Exploring new aspects of orthogonality catastrophe

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Outline

Introduction: Orthogonality Catastrophe

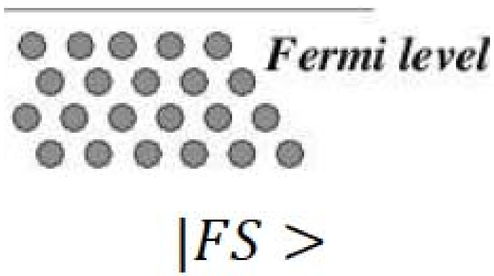
Extended introduction: Orthogonality Catastrophe and RSXS studies of CDW in high Tc cuprates

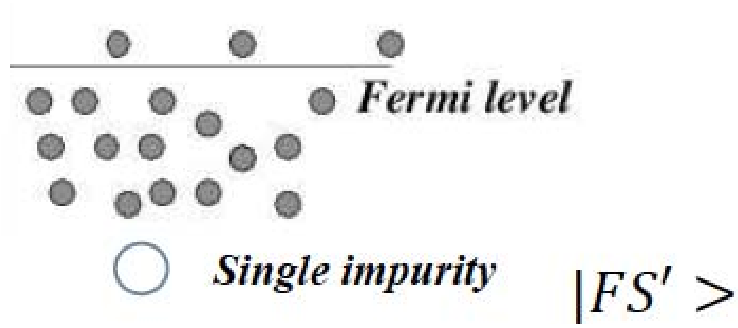
P. Abbamonte, E.D., J.C. Davis, J.-C. Campuzano, arXiv:1112.5112
D. Benjamin, D. Abanin, E.D., unpublished

Exploring Orthogonality Catastrophe with ultracold atoms

M. Knap, A. Shashi, Y. Nishida, A. Imambekov, D. Abanin, ED, arXiv:1206.4962

Anderson orthogonality catastrophe





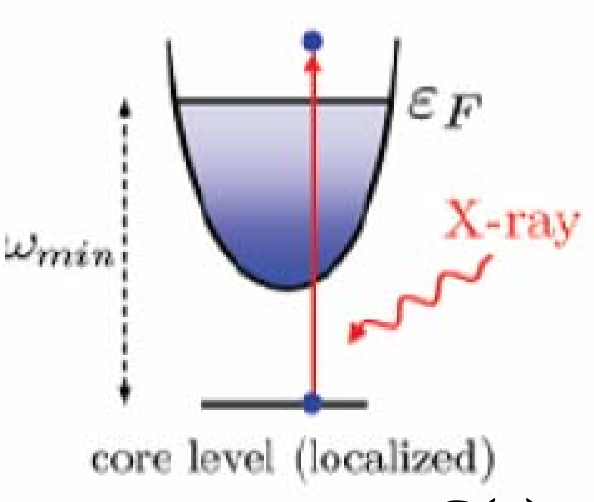
-Overlap $S = \langle FS \mid FS' \rangle$

- $S \rightarrow 0$ as system size $L \rightarrow \infty$, "orthogonality catastrophe"

-Infinitely many low-energy electron-hole pairs produced

Fundamental property of the Fermi gas

Orthogonality catastrophe in X-ray absorption spectra

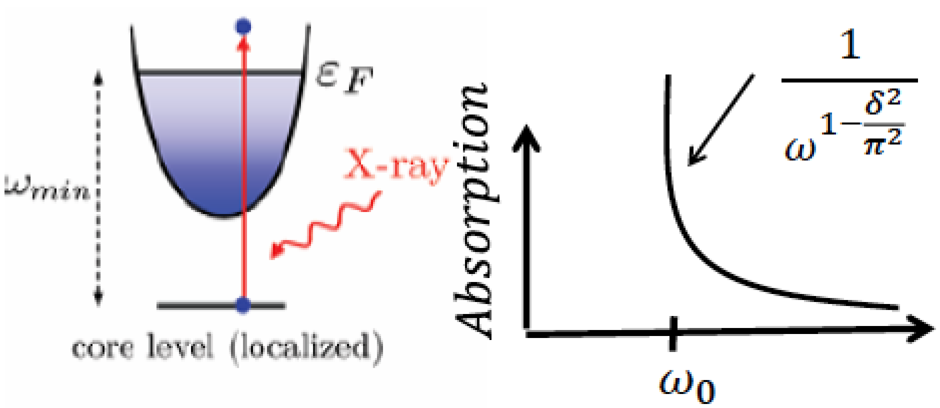


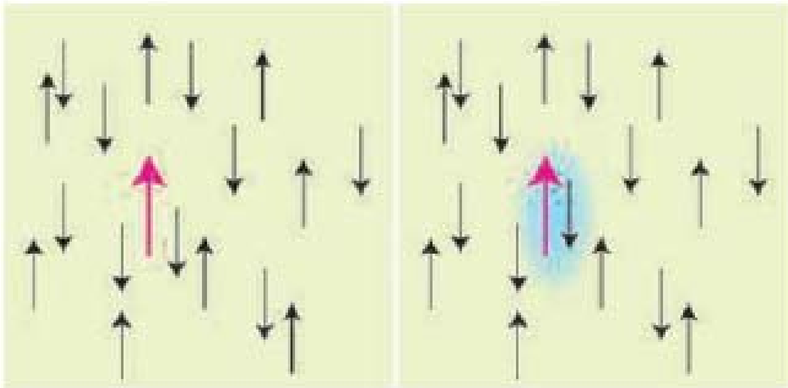
Without impurity *With impurity*

-Relevant overlap: $S(t) = \left\langle FS \,|\, e^{iH_0 t} e^{-iH_f t} \,|\, FS \right\rangle \propto t^{-\delta^2/\pi^2}$

δ -- scattering phase shift at Fermi energy, $\tan\delta = -k_F a$

Orthogonality catastrophe: paradigm of impurity problem in condensed matter





-Edge singularities in the X-ray absorption spectra (exact solution of non-equilibrium many-body problem)

-Kondo effect: entangled state of impurity spin and fermions

Influential area, both for methods (renormalization group) and for strongly correlated materials

