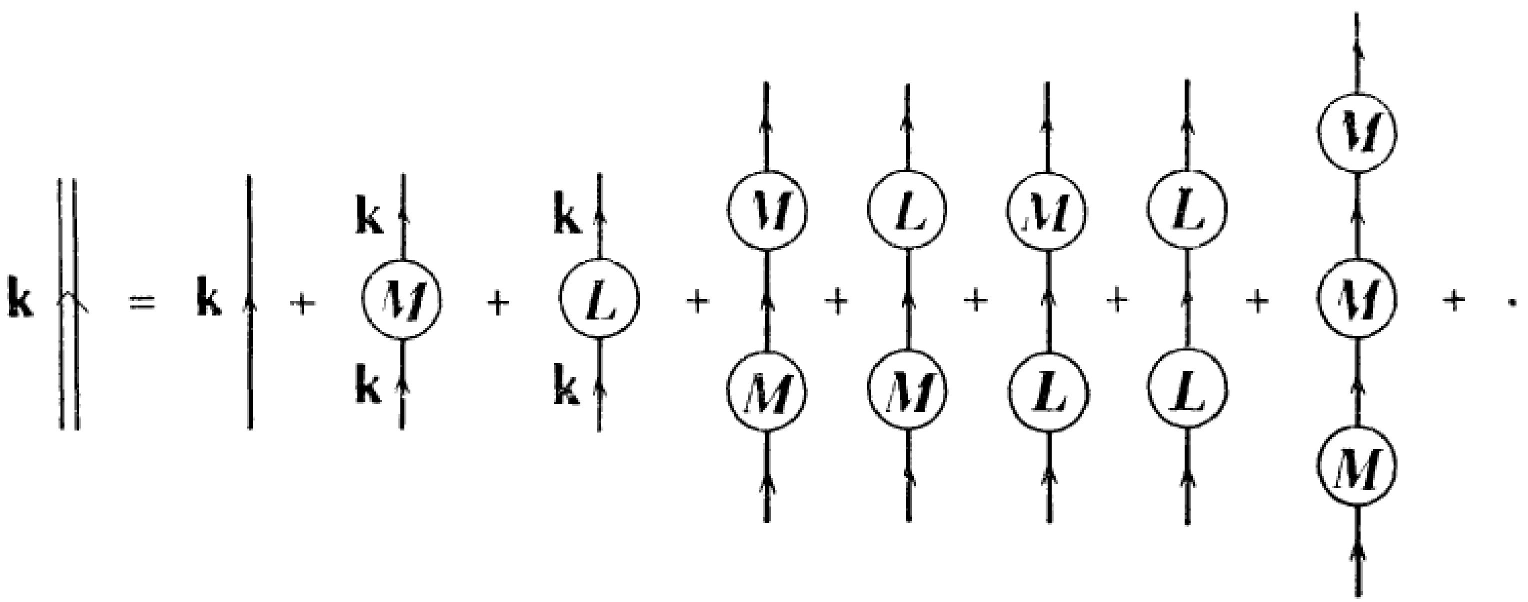
$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega e^{-i\omega(t_2 - t_1)} P_0(\mathbf{r}_G, \mathbf{r}_1, \omega) P(G) P_0(\mathbf{r}_2, \mathbf{r}_G, \omega).$$

$$P(\mathbf{r}_2, \mathbf{r}_1, \omega) =$$

$$= P_0(\mathbf{r}_2, \mathbf{r}_1, \omega) + P_0(\mathbf{r}_G, \mathbf{r}_1, \omega) P(G) P_0(\mathbf{r}_2, \mathbf{r}_G, \omega) + \ldots .$$



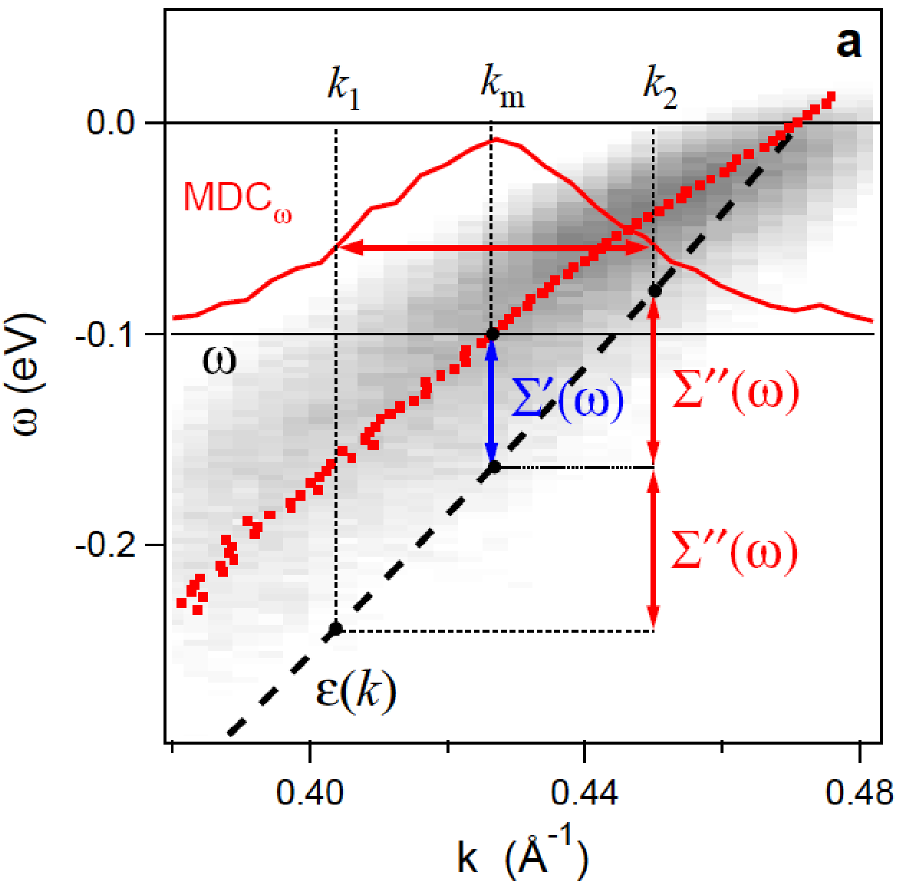
r2
ω
=
r1
+
rG
G
M
rM
· · ·



k
=
+
M
L
· ·

Спектральна функція

$$A(\omega, \mathbf{k}) = -\frac{1}{\pi} \frac{\Sigma''(\omega)}{(\omega - \varepsilon(\mathbf{k}) - \Sigma'(\omega))^2 + \Sigma''(\omega)^2}$$