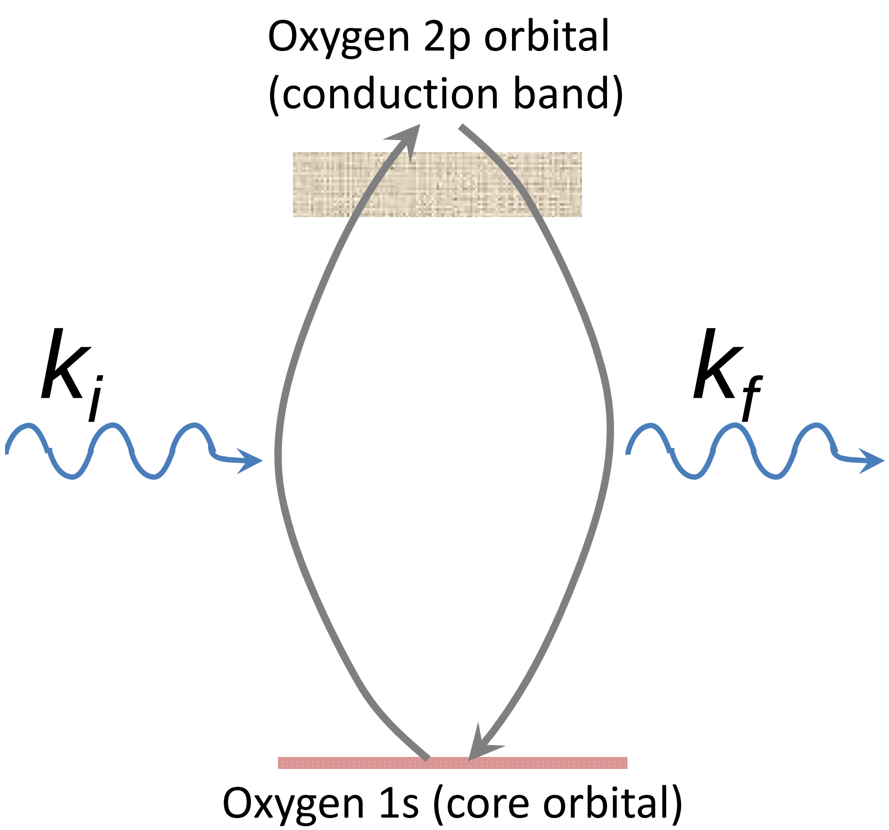
Role of orthogonality catastrophe in RSXS experiments on cuprates

P. Abbamonte, E. D., J. C. Davis, J.-C. Campuzano, arXiv:1112.5112
and
D. Benjamin, D. Abanin, E. D., unpublished

Resonant Soft Xray Scattering (RSXS)

Neutron and X-ray diffraction are mainly sensitive to the nuclear scattering and the core electron scattering.
at the edge of OK level the form factor of the conduction band is enhanced by a factor of 80

$$400\text{eV} < \hbar\omega < 1\text{keV}$$

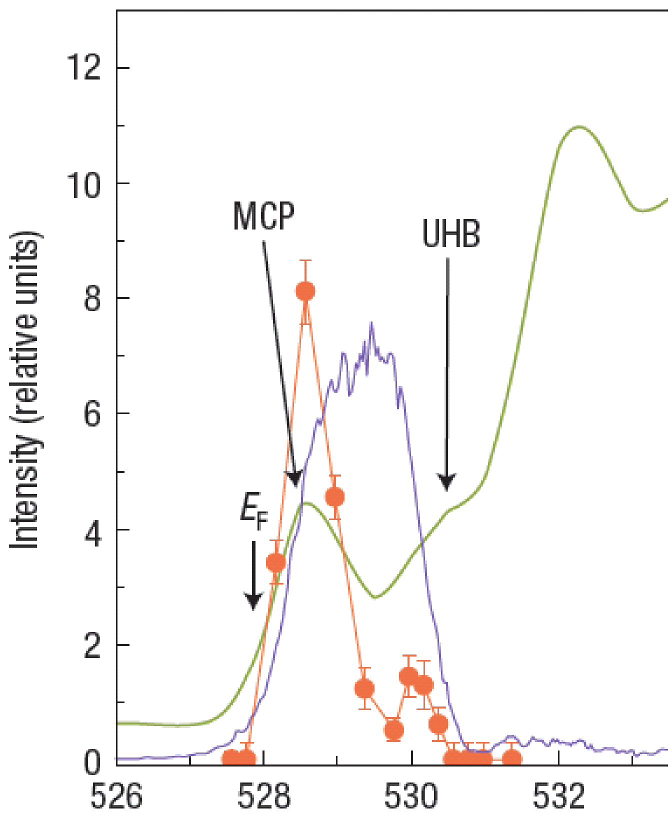


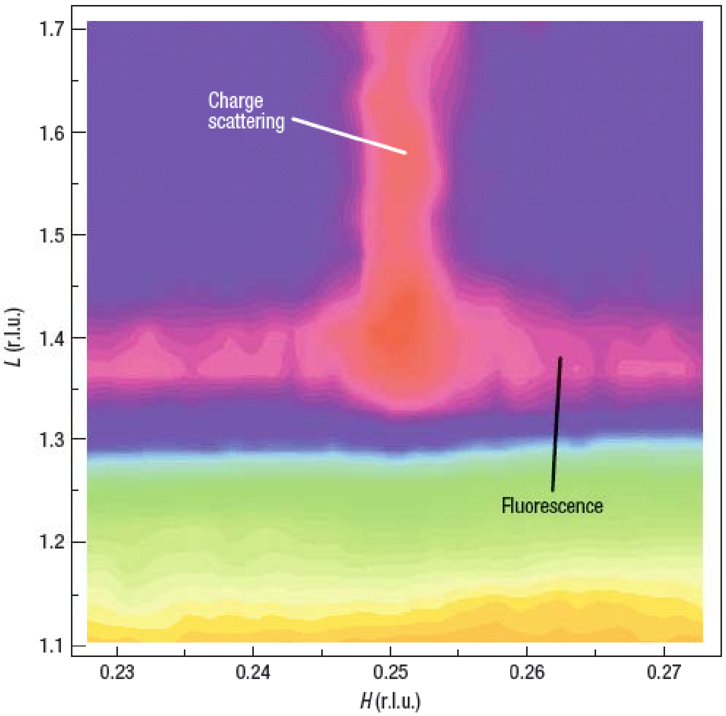
Advantages:
Bulk probe
can be applied to any material

Disadvantages:
energy resolution limited
by lifetime of the core hole
$\Gamma \approx 150$ meV

Observation of period four CDW in cuprates

$La_{2-x}Ba_xCuO_4$ Abbamonte et al., Nature Phys. 1:155 (2005)
$La_{1.8-x}Eu_{0.2}Sr_xCuO_4$ Fink et al., Phys. Rev. B 79:100502 (R) (2009)





Need quantitative analysis of spectra beyond atomic form factors and structure factors

Kramers-Heisenberg formula

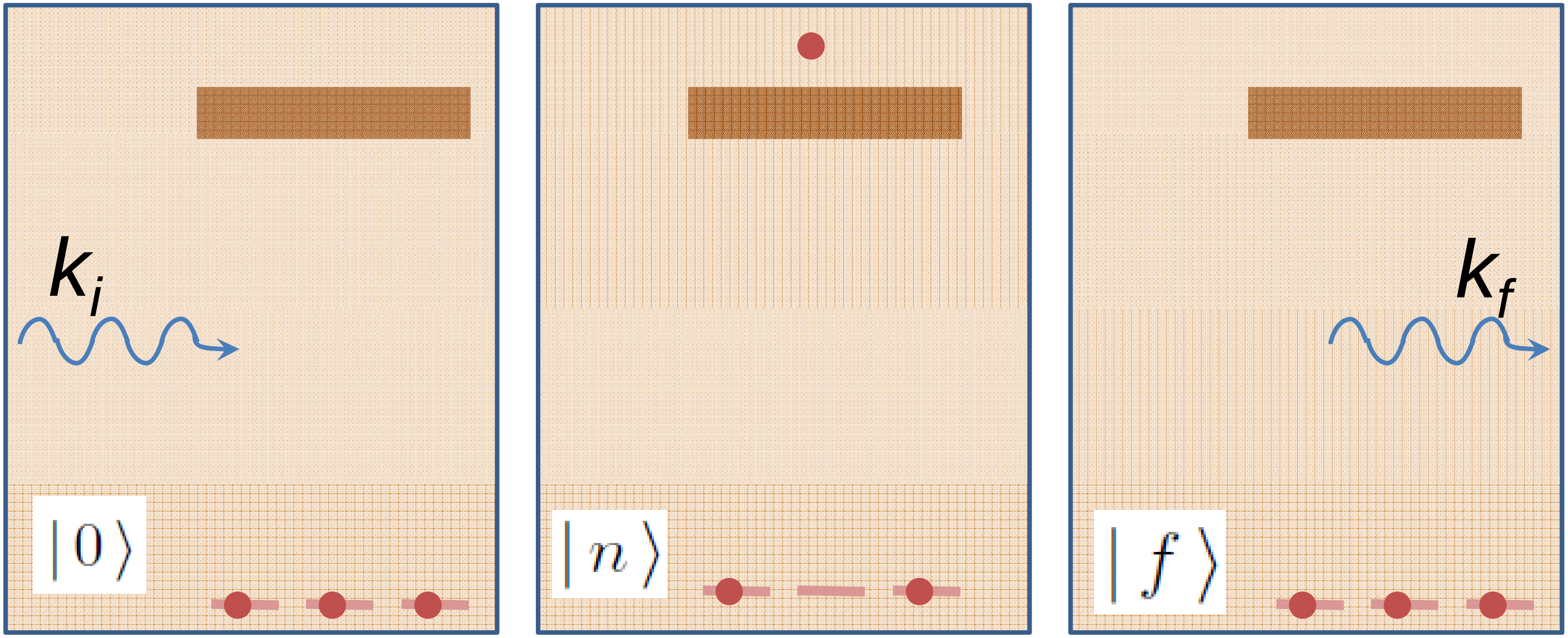
Absorption of initial photon

Emission of final photon

$$T_1 = \sum_j \Psi_j^\dagger c_j a_{k_i} e^{ik_i r_j} + \text{c.c.}$$

$$T_2 = \sum_j c_j^\dagger \Psi_j a_{k_f} e^{ik_f r_j} + \text{c.c.}$$

$$I_{\text{RSXS}} = \sum_f \Big| \sum_n \frac{\langle f|T_2^\dagger|n\rangle\langle n|T_1|0\rangle}{E_0 - E_n + \omega_i + i\Gamma} \Big|^2 \delta(E_0 + \omega_i - E_f - \omega_f)$$



RSXS and response function

Elastic scattering $|\, f\,\rangle \;=\; |\,0\,\rangle$

$$I(q,\omega_i) = |\sum_{nj} \frac{\langle 0|\Psi_j|n\rangle\langle n|\Psi_j^\dagger|0\rangle}{(E_0^N - \tilde{E}_n^{N+1} + \omega_i + i\Gamma)}\; e^{-iqr_j}\;|^2$$

Reminiscent of the local density of states measured in STM

$$\begin{aligned} \mathrm{Im}G(\epsilon, r_j) &= \rho^{\mathrm{STM}}(\epsilon, r_j) \\ &= \sum_n \langle 0|\Psi_j|n\rangle\langle n|\Psi_j^\dagger|0\rangle\delta(\epsilon - (E_n^{N+1} - E_0)) \\ &+ \sum_n \langle 0|\Psi_j^\dagger|n\rangle\langle n|\Psi_j|0\rangle\delta(\epsilon + (E_n^{N-1} - E_0)) \end{aligned}$$

Why we can not relate RSXS and STM in the most general case

- energies of excited states include the core hole potential
- finite core hole lifetime $\tau = \Gamma^{-1}$

RSXS simplified (1)

Neglect the core hole potential
Neglect finite core hole lifetime

$$G^R(r_j,\epsilon) = \sum_n \frac{\langle 0|\Psi_j|n\rangle\langle n|\Psi_j^\dagger|0\rangle}{\epsilon-(E_n^{N+1}-E_0^N)+i0} + \cancel{\sum_n \frac{\langle 0|\Psi_j^\dagger|n\rangle\langle n|\Psi_j|0\rangle}{\epsilon-(E_n^{N-1}-E_0^N)+i0}}$$

RSXS intensity can be related to the electron part of the Green’s function

$$\boxed{I(q,\omega) = |\sum_j \mathrm{ImG}_e(r_j,\omega)e^{-iqr_j}|^2}$$

RSXS intensity can be related to STM Fourier transforms of LDOS

$$\rho^{\mathrm{STM}}(\epsilon,q) = \sum_j \rho^{\mathrm{STM}}(\epsilon,r_j)e^{-iqr_j} = \sum_j \mathrm{Im}G(\epsilon,r_j)e^{-iqr_j}$$

Relating RSXS and STM

Quasiparticle interference in $Bi_2Sr_2CaCu_2O_{8+\delta}$, J. Hoffman et al., Science (2002)

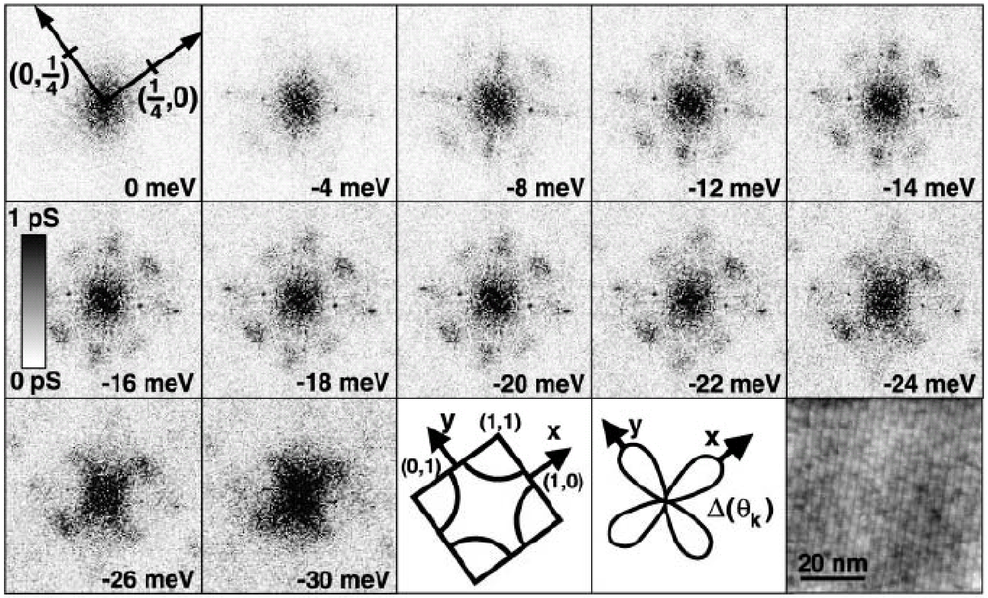


Fig. 3. A series of 12 Fourier transforms of LDOS images measured on a 600 Å square FOV at the energies shown in each panel. The origin and points (1/4, 0) $2\pi/a_0$ and (0, 1/4) $2\pi/a_0$ are labeled.