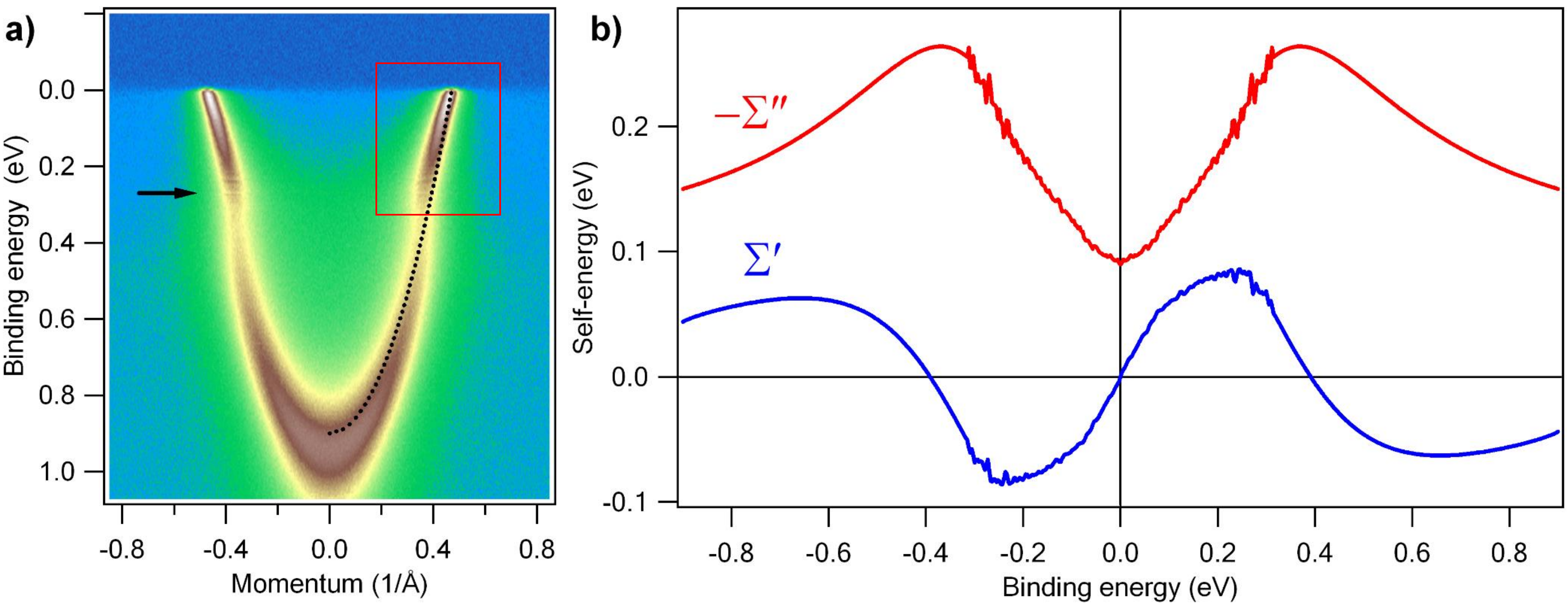
$\mathrm{EDC}(\omega) = A(\omega)_k$

$\mathrm{MDC}(k) = A(k)_\omega$

$$\Sigma'(\omega) = \omega - \varepsilon(k_m)$$

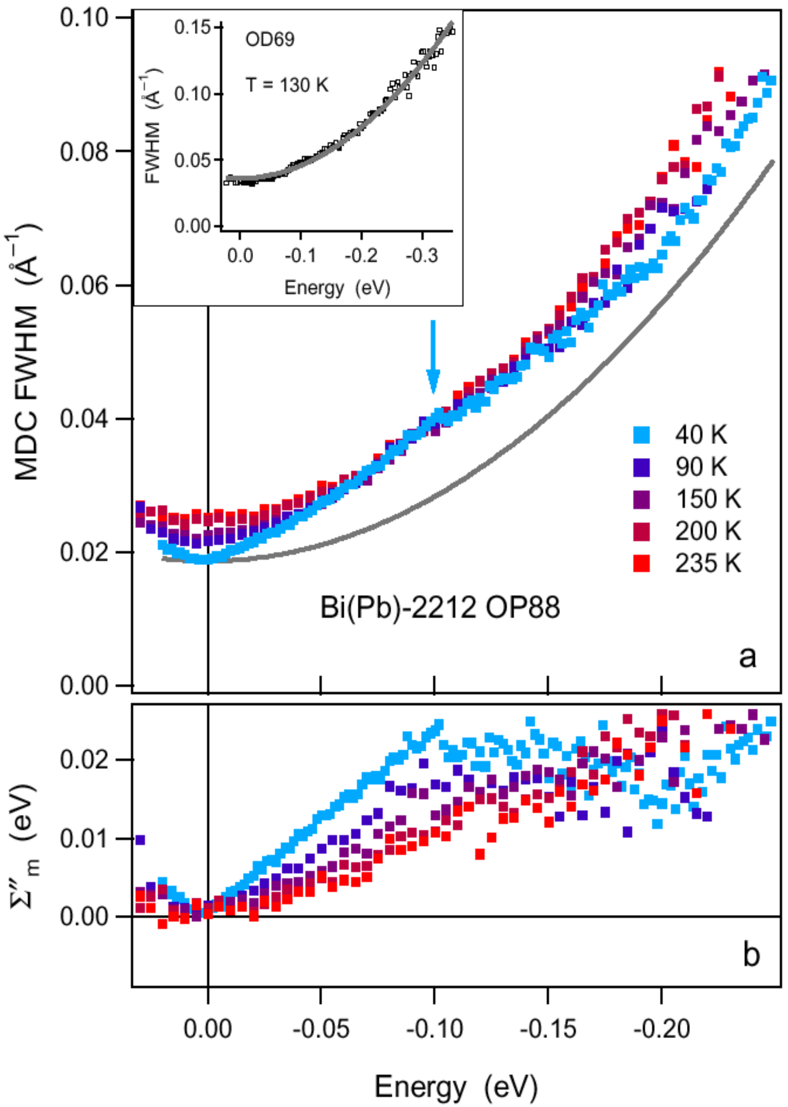
$$\Sigma''(\omega) = -v_F W(\omega)$$

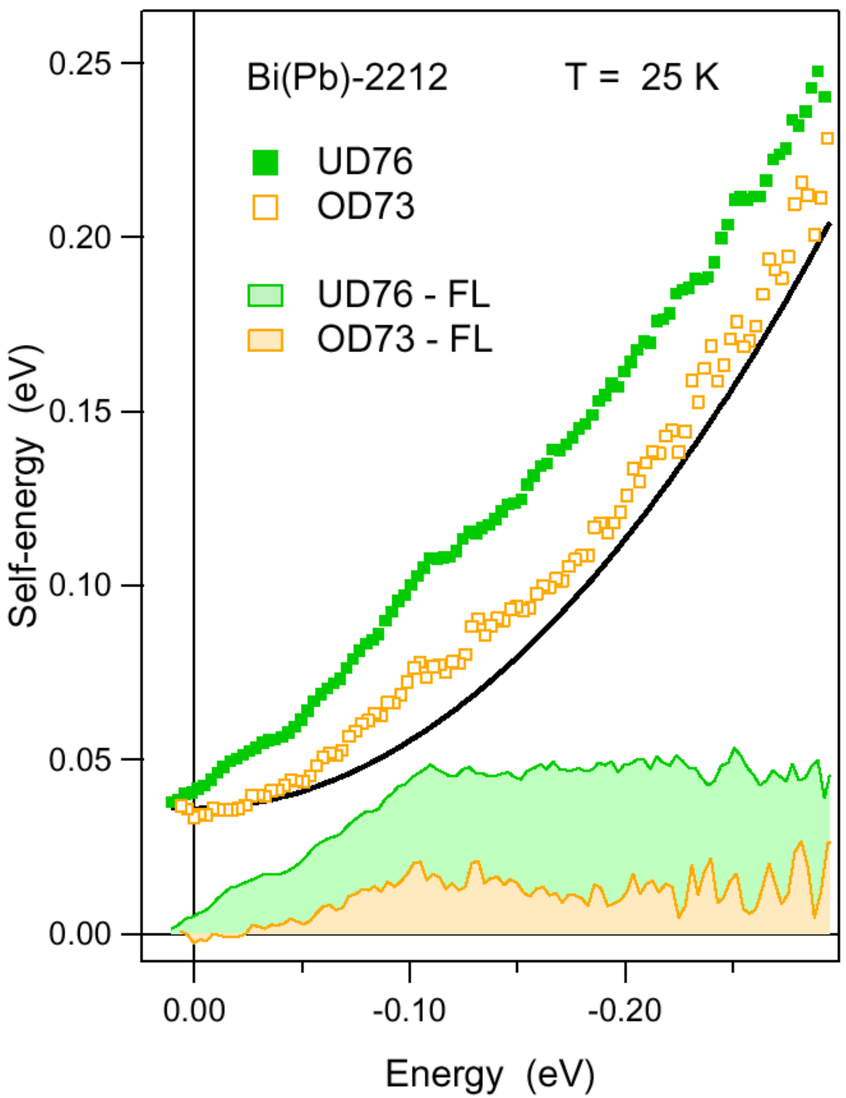
KK



Kordyuk *PRB* 2005

Scattering rate: *T*- and *x*- dependence





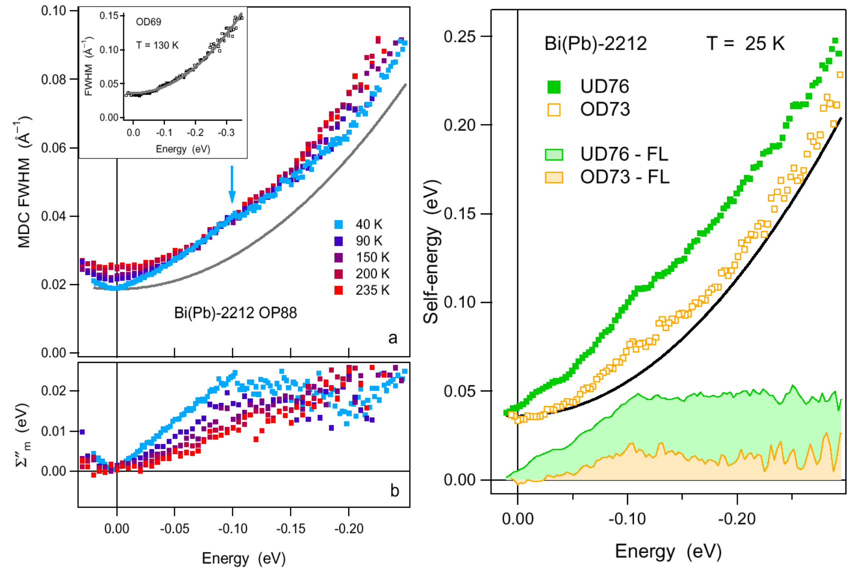
Kordyuk *PRL* 2004

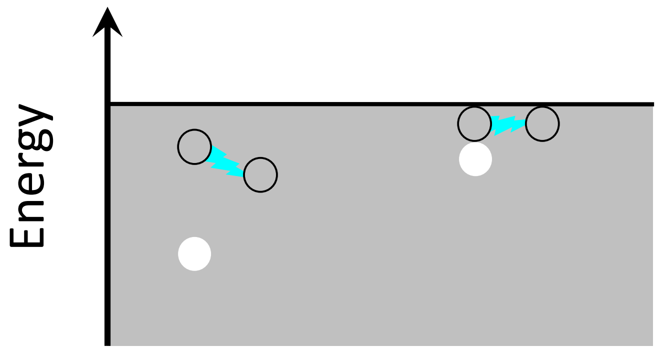
Scattering rate: Two channels

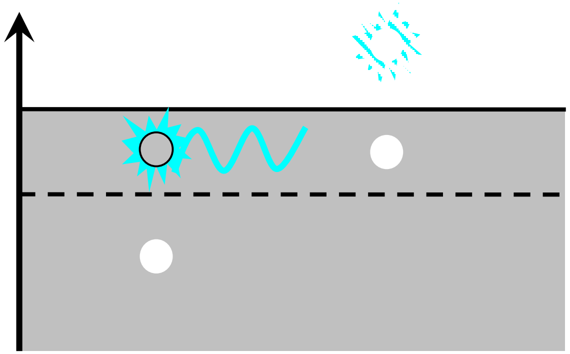
There are two channels:

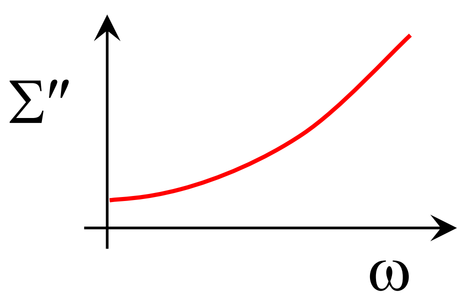
1st electron-electron scattering and

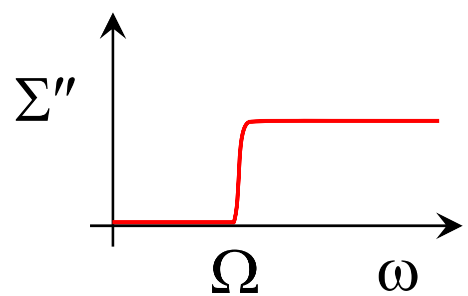
2nd electron-boson scattering

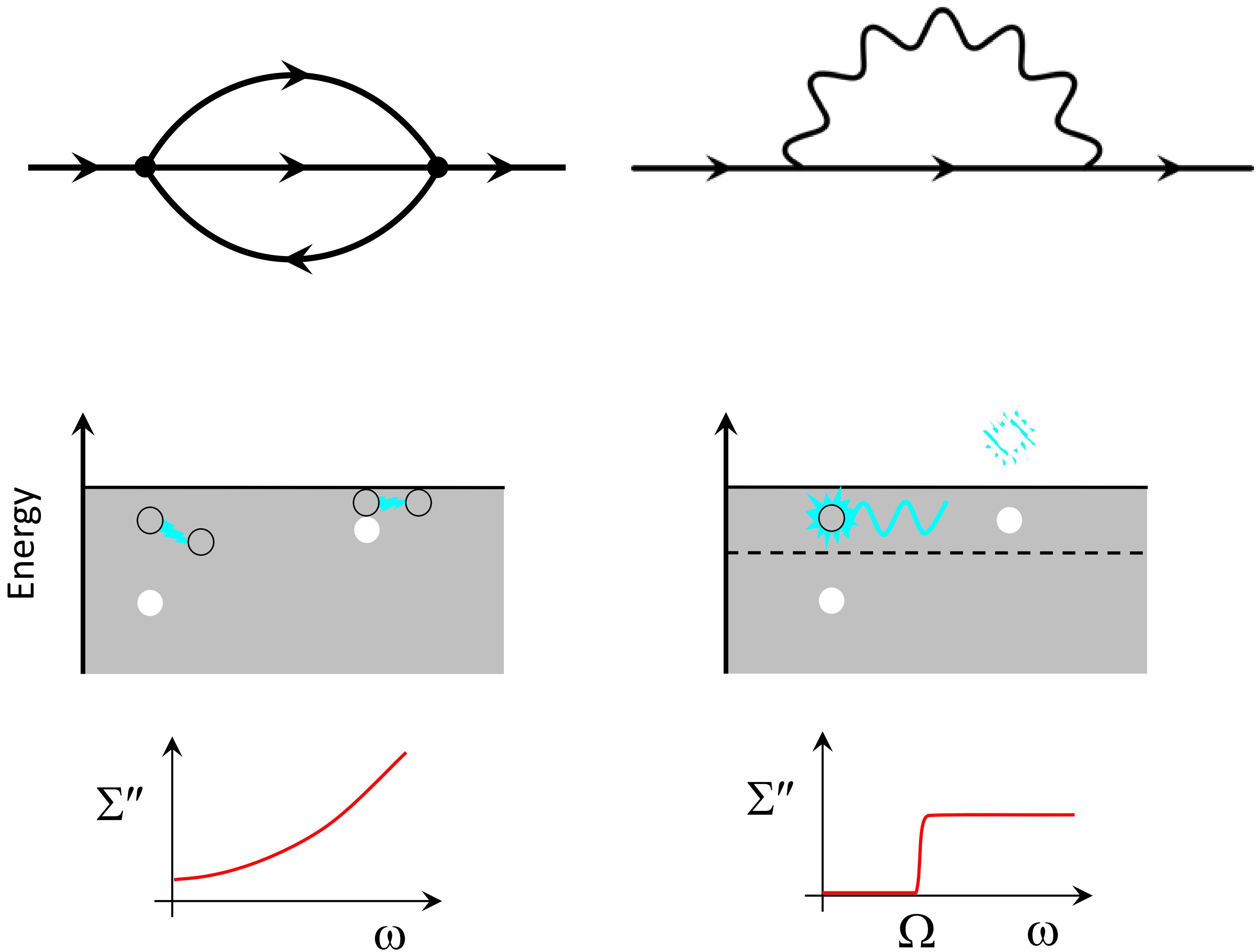




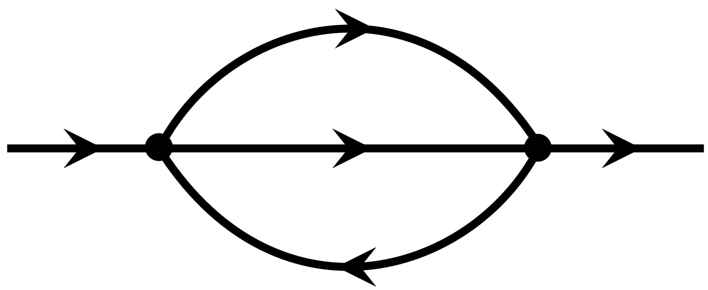


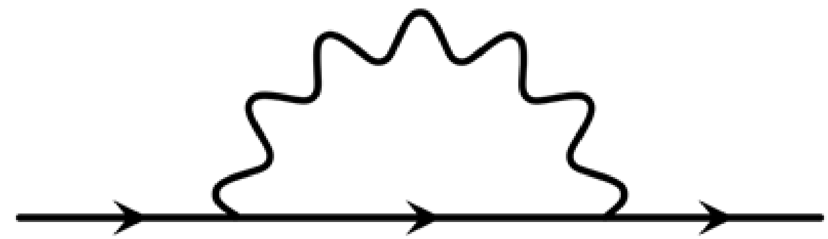




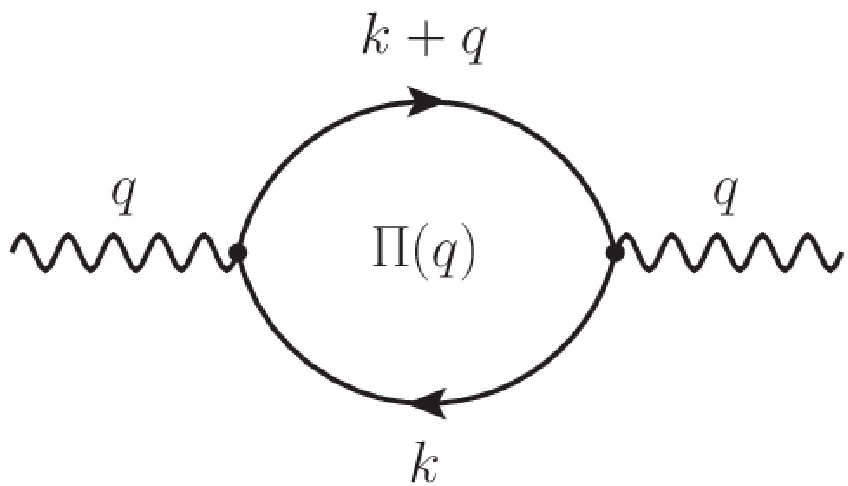

Energy
Σ″
ω
Σ″
Ω
ω

1 particle & 2 particle spectral functions





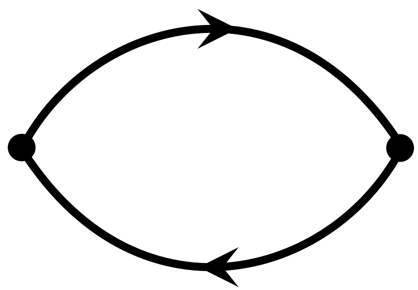
$\Sigma \sim (G \star \chi)_{\mathbf{k},\omega}$



polarization bubble

$\Sigma \sim G \star \chi$

$\Sigma \sim G \star F$

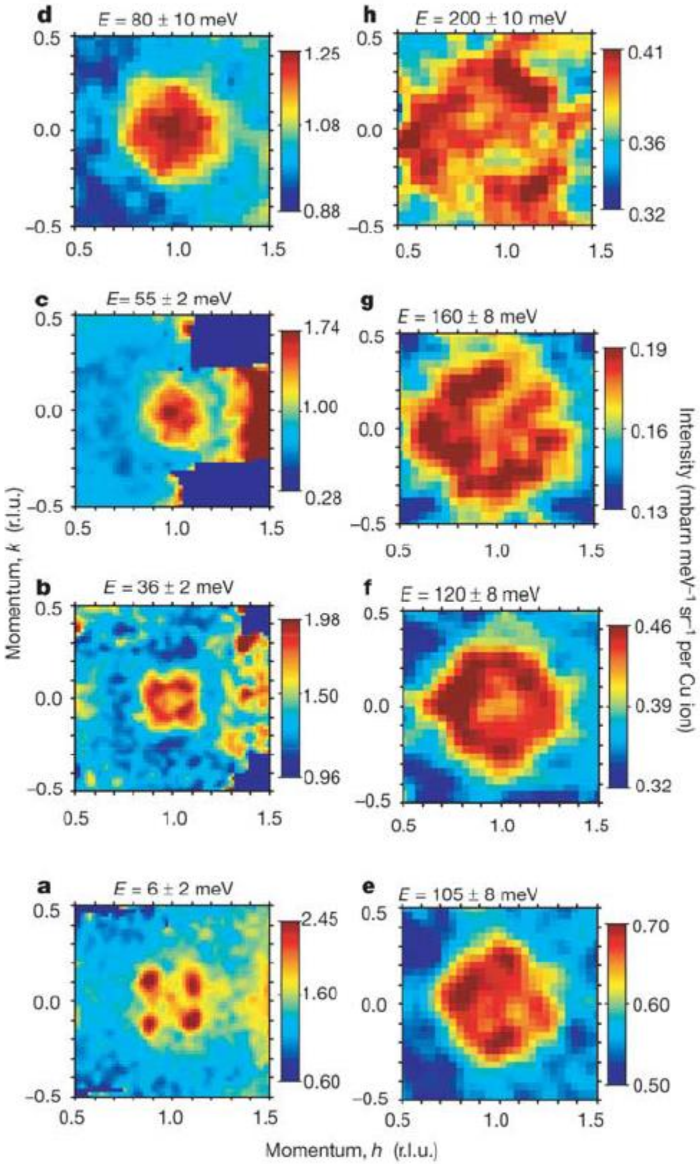


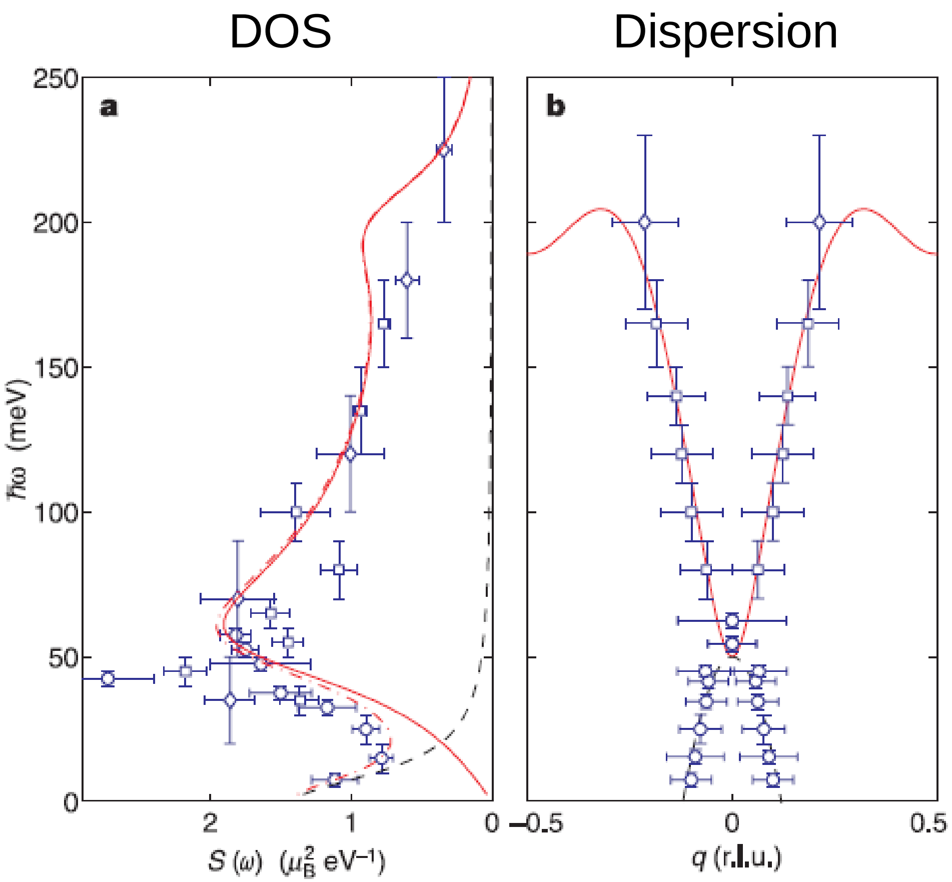
$\chi \sim G \star G$

F

Двохчастинкова функція – функція Лінхардта $\chi(\Omega,\mathbf{q})$

Spin susceptibility structure



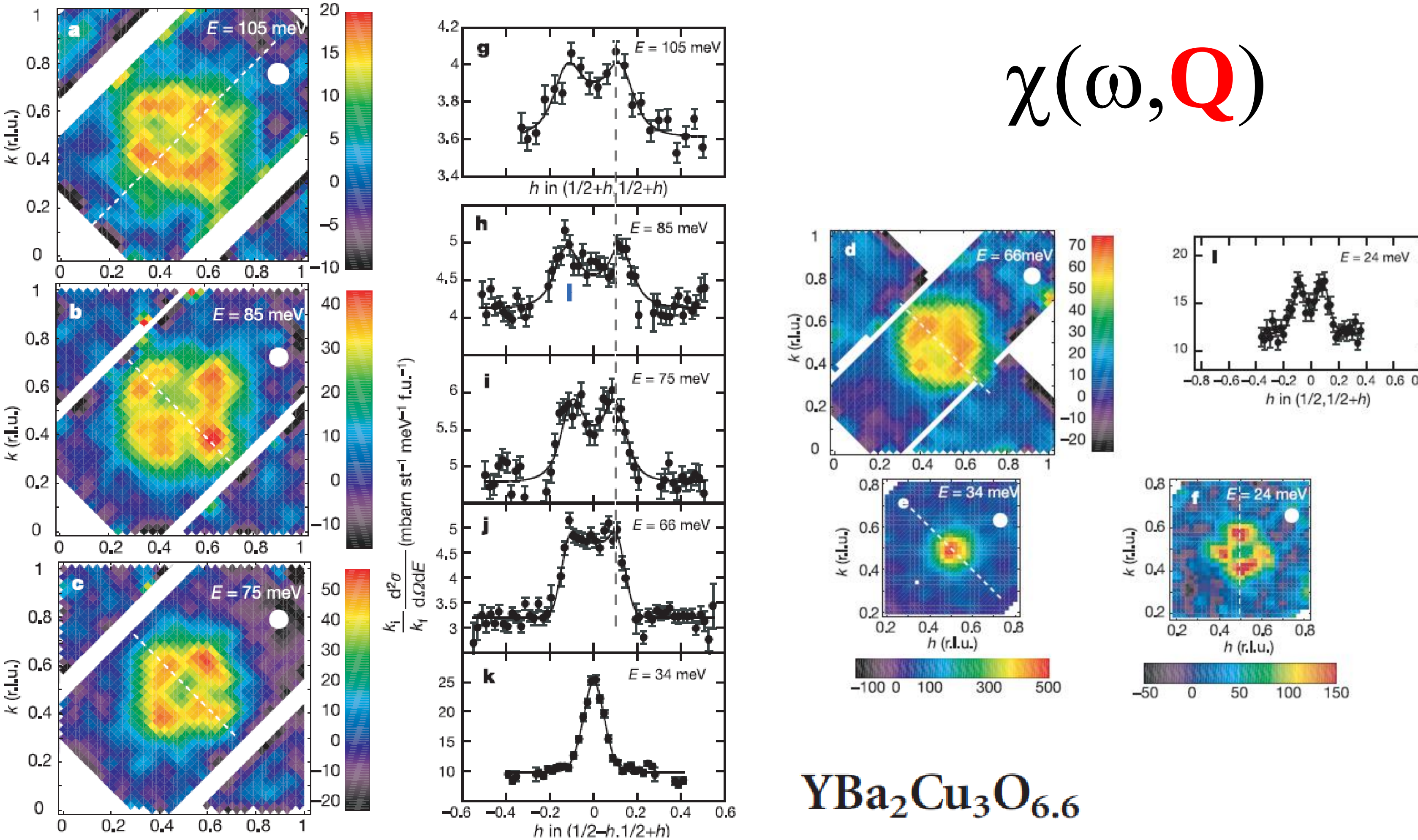


$La_{2-x}Ba_xCuO_4$ (‘Zurich’ oxide)

Tranquada *Nature* 2004

Spin susceptibility structure

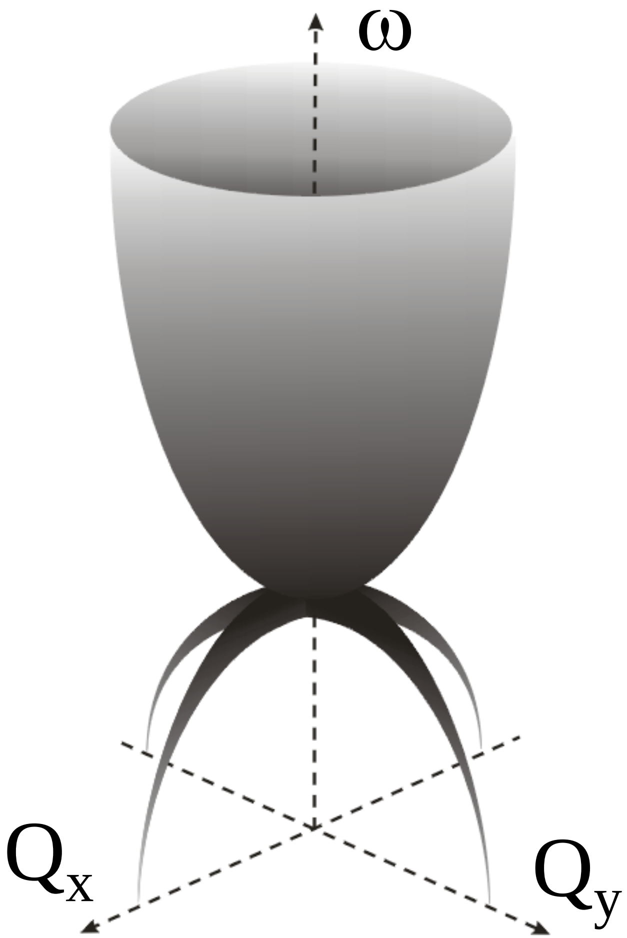
$\chi(\omega,\mathbf{Q})$

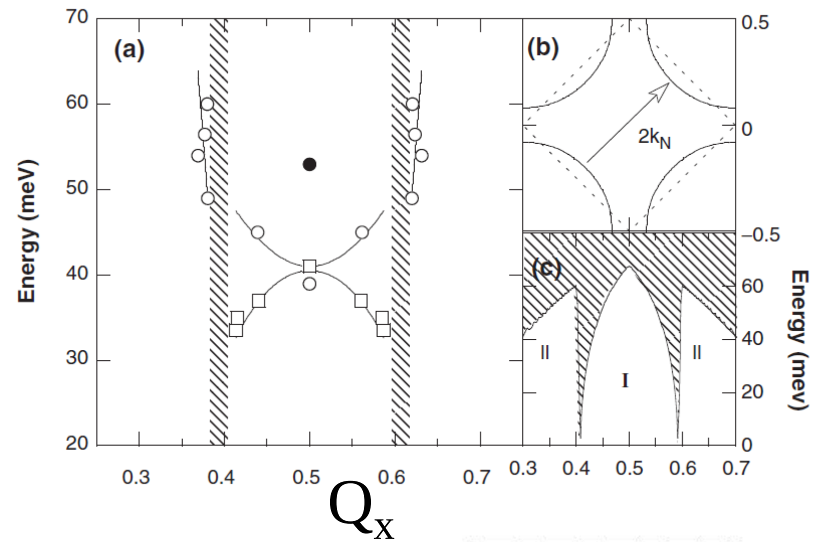


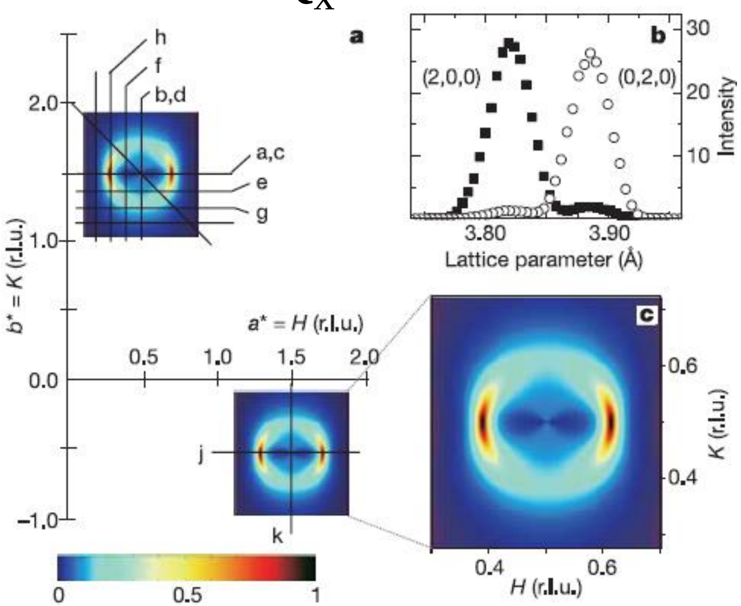
$YBa_2Cu_3O_{6.6}$

Hayden *Nature* 2004

Spin susceptibility structure







$YBa_2Cu_3O_{6.6}$

Hinkov *Nature* 2004

Looking for "fingerprints"

if 2nd order perturbation theory works

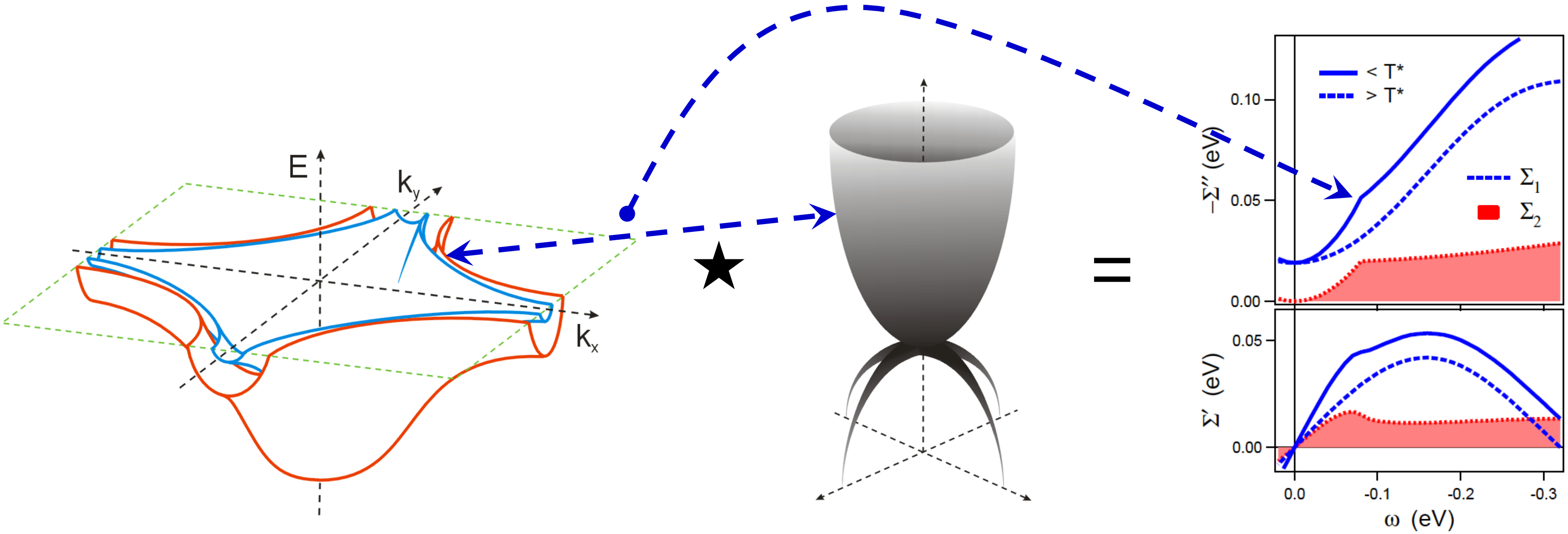
① $(\Delta,\Sigma) = EE(\Delta,\Sigma,\varepsilon,\chi)$ **SC**