RSXS can be related to the electron part of STM spectra

$$I(q,\omega) = \left| \int_0^\infty \frac{\rho_e^{\mathrm{STM}}(\epsilon, q)}{\epsilon - \omega - i0} \right|^2$$

RSXS simplified (2)

Neglect the core hole potential

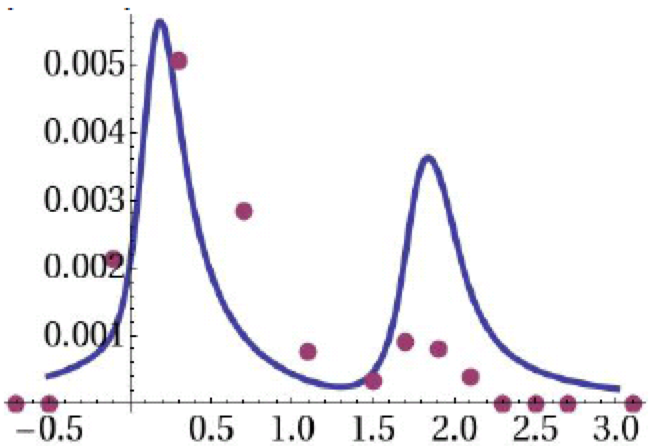
Include the core hole lifetime

$$H = \sum_{\mathbf{k}} \xi_{\mathbf{k}} d^\dagger_{\mathbf{k}} d_{\mathbf{k}} + V \sum_{\mathbf{k}} \left(d^\dagger_{\mathbf{k}+\mathbf{Q}} d_{\mathbf{k}} + d^\dagger_{\mathbf{k}} d_{\mathbf{k}+\mathbf{Q}} \right)$$

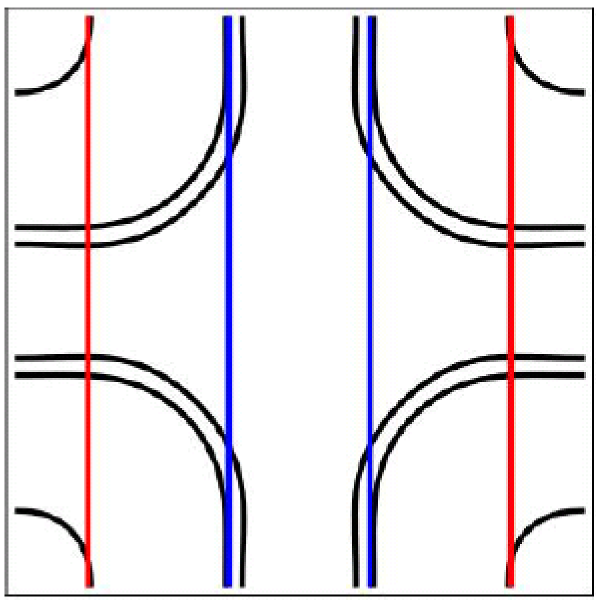
$$\xi_{\mathbf{k}} = -t(\cos k_x + \cos k_y) + 4t_1 \cos k_x \cos k_y - 2t_2(\cos 2k_x + \cos 2k_y)$$

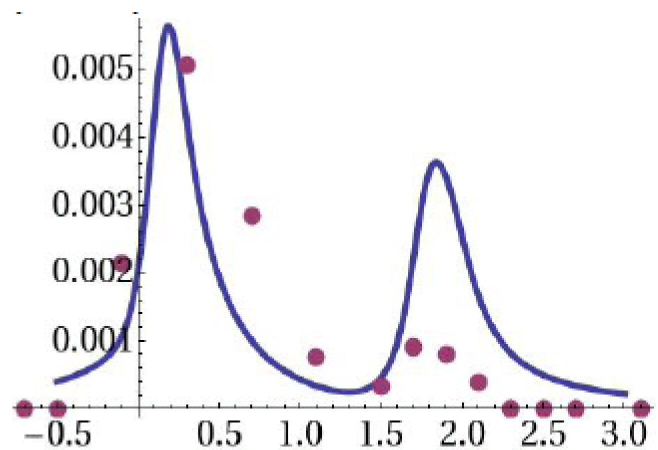
Take “canonical” parameters from ARPES and DFT

$$I(q,\omega_i) = |\sum_{nj} \frac{\langle 0|\Psi_j|n\rangle\langle n|\Psi^\dagger_j|0\rangle}{(E^N_0 - E^{N+1}_n + \omega_i + i\Gamma)} e^{-iqr_j}|^2$$



Two peak structure in RSXS: dynamic nesting





Including core hole potential: orthogonality catastrophe

$$I_{\mathrm{RSXS}} = |\sum_{nj} e^{-iqr_j} \frac{\langle 0|\Psi_j|n\rangle\langle n|\Psi_j^\dagger|0\rangle}{E_0 - \tilde{E}_n + \omega_i + i\Gamma}|^2\,\delta(E_0 + \omega_i - E_f - \omega_f)$$

Introduce local on-site potential $\mathcal{H}_1 = \mathcal{H}_0 + V n_j$

Express I_{RSXS} in a way reminiscent of Orthogonality Catastrophe

$$\sum_n \frac{|n\rangle\langle n|}{E_0 - \tilde{E}_n + \omega_i + i\Gamma} = \int_0^\infty e^{i(\mathcal{H}_1 - E_0 - \omega_i)t - \Gamma t}$$

$$\boxed{I_{RSXS} = |\sum_j e^{-iqr_j} \int_0^\infty dt\, e^{-\Gamma t}\,\langle 0|\Psi_j e^{i\mathcal{H}_1 t}\Psi_j^\dagger e^{i\mathcal{H}_0 t}|0\rangle\,|^2}$$

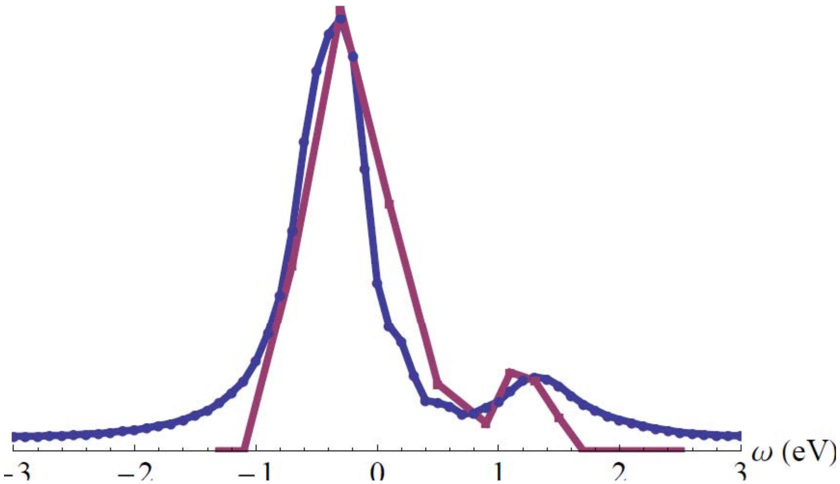
RSXS

Use functional determinant approach to relate expectation value over many-body state to summation over single particle states
Klich 2003; d'Ambrumenil, Muzykantsky 2005; Abanin, Levitov 2005

$$\langle 0|\Psi_i e^{i\mathcal{H}_1 t}\Psi_j^\dagger|0\rangle = \det[1+(e^{i\mathcal{H}_1 t}-1)n]\,\langle j|[\frac{\hat{n}}{1-\hat{n}}+e^{-i\mathcal{H}_1 t}]^{-1}|j\rangle$$

$$\mathcal{H}_1 = \mathcal{H}_0 + V|j\rangle\langle j|$$

$$\hat{n} = \frac{e^{-\beta\mathcal{H}_0}}{1+e^{-\beta\mathcal{H}_0}}$$



Including the core hole potential V=-0.75eV

Summary of part I

Established formalism for relating RSXS intensity to correlation functions of electrons in the conduction band

RSXS experiments on cuprates can be described quantitatively by a combination of dynamical nesting of band structure and orthogonality catastrophe on the hole potential

Difficulties of probing universal features of orthogonality catastrophe in solid state systems

-Many unknowns;
Simple models hard to test
(complicated band structure, unknown impurity parameters, coupling to phonons)

-Limited probes
(usually only absorption spectra)

-Dynamics beyond linear response out of reach
(relevant time scales GHz-THz, experimentally difficult)

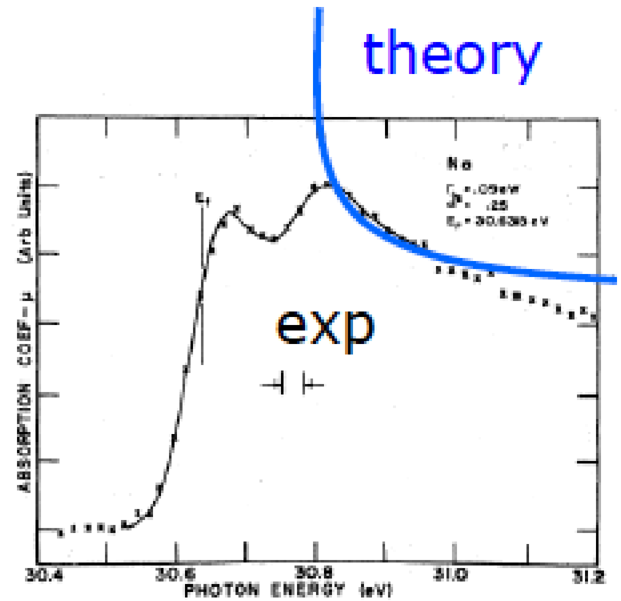


FIG. 6. SKA spectrum for Na at 100 K.

X-ray absorption in Na

Exploring orthogonality catastrophe with ultracold atoms

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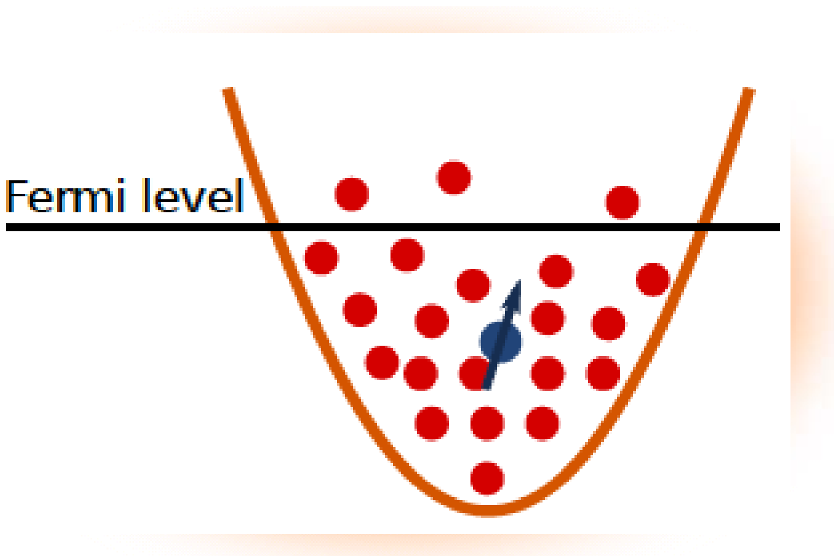
arXiv:1206.4962

Orthogonality catastrophe with cold atoms: Setup



- Fermi gas+single impurity

- Two pseudospin states of impurity, $|\uparrow\rangle$ and $|\downarrow\rangle$

- $|\uparrow\rangle$ -state scatters fermions
  $|\downarrow\rangle$ -state does not

- Scattering length a

- Fermion Hamiltonian for pseudospin $|\uparrow\rangle, |\downarrow\rangle$ -- H_0, H_f

Earlier theoretical work on Kondo and FES with relation to cold atoms: Zwerger, Lamacraft, Imambekov, Kamenev, Gangardt, Giamarchi, Kollath,.

Ramsey fringes – new manifestation of OC

-Utilize control over spin

-Access coherent coupled dynamics of spin and Fermi gas

-Ramsey interferometry

1) $\pi/2$ pulse $$|\downarrow\rangle|FS\rangle \to \frac{1}{\sqrt{2}}|\downarrow\rangle|FS\rangle + \frac{1}{\sqrt{2}}|\uparrow\rangle|FS\rangle$$