$\Sigma \sim (G \star \chi)_{\mathbf{k},\omega}$ **N**

② $\chi_{it} \sim (G \star G)_{\mathbf{k},\omega}$ "itinerant" magnetism

① $G \star \chi \sim \Sigma$

$$\Sigma(\mathbf{k},\omega) \sim \int G(\mathbf{k}+\mathbf{Q},\omega+\Omega)\,\chi(\mathbf{Q},\Omega)\,d\mathbf{Q}\,d\Omega$$



k, ω

Q, Ω

k, ω

①

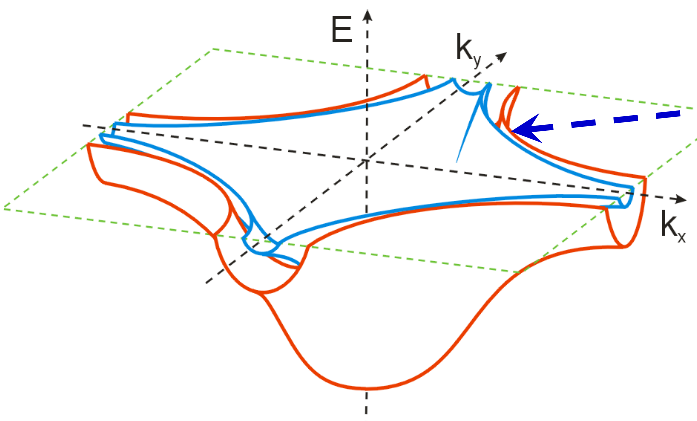
LDA or ARPES

$$G_0 \star \chi_{exp} \sim \Sigma_i$$

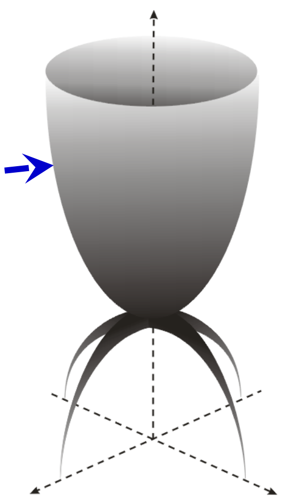
INS

$$G_i^{-1} = G_0^{-1} + \Sigma_i$$

ARPES



★



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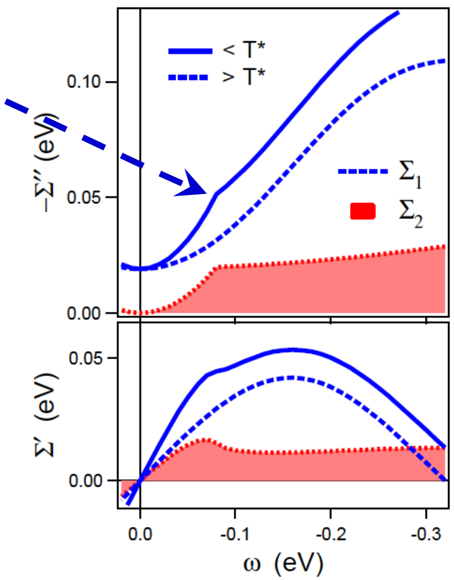
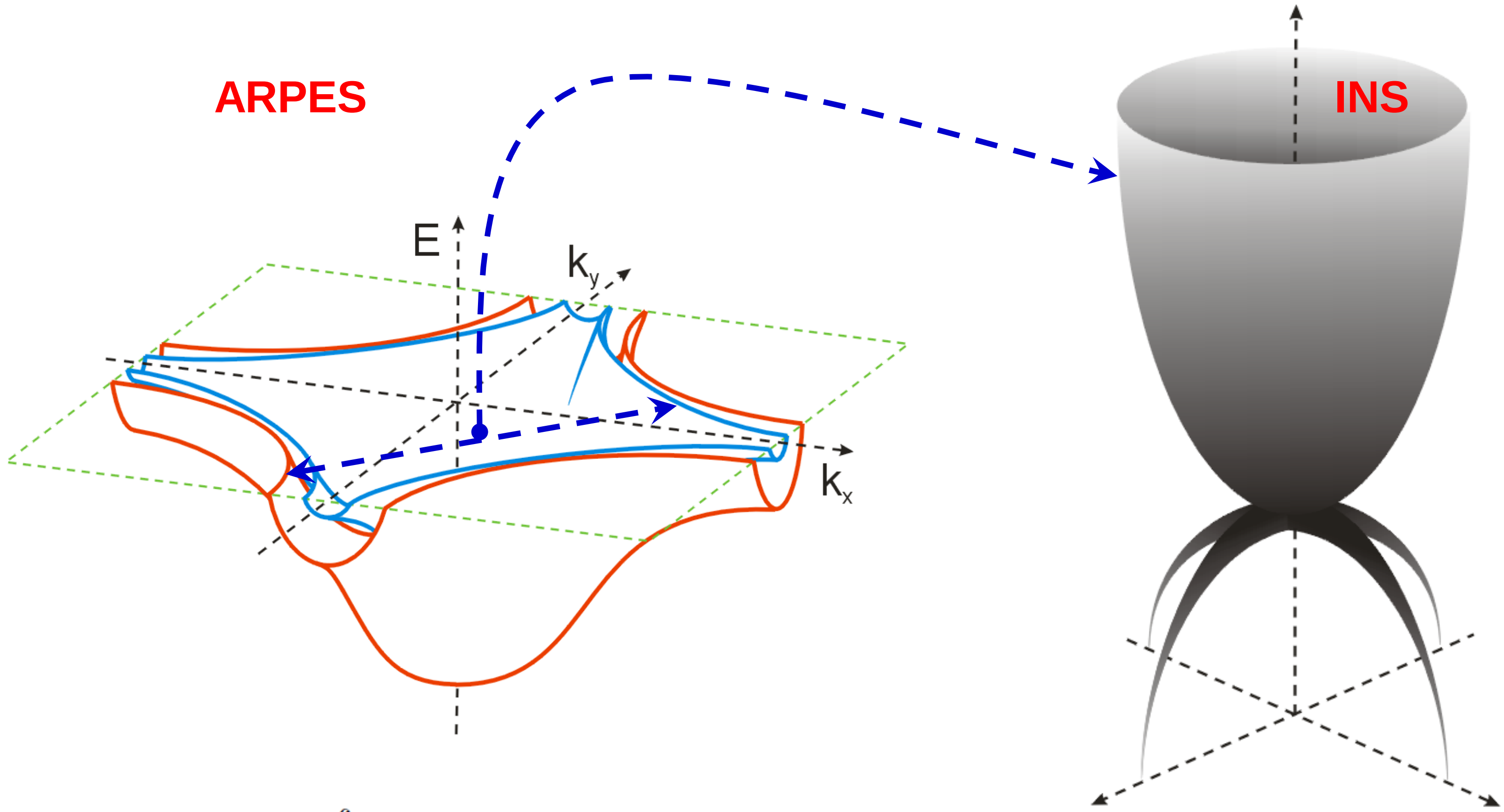


k, ω　　**Q**, Ω　　**k**, ω

we + Hinkov & Keimer + Dahm & Scalapino 2006

② itinerant $\chi \sim G \star G$



$$\chi_0(\mathbf{Q},\Omega) \propto -2i \int G(\mathbf{k},\omega) G(\mathbf{k}+\mathbf{Q},\omega+\Omega)\, d^2k\, d\omega$$

$$\chi(\mathbf{Q},\Omega) = \chi_0(\mathbf{Q},\Omega)/[1 + J_Q\, \chi_0(\mathbf{Q},\Omega)]$$ RPA

we + Eremin 2006

② $\chi \sim G \star G$

$$\chi_0(\mathbf{Q}, i\Omega_n) = \frac{1}{\pi^2} \int \sum_m G(\mathbf{k}, i\omega_m) G(\mathbf{k}+\mathbf{Q}, i\omega_m + i\Omega_n) \mathrm{d}\mathbf{k}$$

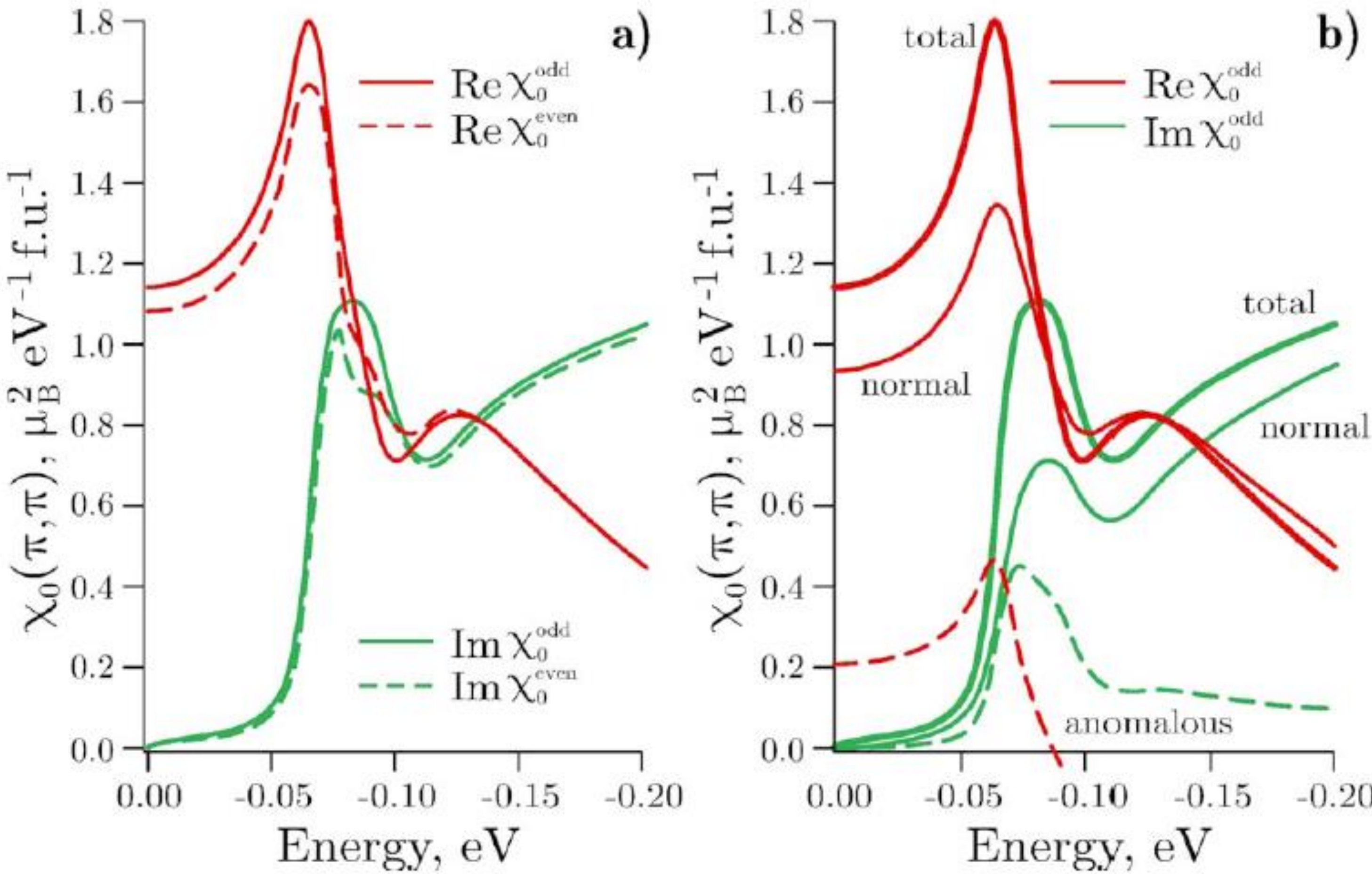
$$\chi_0^{\mathrm{o,e}}(\mathbf{Q}, \Omega) = \sum_{\substack{i=j(\mathrm{o}) \\ i \neq j(\mathrm{e})}} \iint_{-\infty}^{+\infty} C_{ij}(\mathbf{k}, \epsilon, \nu) \frac{n_{\mathrm{f}}(\nu) - n_{\mathrm{f}}(\epsilon)}{\Omega + \nu - \epsilon + i\Gamma} \mathrm{d}\nu\, \mathrm{d}\epsilon$$

where

$$C_{ij}(\mathbf{k}, \epsilon, \nu) = \frac{1}{\pi^2} \int [\mathrm{Im}\, G_i(\mathbf{k}, \epsilon)\, \mathrm{Im}\, G_j(\mathbf{k}+\mathbf{Q}, \nu) + \mathrm{Im}\, F_i(\mathbf{k}, \epsilon) \mathrm{Im}\, F_j(\mathbf{k}+\mathbf{Q}, \nu)]\, \mathrm{d}\mathbf{k}.$$

Inosov PRB 2007

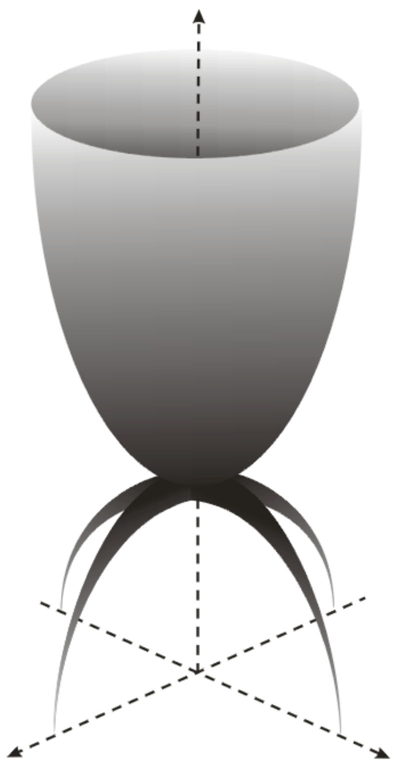
②

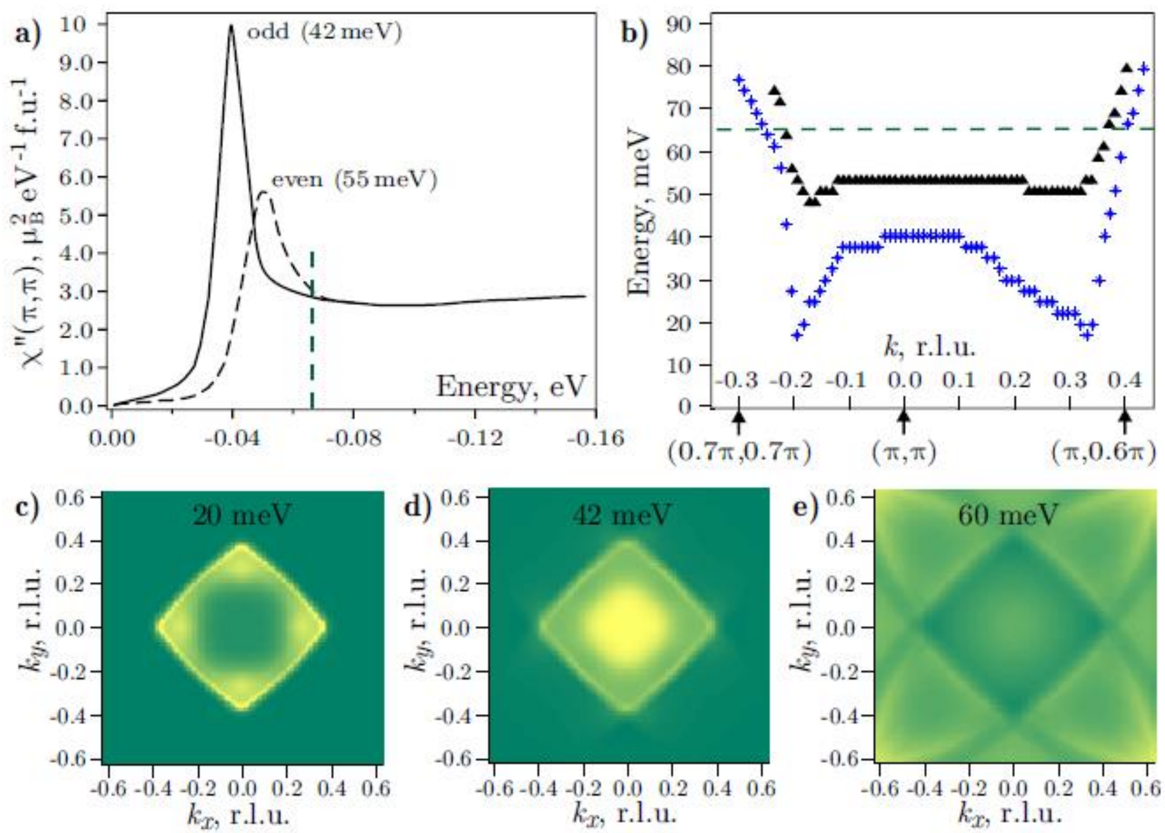


Inosov PRB 2007

②

$$\chi^{o,e}(\mathbf{Q},\Omega) = \chi_0^{o,e}(\mathbf{Q},\Omega)/[1 - J_Q^{o,e}\chi_0^{o,e}(\mathbf{Q},\Omega)]$$





Inosov PRB 2007

Fourier transform (FT) & Correlation

Fourier transform (FT)

$$F(\omega) = \int_{-\infty}^{\infty} f(t) e^{-i\omega t} dt$$

$$f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\omega) e^{i\omega t} d\omega$$

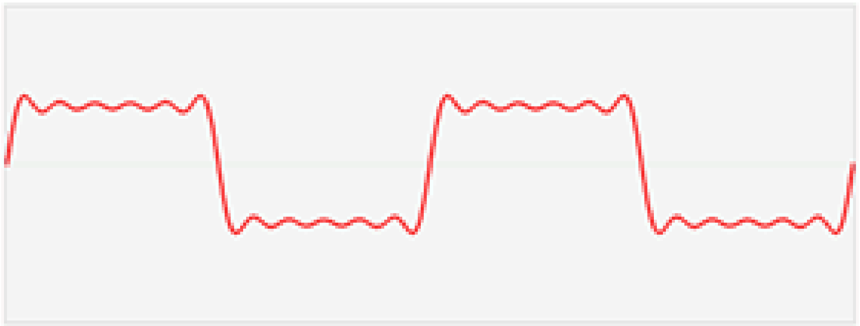
Fourier transform (FT)

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} f(x)\, e^{-2\pi i x \xi}\, dx,$$

$$f(x) = \int_{-\infty}^{\infty} \hat{f}(\xi)\, e^{2\pi i x \xi}\, d\xi,$$

https://youtu.be/spUNpyF58BY

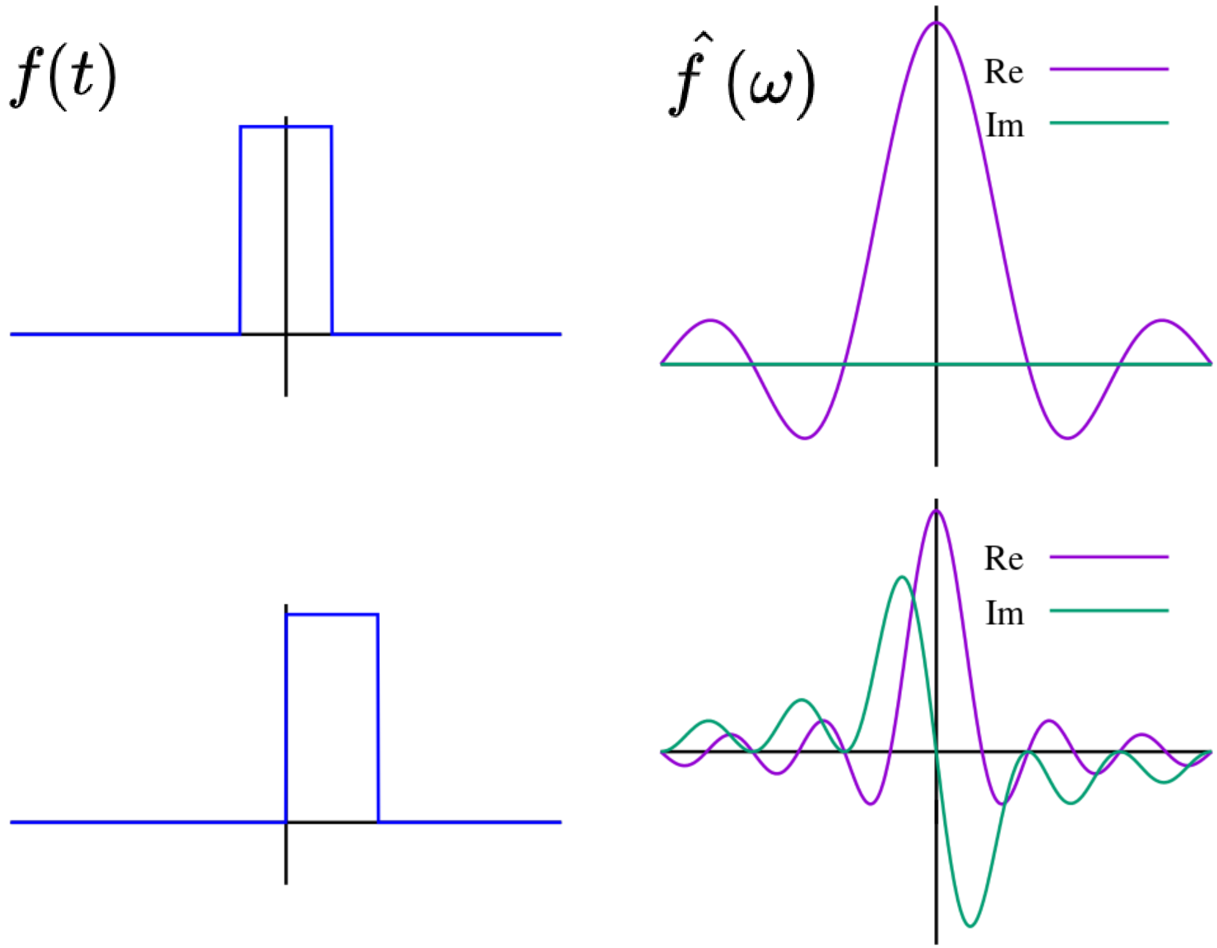
Fourier series



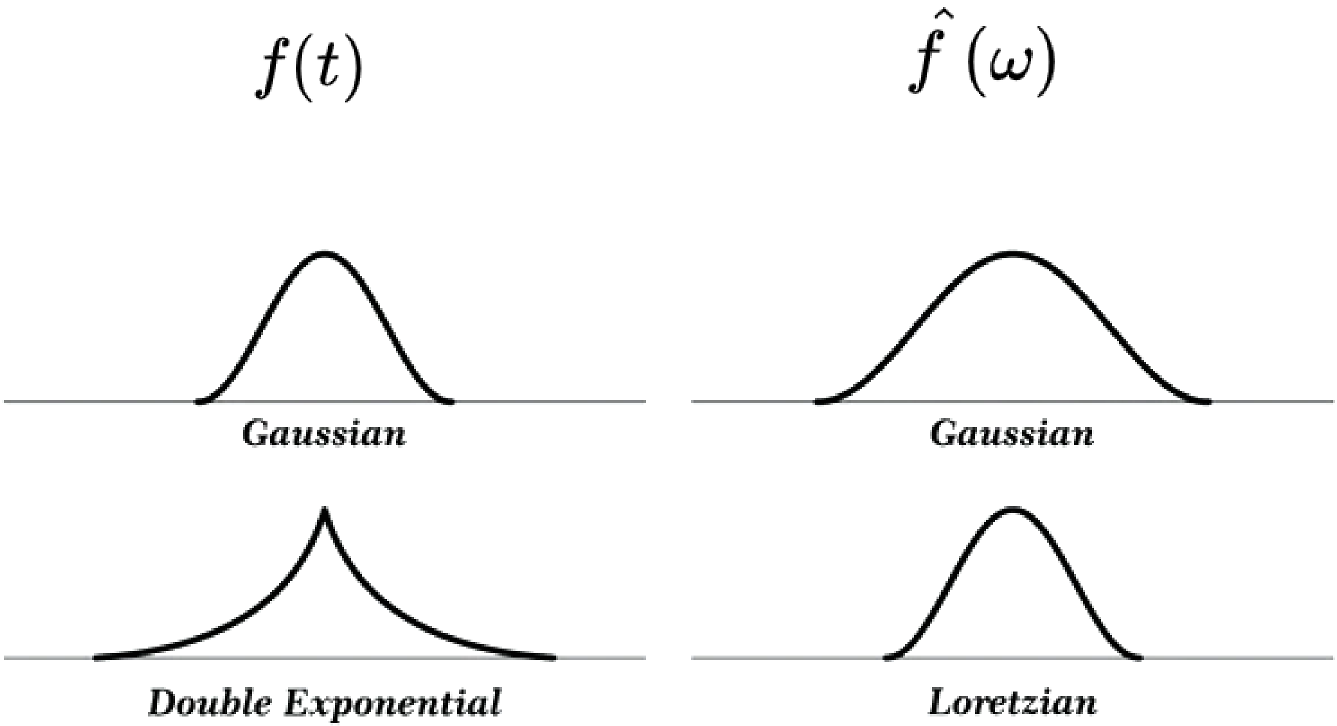
$$f(x) = \sum_{n=-\infty}^{\infty} c_n \, e^{2\pi i \left(\frac{n}{T}\right) x}$$

$$c_n = \frac{1}{T} \int_{-\frac{T}{2}}^{\frac{T}{2}} f(x) \, e^{-2\pi i \left(\frac{n}{T}\right) x} \, dx.$$

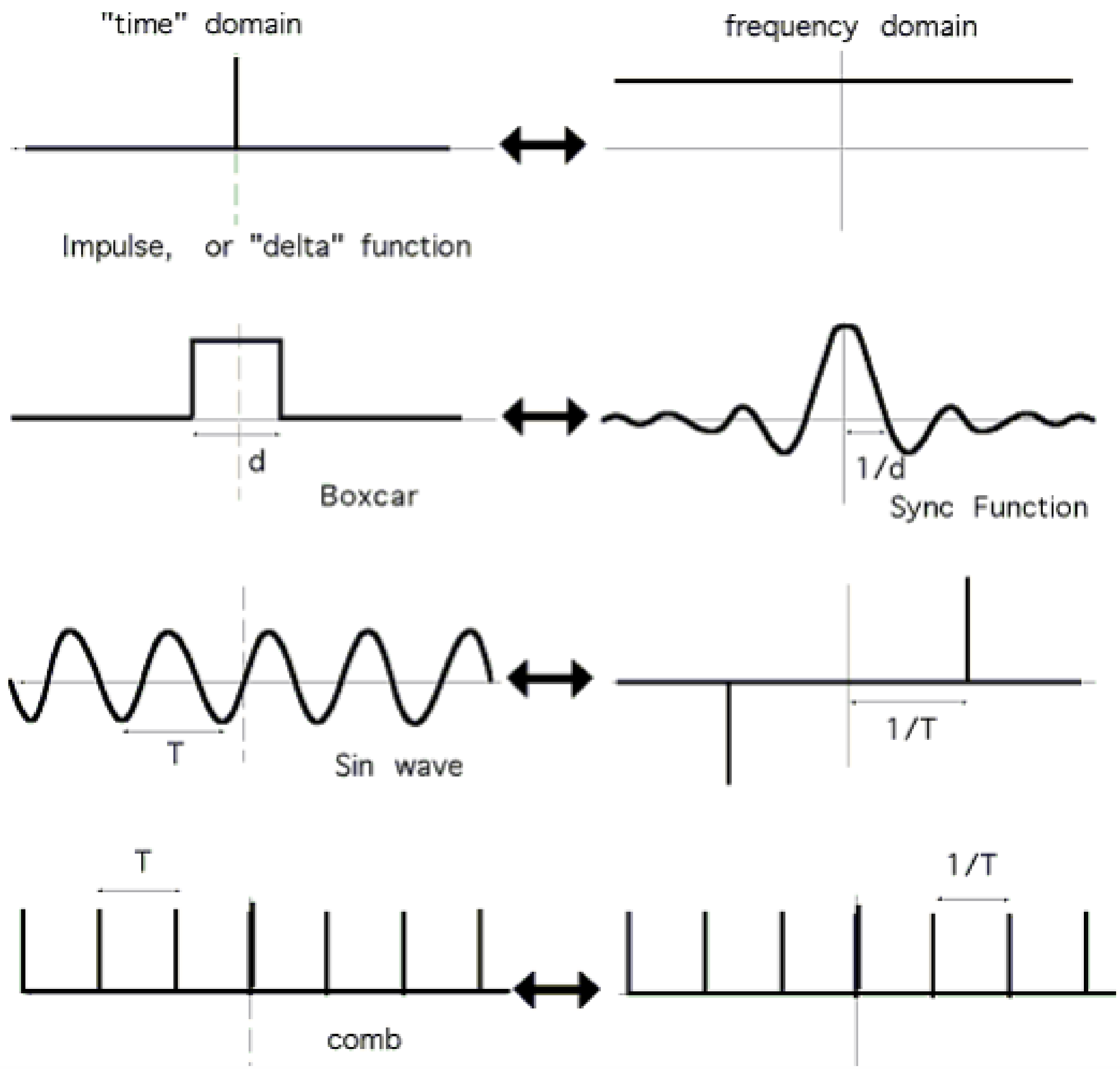
Fourier transform (FT)



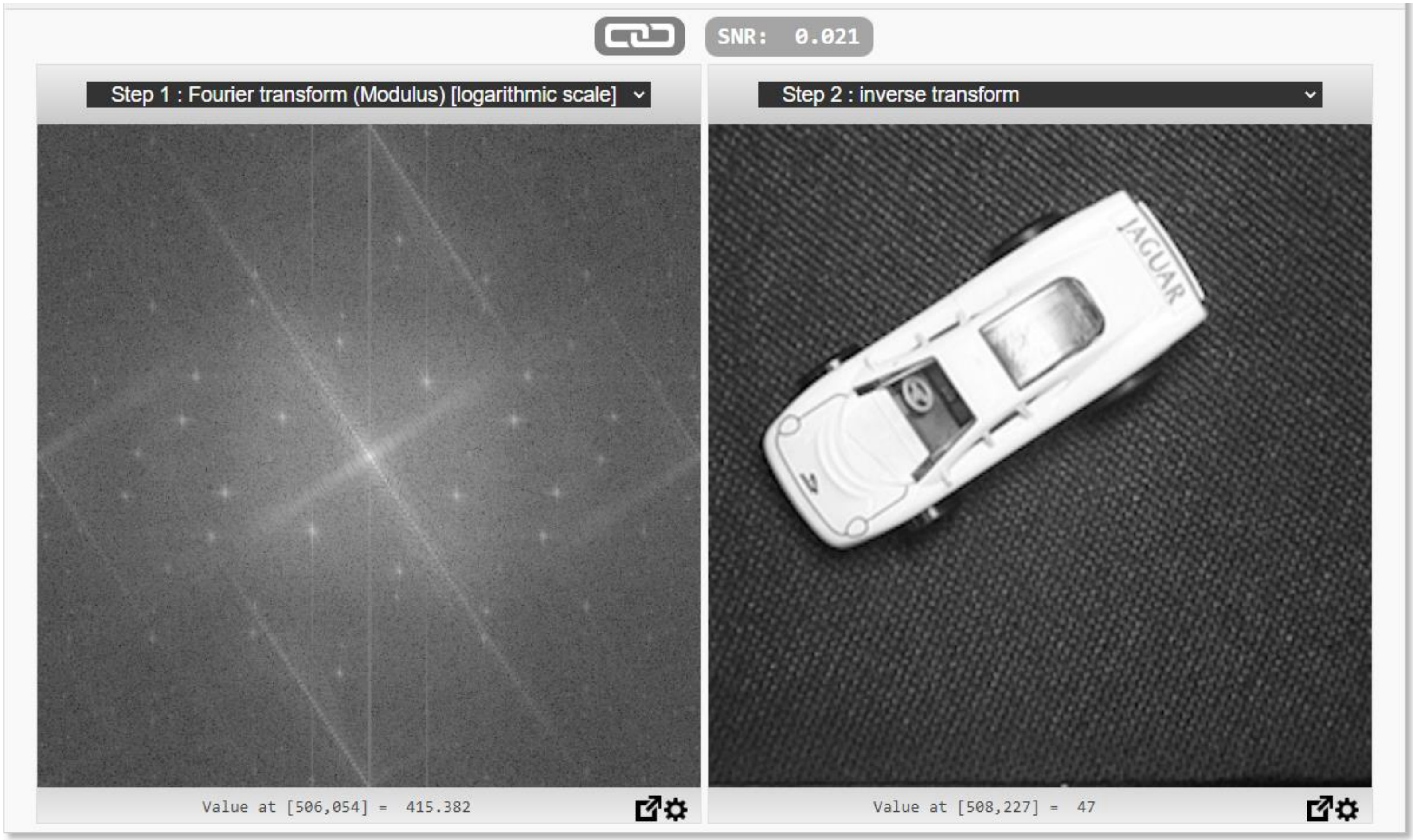
Fourier transform (FT)