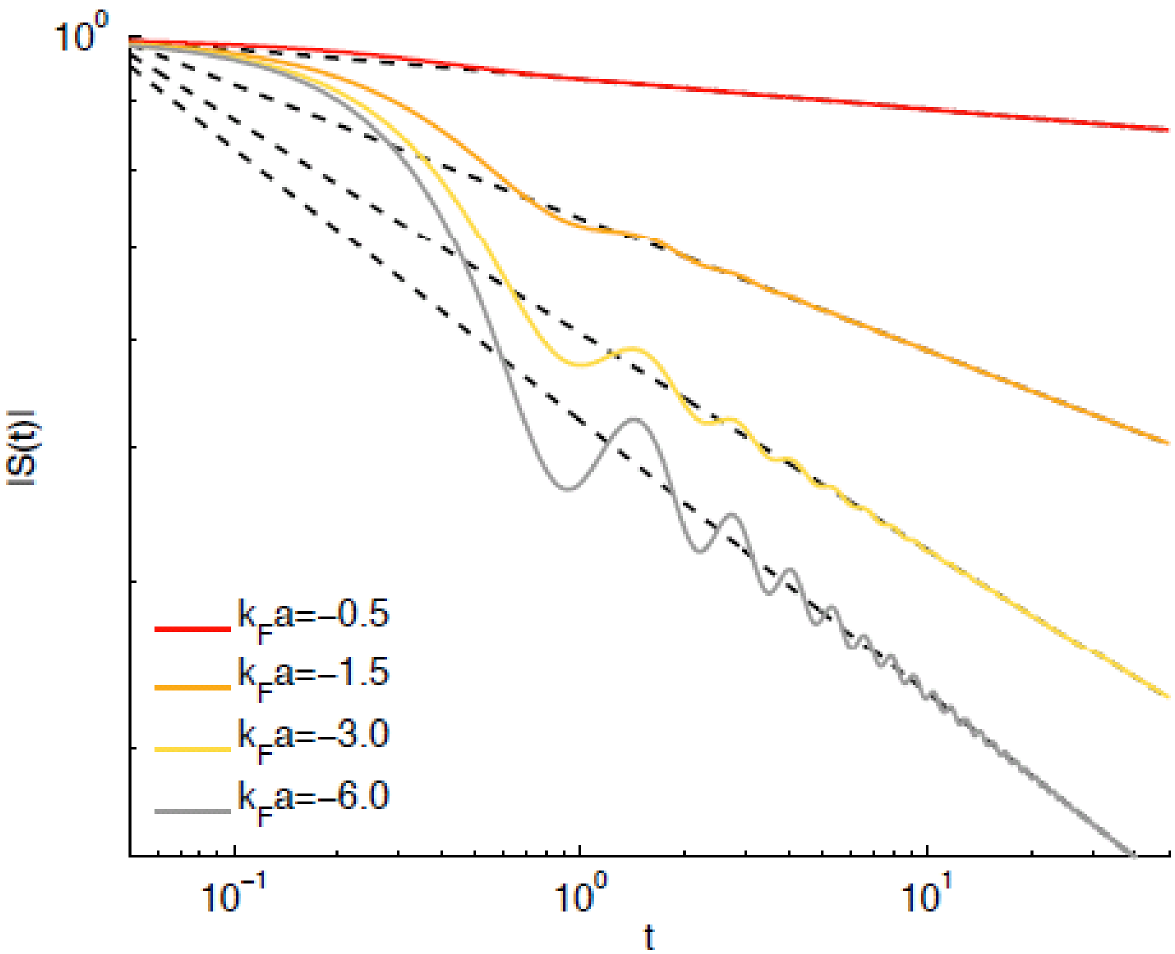
2) Evolution $$\frac{1}{\sqrt{2}}|\downarrow\rangle e^{-iH_0 t}|FS\rangle + \frac{1}{\sqrt{2}}|\uparrow\rangle e^{-iH_f t}|FS\rangle$$

3) Use $\pi/2$ pulse to measure $$< S_x >= \mathrm{Re}[S(t)]$$

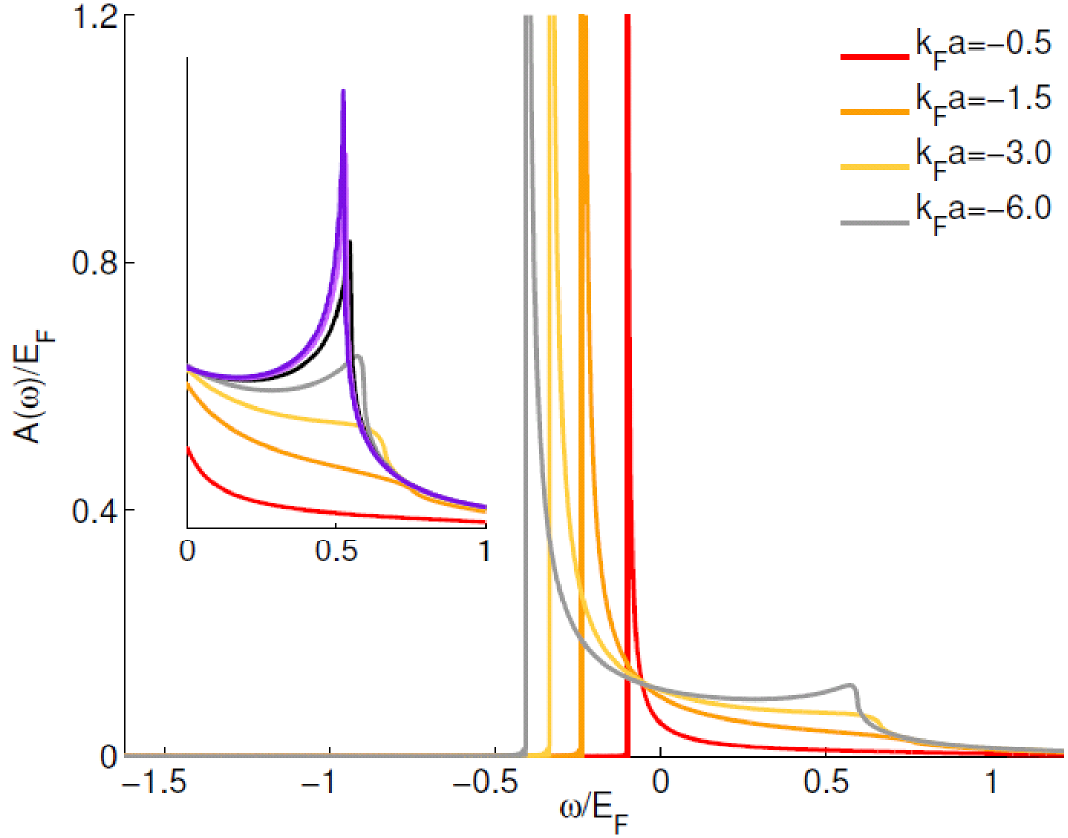
$$S(t) = \left\langle FS \,|\, e^{iH_0 t} e^{-iH_f t} \,|\, FS \right\rangle$$

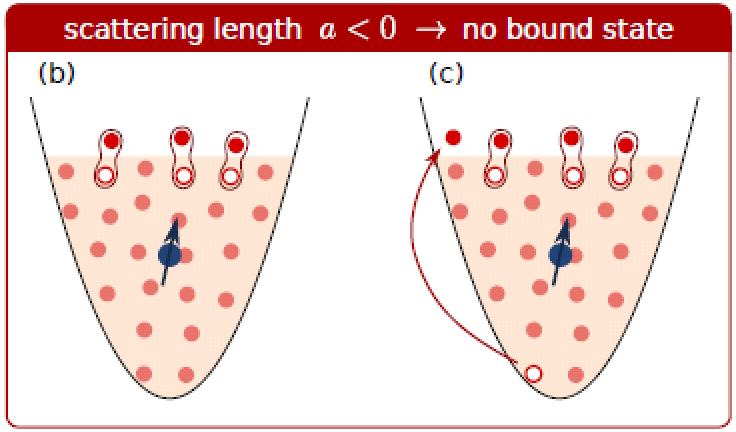
Direct measurement of OC in the time domain