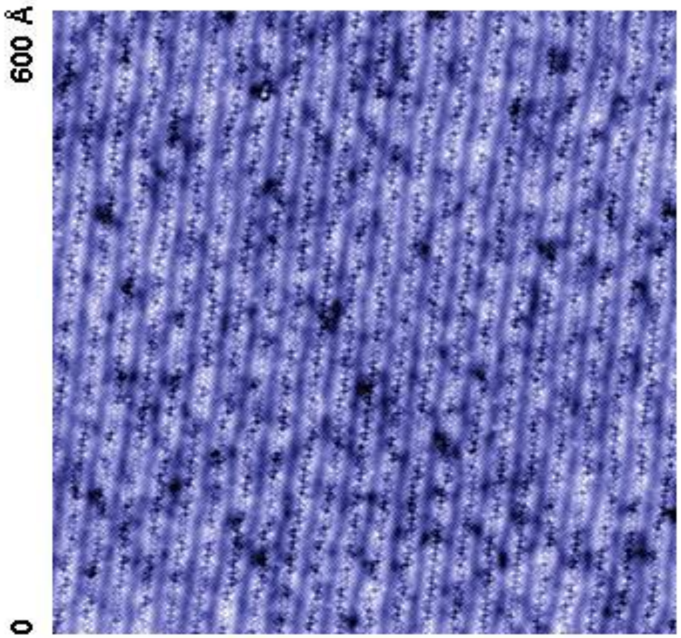
Fourier transform (FT)

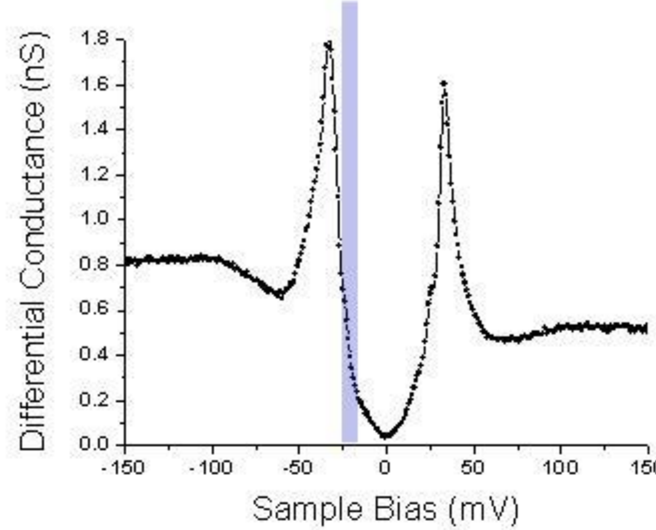


Fourier transform (FT)

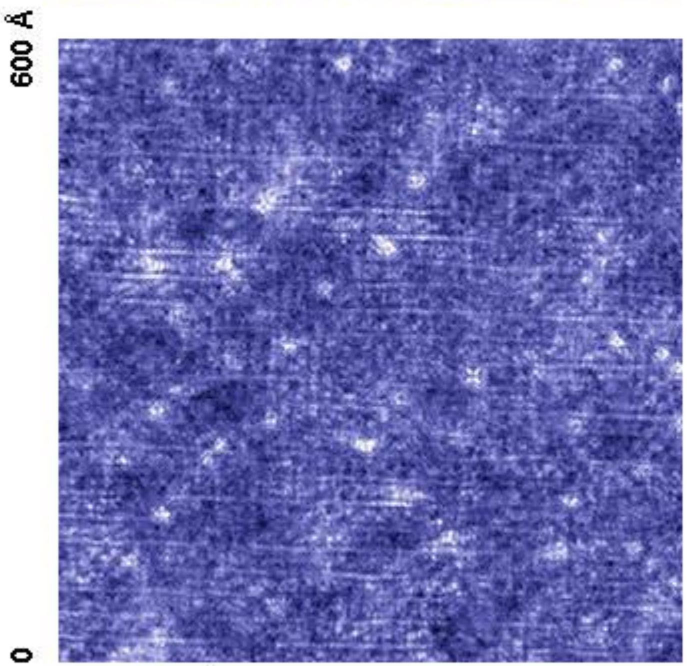


http://bigwww.epfl.ch/demo/ip/demos/FFT/



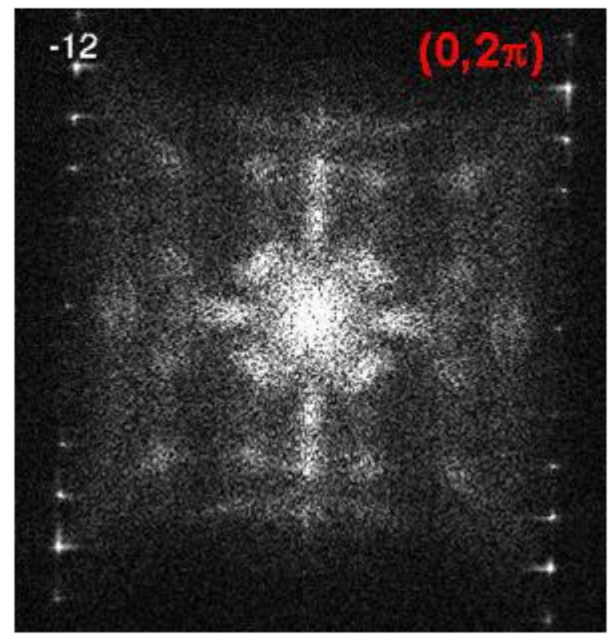


Point dI/dV $\equiv g(\vec{r}, E)$ Spectrum



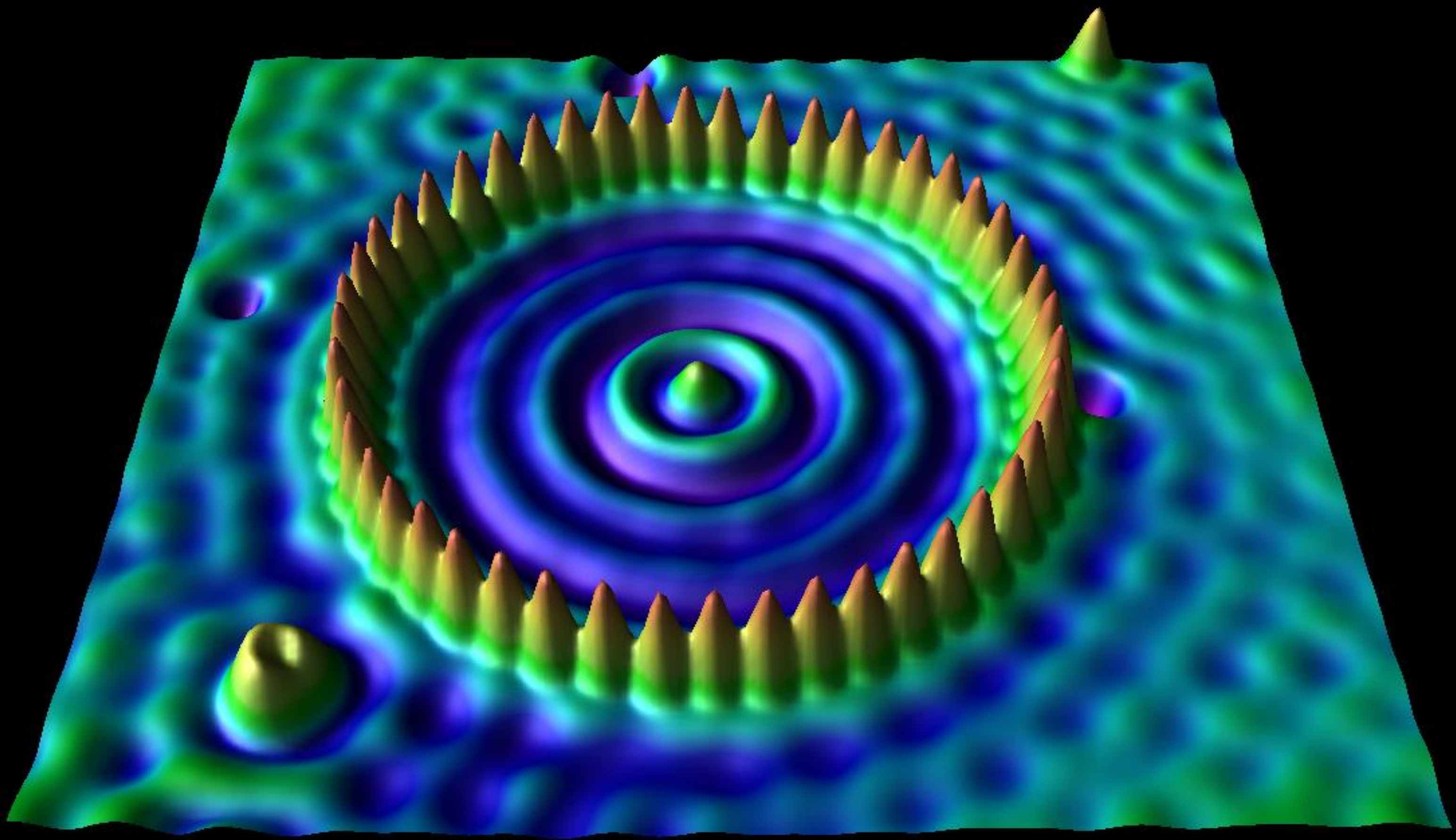
$g(\vec{r}, E = -12meV)$

FFT shows q-vector of LDOS modulations

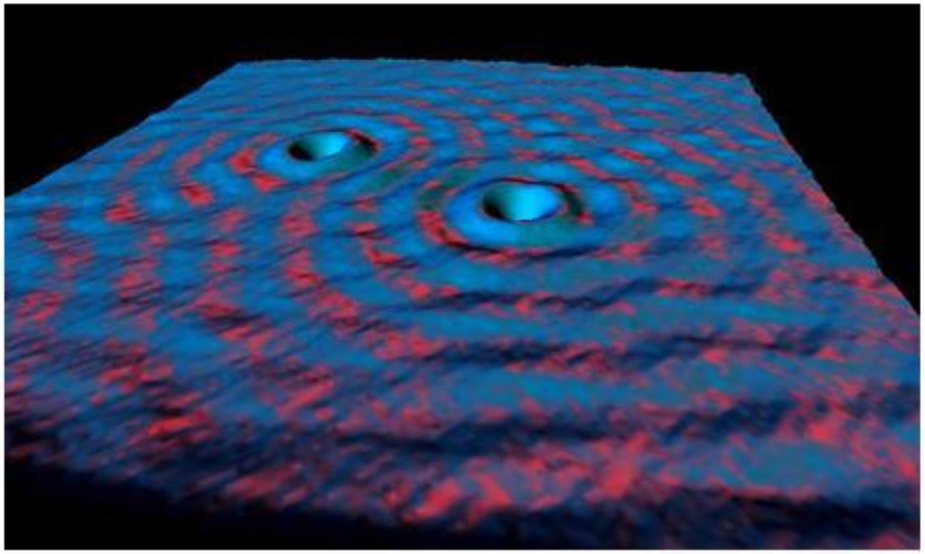


$g(\vec{q}, E = -12\, meV)$

McElroy, 2004



Quasiparticle Interference at Impurity Atoms

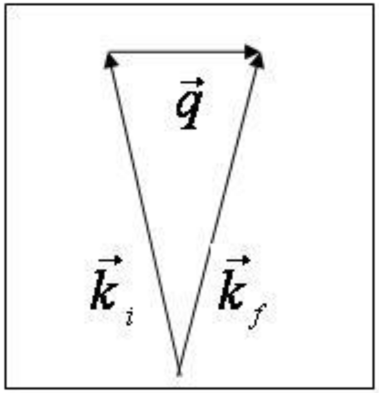


Crommie, Lutz & Eigler, Nature 363, 524 (1993)

•Mixing of $\left|\vec{k}_1\right\rangle$ and $\left|\vec{k}_2\right\rangle$ by scattering creates
interference term, with wavevector

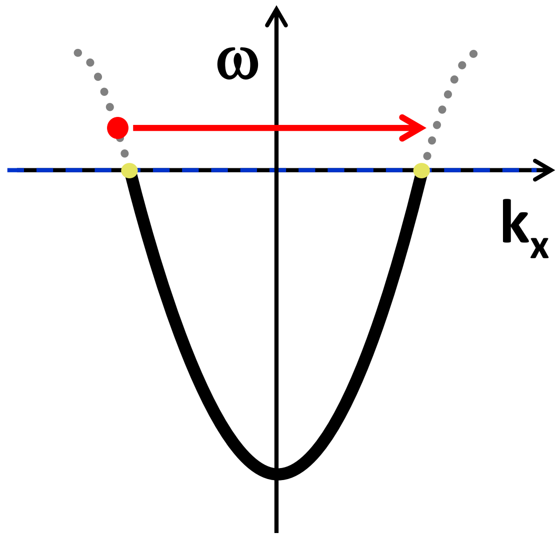
$$\vec{q} = \vec{k}_2 - \vec{k}_1$$

•Interference results in modulations in LDOS with wavelength $\lambda = \frac{2\pi}{|\vec{q}\,|}$

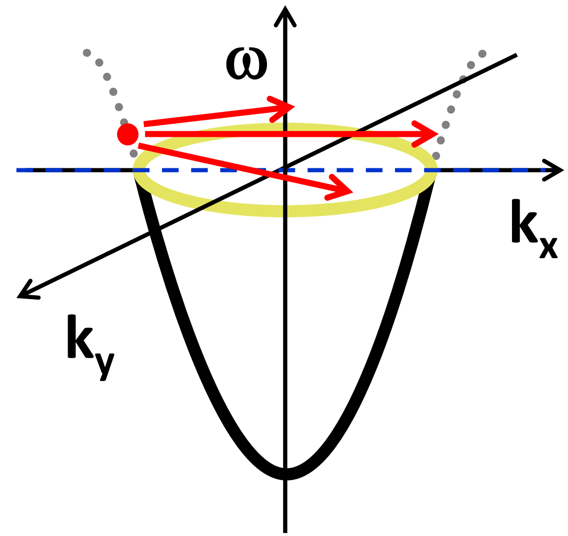


McElroy, 2004

Impurity scattering

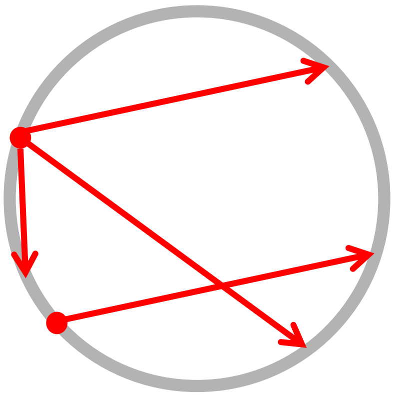


1D

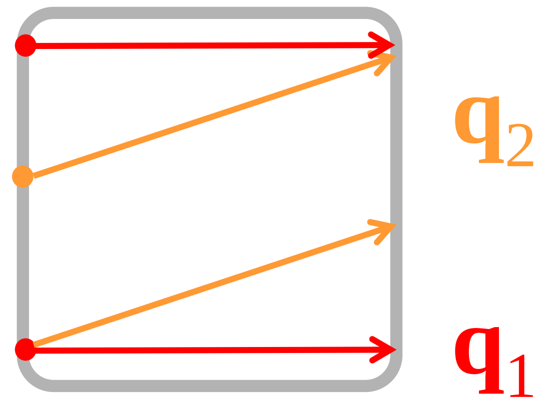


2D

$$\chi \sim G \star G \sim \int A(\mathbf{k})A(\mathbf{k}+\mathbf{q})d\mathbf{k}$$