Ramsey fringes as a probe of OC
First principle calculations



Exact RF spectra



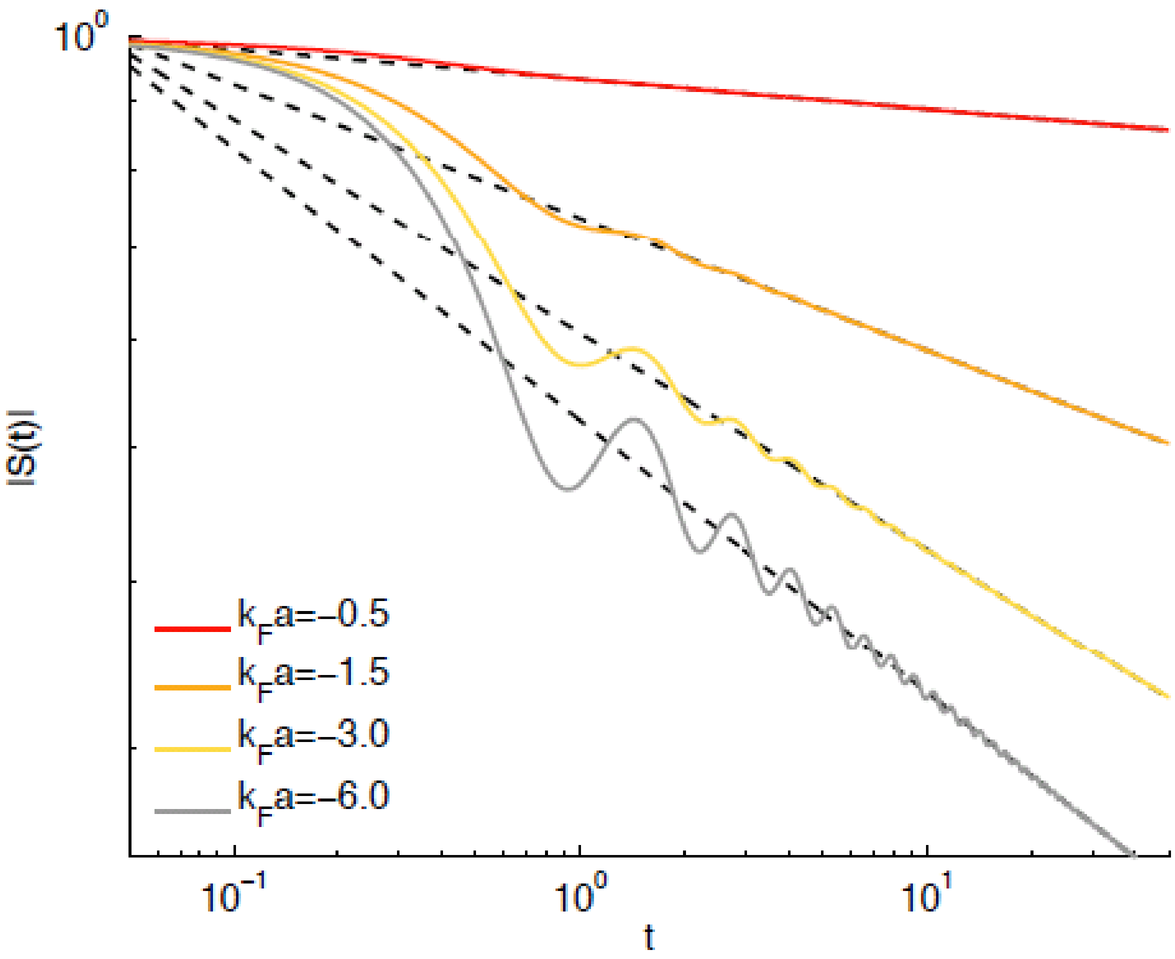


a<0; no impurity bound state

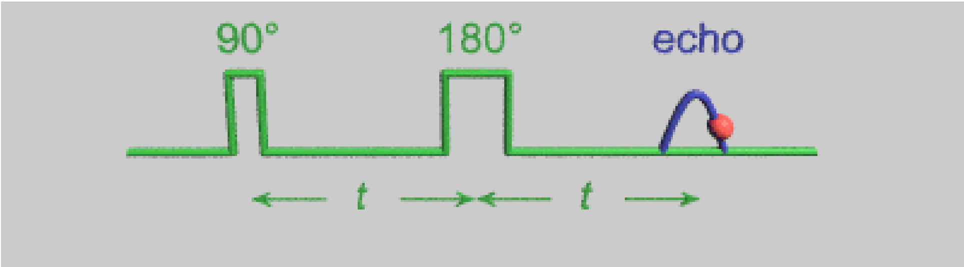
Cusp at E_F

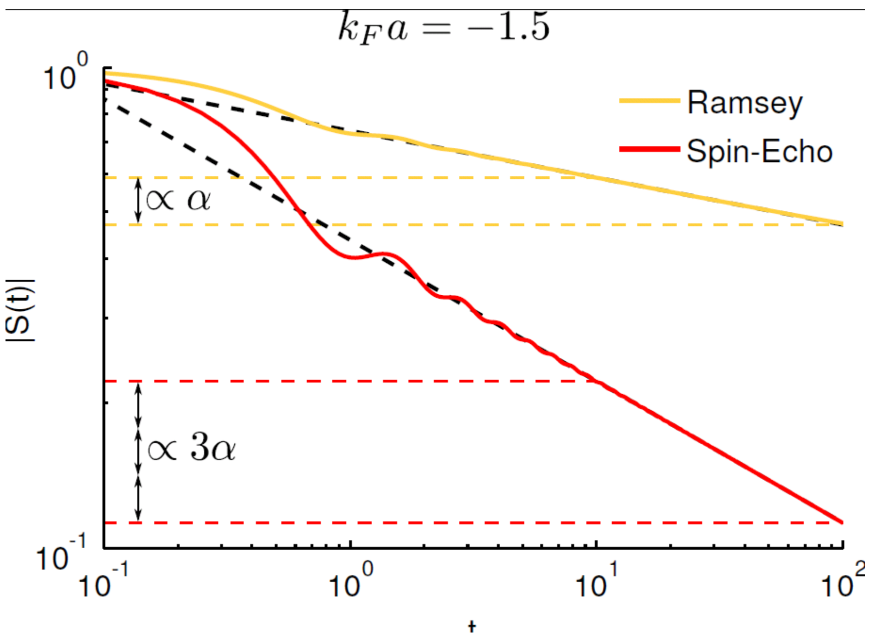
Single threshold in absorption

Ramsey fringes as a probe of OC
First principle calculations



Spin echo: probing non-trivial dynamics of the Fermi gas





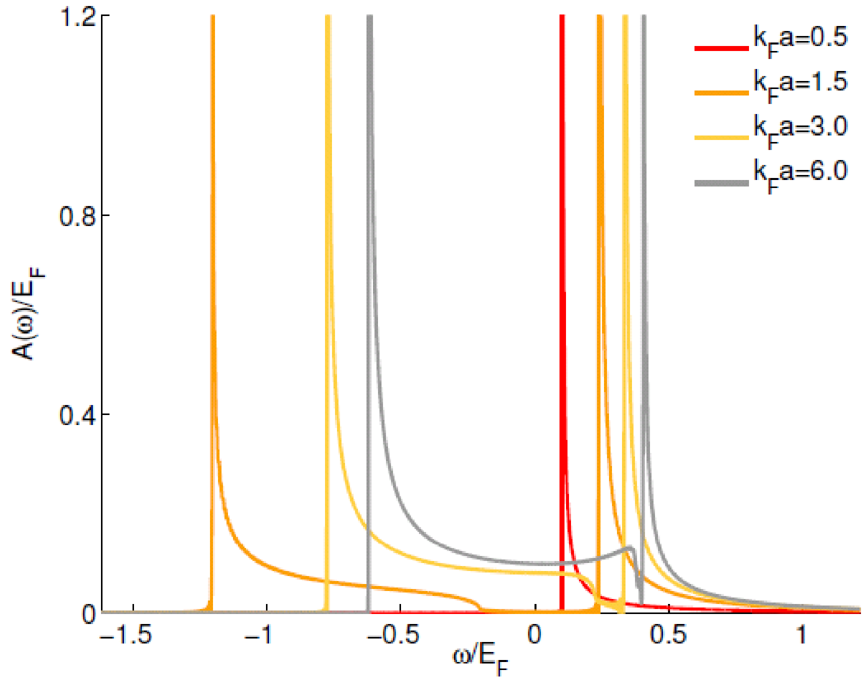
-Unlike the usual situation (spin-echo decays slower than Ramsey)