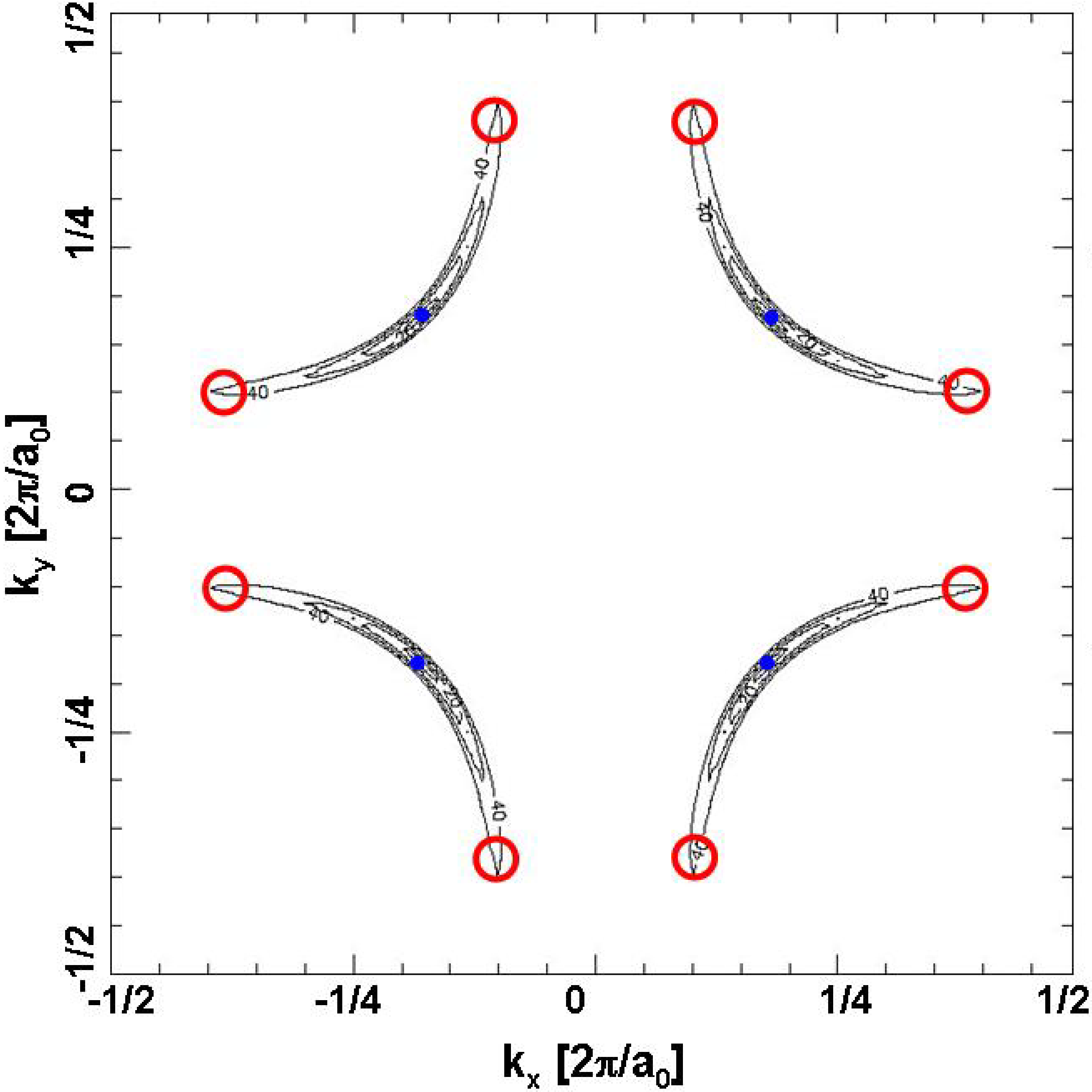


$$\mathbf{q} = \mathbf{k}_1 - \mathbf{k}_0$$



$$\chi(\mathbf{q}_1) > \chi(\mathbf{q}_2)$$

Octet of regions at ends of ‘bananas’ have smallest dE/|dk|

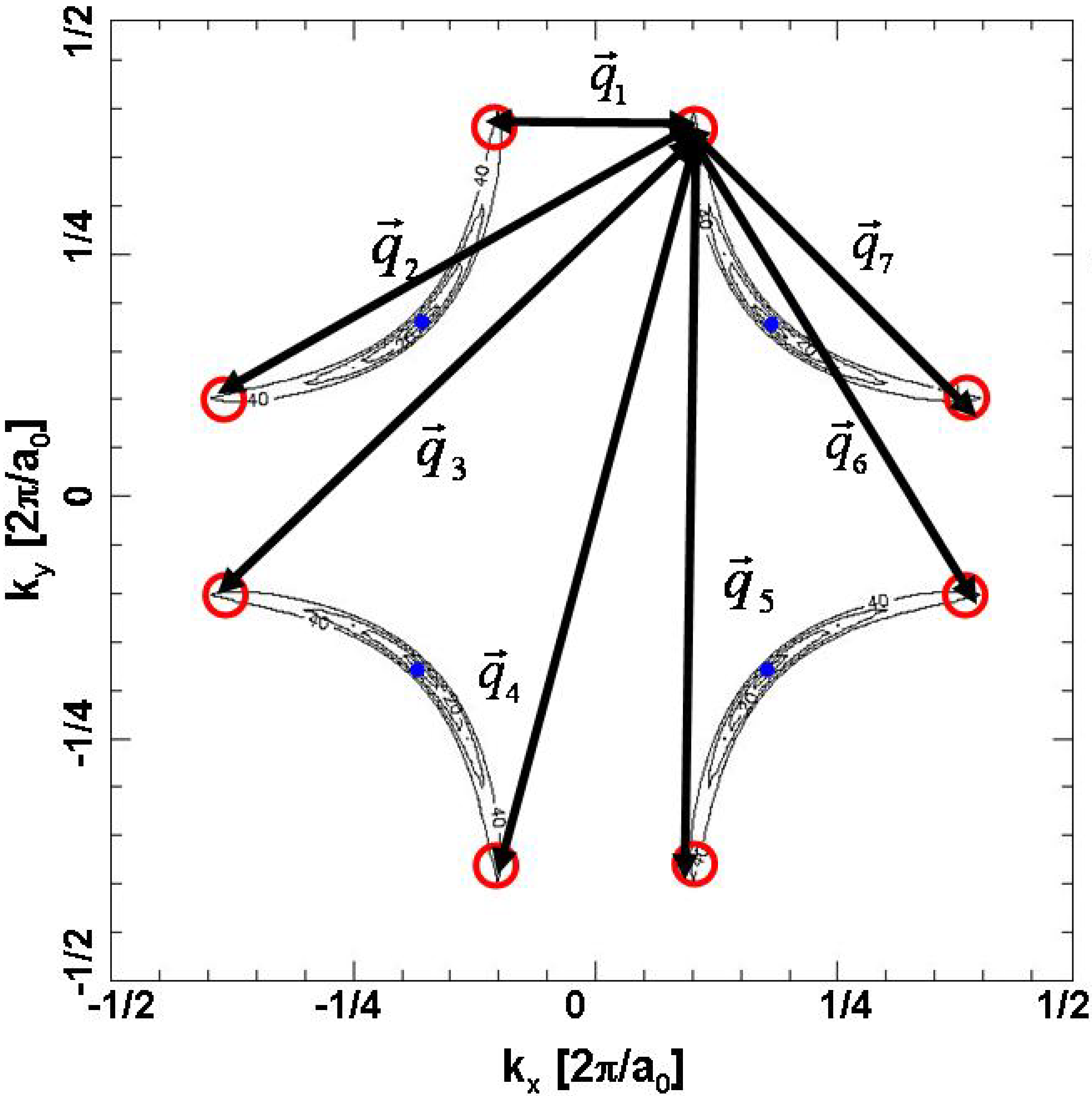


Density of States

$$n(E) = \oint_{E(k)=E} \frac{1}{\left|\nabla_k E(\vec{k})\right|} dk$$

This octet of locations at the tips of the ‘bananas’ provide maximum contribution to $n_f(E)$ and thus dominate elastic scattering processes.

Octet of regions at ends of 'bananas' have smallest dE/|dk|



Density of States

$$n(E) = \oint_{E(k)=E} \frac{1}{\left|\nabla_k E(\vec{k})\right|} dk$$

Characteristic set of quasiparticle interference wavevectors which is different at each energy.

McElroy, 2004

Way to ARPES

Impurity scattering hypothesis: $\left|\mathcal{F}\, S(\mathbf{r})\right| = \mathrm{AC}\, A(\mathbf{k})$

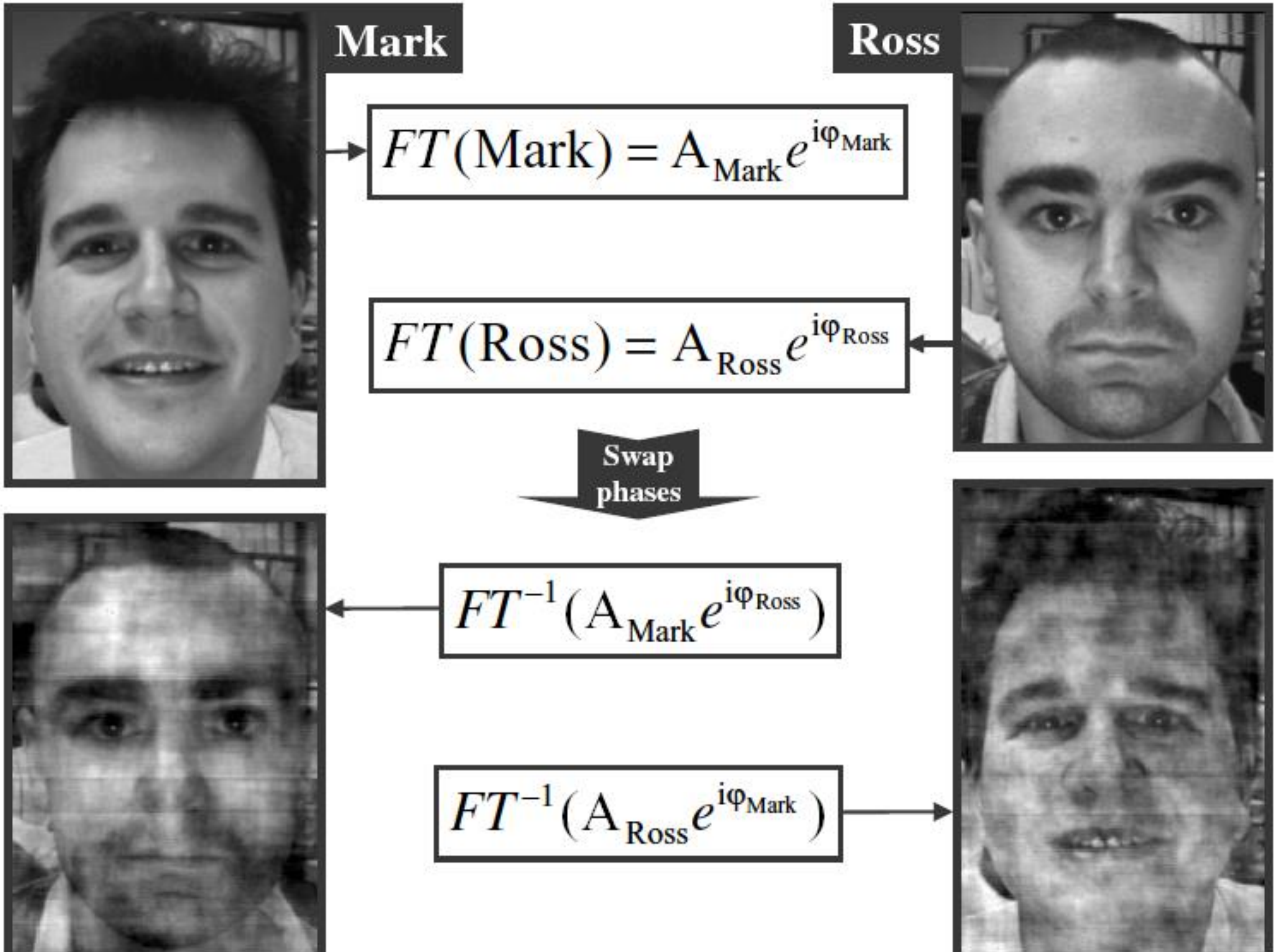
Definition of autocorrelation: $\mathrm{AC}\, A(\mathbf{k}) = \int A(\mathbf{k}) A(\mathbf{k}+\mathbf{q})\, d\mathbf{k}$

Another definition through the Fourier transform (Wiener-Khinchin theorem): $\mathrm{AC}\, A(\mathbf{k}) = \mathcal{F}\left|\mathcal{F} A(\mathbf{k})\right|^2$

$$\left|\mathcal{F} A(\mathbf{k})\right| = \sqrt{\mathcal{F}\left|\mathcal{F}\, S(\mathbf{r})\right|} = R(\boldsymbol{\rho})$$

Phase retrival algorithm: $A(\mathbf{k}) = \mathrm{PRA}\sqrt{\mathcal{F}\left|\mathcal{F}\, S(\mathbf{r})\right|}$

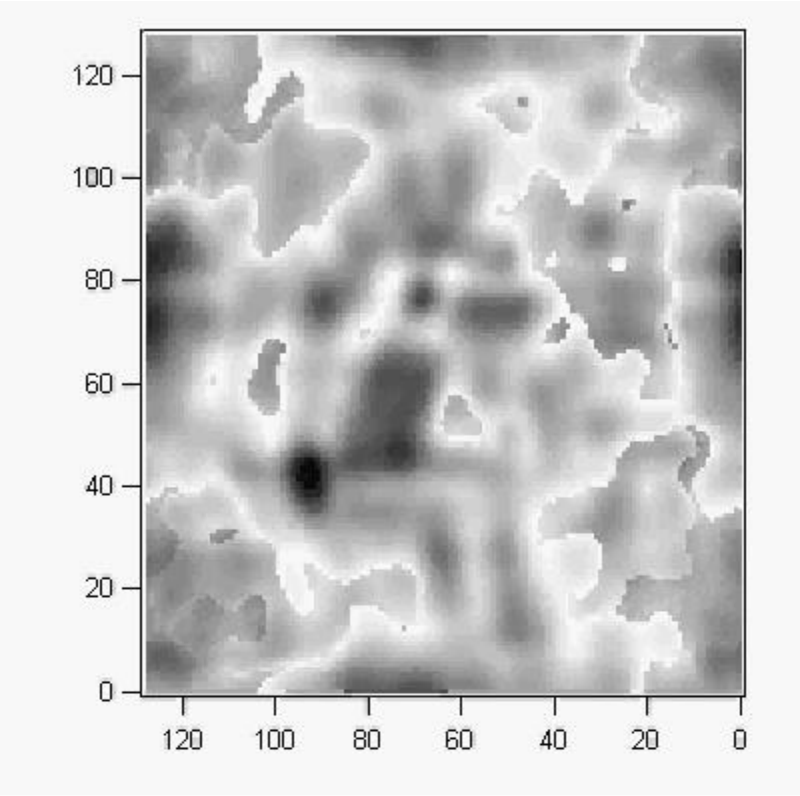
Phase retrival algorithm

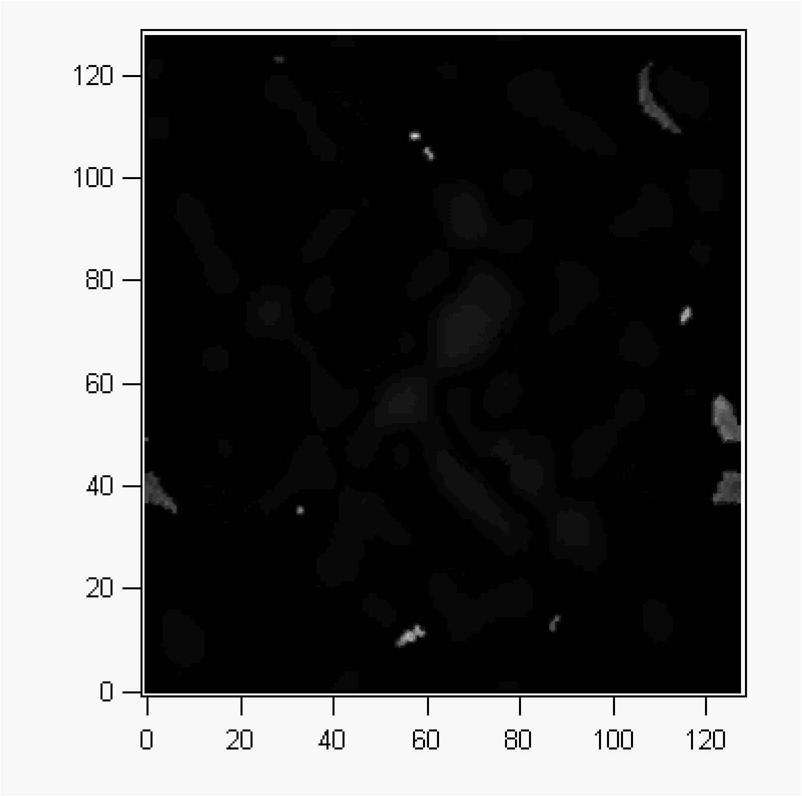


J. Phys.: Condens. Matter **13** (2001) 10689

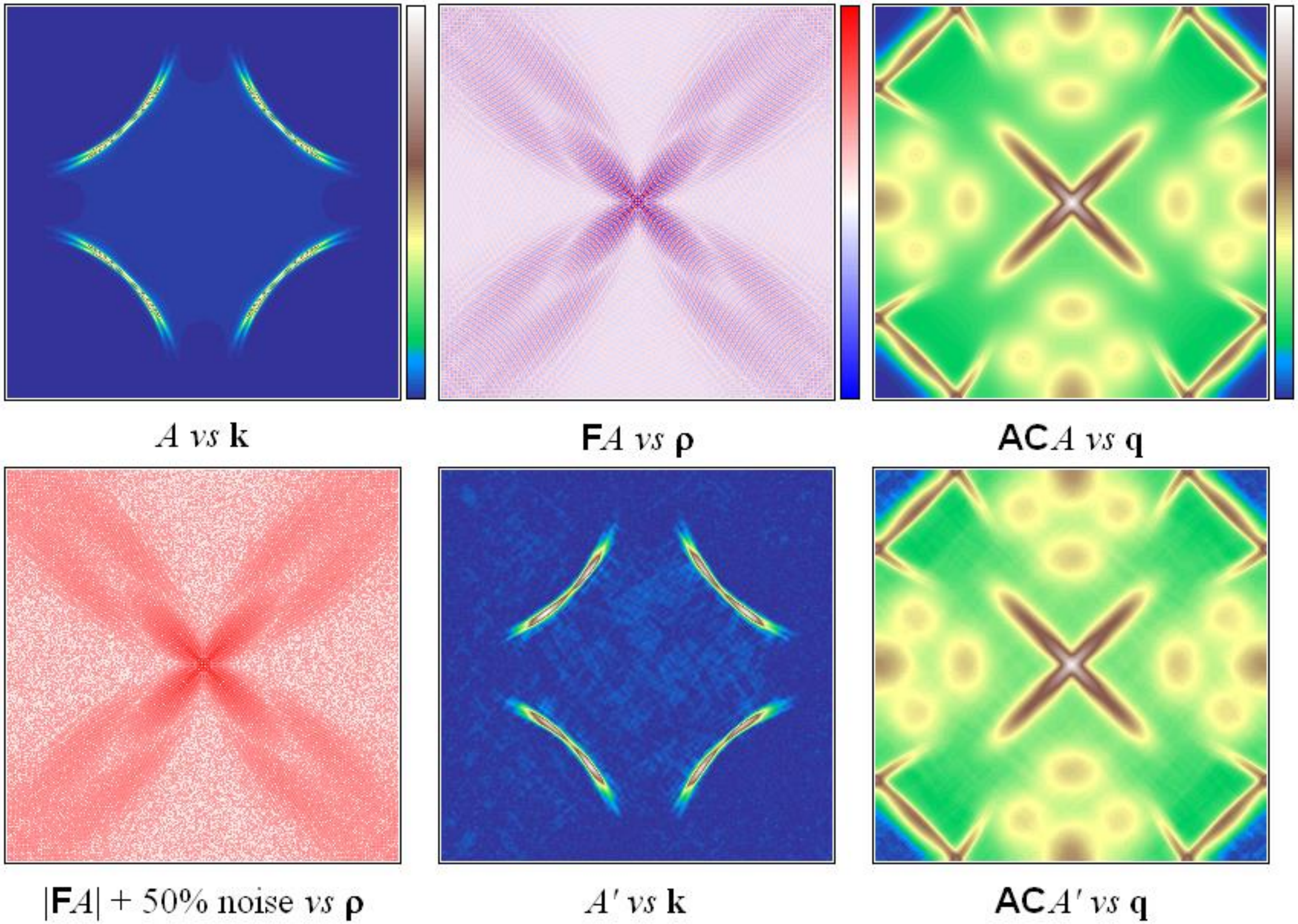
Phase retrival algorithm

$$A(\mathbf{k}) = \text{PRA}\ \left|\mathrm{F}A(\mathbf{k})\right|$$



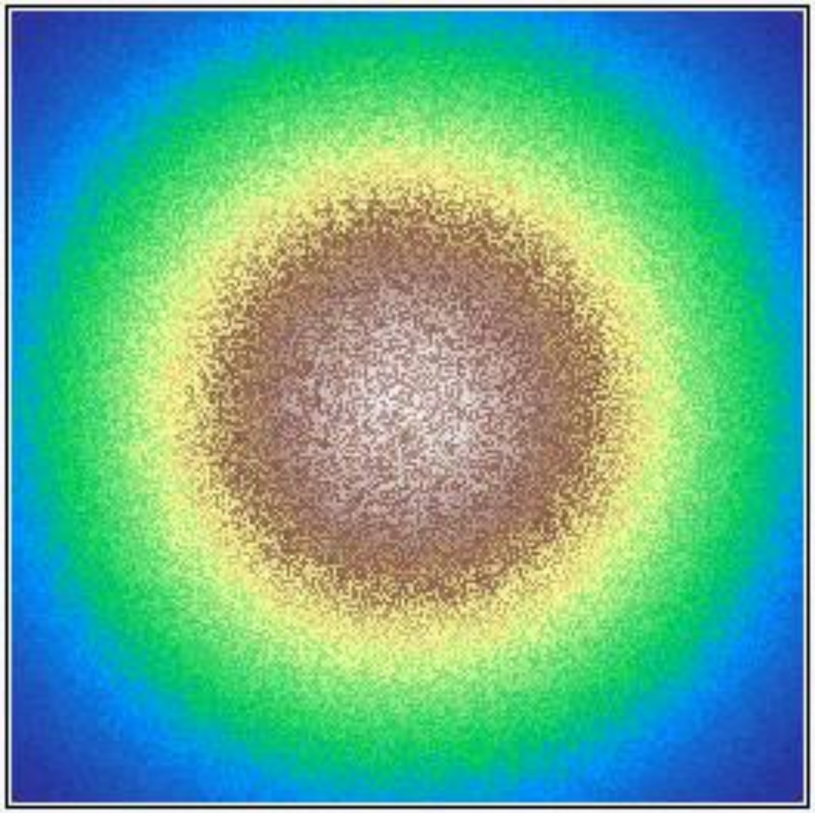


Representations of quasiparticles in different spaces of high-*T*c cuprates:



Kordyuk JES 2007

Phase retrival algorithm



$$\mathcal{R}_n = \mathbf{F} A_n,$$

$$\mathcal{R}'_n = R \exp[i \arg(\mathcal{R}_n)],$$

$$\mathcal{A}'_n = \mathbf{F}^{-1} \mathcal{R}'_n,$$

$$A_{n+1} = \begin{cases} \mathrm{Re}(\mathcal{A}'_n) & \text{if } \mathrm{Re}(\mathcal{A}'_n) \geq 0, \\ \mathrm{Re}(A_n - \beta \mathcal{A}'_n) & \text{if } \mathrm{Re}(\mathcal{A}'_n) < 0, \end{cases}$$

Kordyuk JES 2007

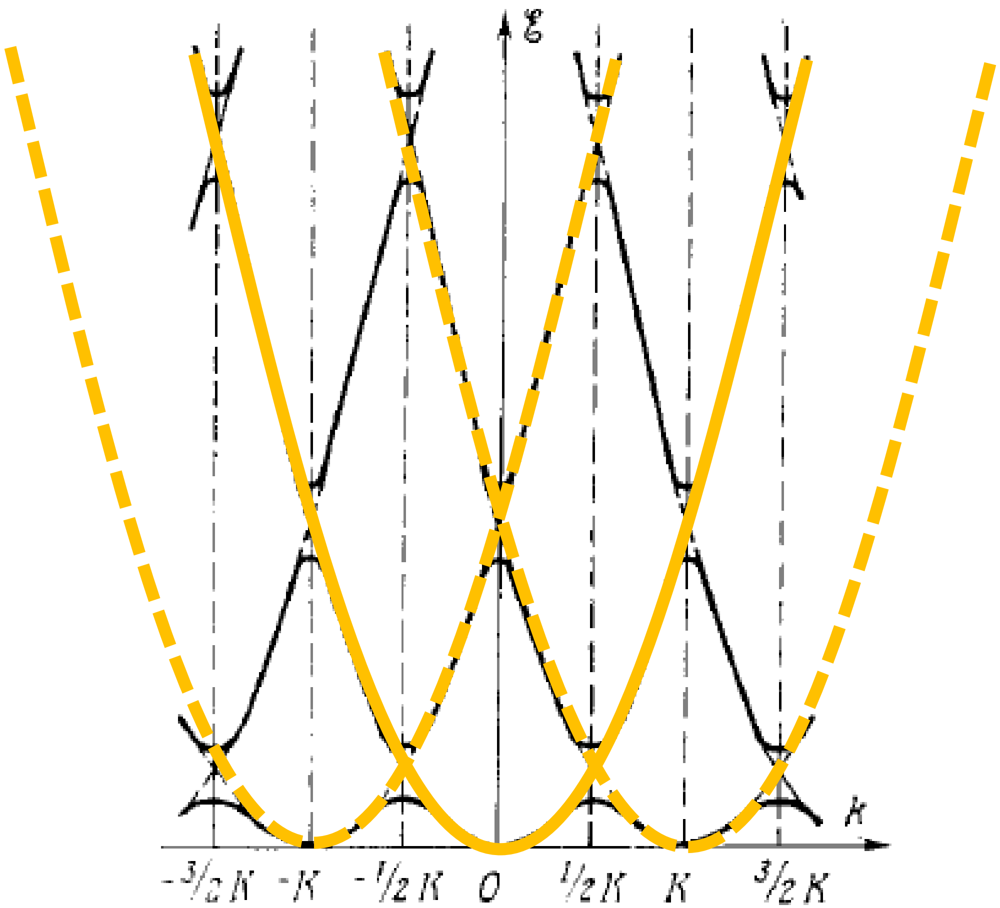
Теорема Блоха

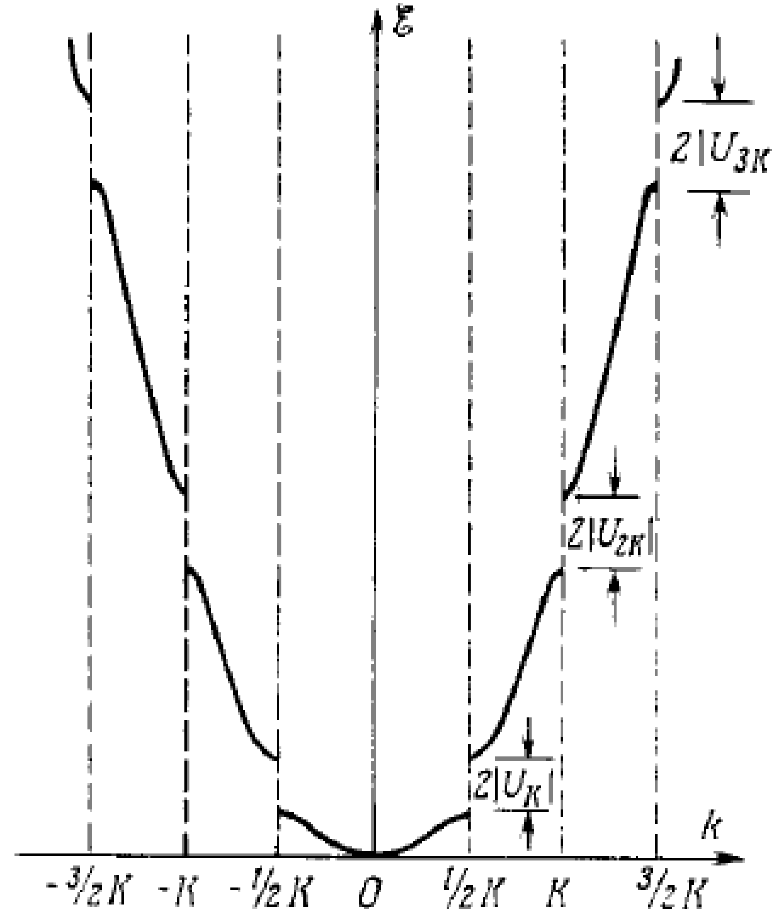
$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u(\mathbf{r})$$

$$\psi_{n,\,\mathbf{k}+\mathbf{K}}(\mathbf{r}) = \psi_{n\mathbf{k}}(\mathbf{r})$$

$$\mathcal{E}_{n,\,\mathbf{k}+\mathbf{K}} = \mathcal{E}_{n\mathbf{k}}$$

$$\mathcal{E} = \frac{1}{2}\left(\mathcal{E}^0_{\mathbf{q}} + \mathcal{E}^0_{\mathbf{q}-\mathbf{K}}\right) \pm \left[\left(\frac{\mathcal{E}^0_{\mathbf{q}} - \mathcal{E}^0_{\mathbf{q}-\mathbf{K}}}{2}\right)^2 + |U_{\mathbf{K}}|^2\right]^{1/2}$$





2H-Cu_xTaSe_2