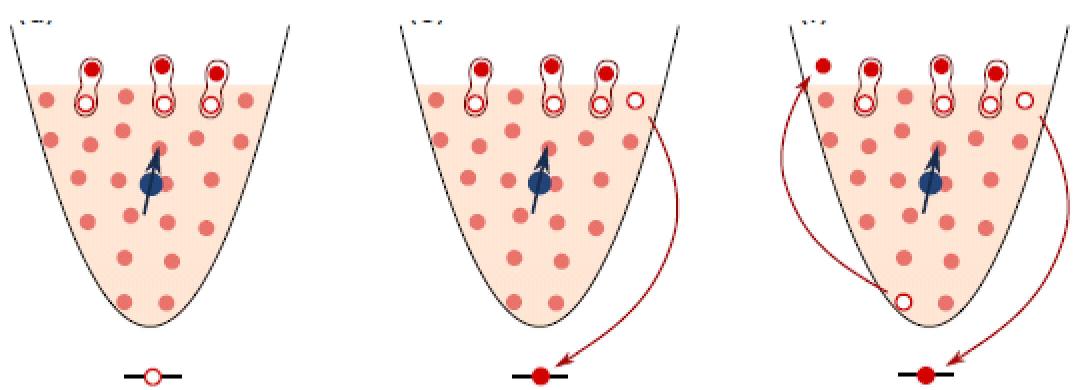
-Cancels magnetic field flutuations

-Universal

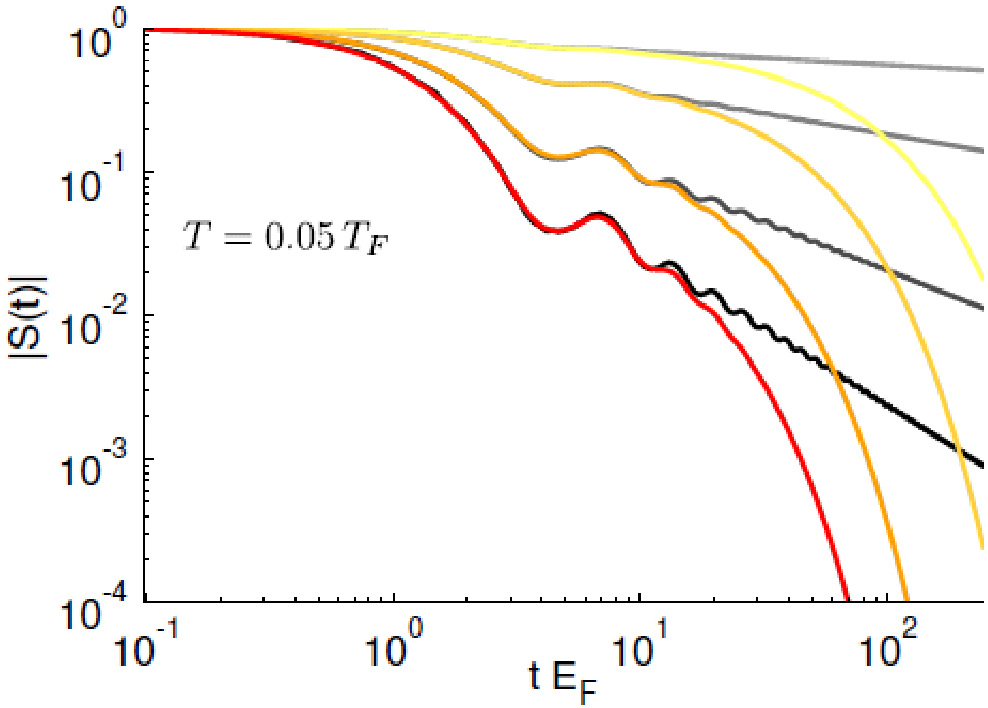
-Generalize to n pi-pulses to study even more complex response functions

Ramsey fringes as a probe of OC
First principle calculations

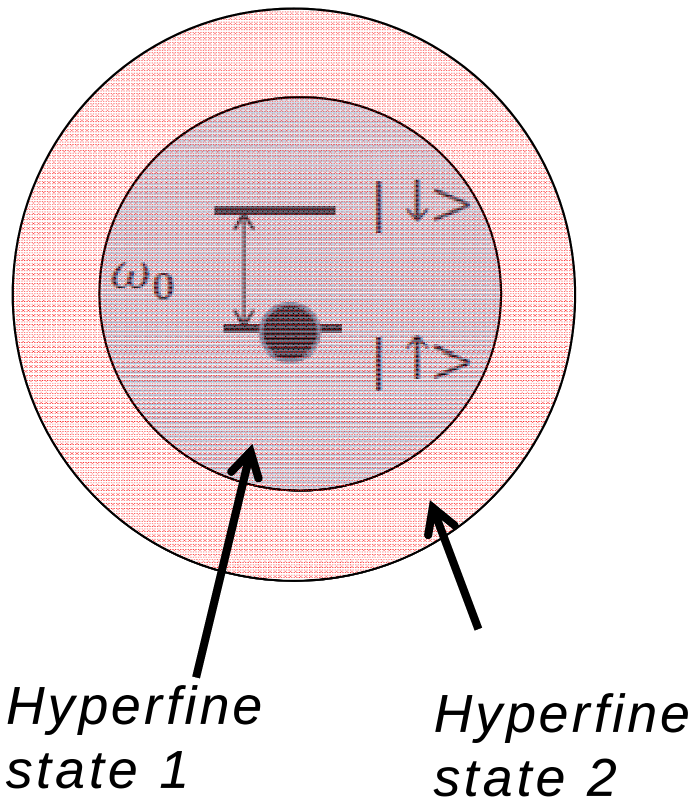




Ramsey fringes as a probe of OC
First principle calculations



Generalizations: non-equilibrium OC, non-abelian Riemann-Hilbert problem



-Multi-component Fermi gas coupled to impurity

-Imbalance different species

-Mix them by pi/2 pulses

-Realization of non-equilibrium OC problem

-”Simulator” of quantum transport and non-abelian Riemann-Hilbert problem

-Charge full counting statistics can be probed

Summary of part II

RSXS intensity can be related to correlation function of conduction band

RSXS experiments on cuprates can be described quantitatively by a combination of dynamical nesting and orthogonality catastrophe on the hole potential