Quantum dynamics in many-body systems

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Outline

Examples of theory addressing experimental puzzles

Role of non-equilibrium processes in resonant XRay

Chiral prethermalization in non-uniformly split condensates
Role of nonequilibrium dynamics in Resonant Soft Xray Scattering experiments on high Tc cuprates


D. Benjamin, I. Klich, E. Demler, arXiv:1312.6642
Resonant Elastic XRay Scattering (REXS)
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
- \( \Gamma \approx 150 \text{meV} \)
Observation of period four CDW in cuprates

La$_{2-x}$Ba$_x$CuO$_4$  Abbamonte et al., Nature Phys. 1:155 (2005)
La$_{1.8-x}$Eu$_{0.2}$Sr$_x$CuO$_4$ Fink et al., Phys. Rev. B 79:100502 (R) (2009)

Peak separation is too small for the Hubbard gap
If second peak is Mott, it should be strong at Cu edge and weak at O edge. Experimentally it is the opposite.
Kramers-Heisenberg formula

Absorption of initial photon

\[ T_1 = \sum_j \Psi_j^\dagger c_j a_k e^{ik_ir_j} + \text{c.c.} \]

Emission of final photon

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

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

Elastic scattering \( |f\rangle = |0\rangle \)

\[
I(q, \omega_i) = \sum_{n_j} \frac{\langle 0|\Psi_j|n\rangle \langle n|\Psi_j^\dagger|0\rangle}{(E_0^N - E_n^{N+1} + \omega_i + i\Gamma)} e^{-iqr_j} |^2
\]

Reminiscent of the local density of states measured in STM

\[
\text{Im} G(\epsilon, r_j) = \rho_{\text{STM}}(\epsilon, r_j)
\]

\[
= \sum_n \langle 0|\Psi_j|n\rangle \langle n|\Psi_j^\dagger|0\rangle \delta(\epsilon - (E_n^{N+1} - E_0)) + \sum_n \langle 0|\Psi_j^\dagger|n\rangle \langle n|\Psi_j|0\rangle \delta(\epsilon + (E_n^{N-1} - E_0))
\]

Why we cannot relate REXS and STM in the most general case
- energies of excited states include the core hole potential
- finite core hole lifetime \( \tau = \Gamma^{-1} \)
REXS simplified (1)

Neglect the core hole potential
Neglect finite core hole lifetime

\[ \mathcal{G}_R(r_j, \epsilon) = \sum_n \frac{\langle 0 | \Psi_j | n \rangle \langle n | \Psi_j^\dagger | 0 \rangle}{\epsilon - (E_{n+1}^N - E_0^N) + i0} + \sum_n \frac{\langle 0 | \Psi_j^\dagger | n \rangle \langle n | \Psi_j | 0 \rangle}{\epsilon - (E_{n-1}^N - E_0^N) + i0} \]

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

\[ I(q, \omega) = | \sum_j \text{Im} G_e(r_j, \omega) e^{-iqr_j} |^2 \]

RSXS intensity can be related to STM Fourier transforms of LDOS

\[ \rho_{\text{STM}}(\epsilon, q) = \sum_j \rho_{\text{STM}}(\epsilon, r_j) e^{-iqr_j} = \sum_j \text{Im} G(\epsilon, r_j) e^{-iqr_j} \]
Relating REXS and STM

Quasiparticle interference in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, J. Hoffman et al., Science (2002)

RSXS can be related to the electron part of STM spectra

\[ I(q, \omega) = \left| \int_0^\infty \frac{\rho_e^{STM}(\epsilon, q)}{\epsilon - \omega - i0} \right|^2 \]
REXS simplified (2)

Neglect the core hole potential

Include the core hole lifetime

\[ H = \sum_k \xi_k d_k \dagger d_k + V \sum_k \left( d_{k+Q} \dagger d_k + d_k \dagger d_{k+Q} \right) \]

\[ \xi_k = -t (\cos k_x + \cos k_y) + 4t_1 \cos k_x \cos k_y - 2t_2 (\cos 2k_x + \cos 2k_y) \]

Take “canonical” parameters from ARPES and DFT

\[ I(q, \omega_i) = \left| \sum_{n_j} \frac{\langle 0 | \Psi_j | n \rangle \langle n | \Psi_j \dagger | 0 \rangle}{(E_0^n - E_n^{N+1} + \omega_i + i\Gamma)} e^{-iqr_j} \right|^2 \]
Two peak structure in REXS: dynamic nesting
REXS as dynamic problem

\[ A_{i\rightarrow i} = \sum_{m} e^{i(k_f-k_i)\cdot R_m} \langle i|d_m(\omega + H_m - E_i + i\Gamma)^{-1}d^\dagger_m|i \rangle \]

\[ = \int_{0}^{\infty} dt \ e^{i(\omega - \Gamma)t} \sum_{m} e^{iQ_{CDW}\cdot R_m} \langle i|d_m e^{-iH_m t}d^\dagger_m e^{-iH_0 t}|i \rangle \]

= Fourier transform of a history: excite, propagate, de-excite
REXS cross section from functional determinant formalism

\[ S_m(t) = \langle i | d_m e^{-iH_m t} d_m^\dagger e^{-iH_0 t} | i \rangle \]

\[ = \det \left( (1 - N) + U_m(t)N \right)^2 \langle m | \left( \frac{N}{1 - N} + U_m^{-1}(t) \right)^{-1} | m \rangle, \]

\[ \quad \text{Fermi sea} \quad \text{photoexcited electron} \]

\[ N \equiv (1 + \exp(\beta h_0))^{-1}, \quad U_m(t) \equiv e^{-i h_m t} e^{i h_0 t} \]

- \( N \): single-particle Fermi sea occupation
- \( U_m \): single-particle time-evolution with core hole at \( \mathbf{R}_m \)
- \( \det \): device for matrix elements of Slater determinant state
- \( \det()^2 \): one Fermi sea for each spin
- \( (1 - N) + U_m(t)N \): time-evolve only occupied states.
- \( |m\rangle \): Wannier orbital at \( \mathbf{R}_m \).
- \( \langle m| |m\rangle \): Propagator \( \langle m|U_m(t)|m\rangle \) for \( N = 0 \), Pauli-blocking 0 for \( N = 1 \).
Consider $\langle e^X \rangle = \text{tr} \left[ e^X e^{-\beta H} \right] / \text{tr} \left[ e^{-\beta H} \right]$ for quadratic $X, H$.

- In basis where $X = \sum_\alpha \omega_\alpha \hat{n}_\alpha$

$$\text{tr} \left[ e^X \right] = \prod_\alpha \sum_{n_\alpha = 0,1} e^{n_\alpha \omega_\alpha} = \prod_\alpha (1 + e^{\omega_\alpha}) = \det (1 + e^X)$$

- BCH: $e^X e^Y = e^Z$, $Z$ quadratic, $\text{tr} \left[ e^X e^Y \right] = \det (1 + e^X e^Y)$

- Insertions: $\text{tr} \left[ d_m^\dagger d_n e^Z \right] = \sum_{\alpha, \beta} \langle \alpha|n\rangle \langle m|\beta\rangle \text{tr} \left[ d_\alpha^\dagger d_\beta e^Z \right] = \sum_\alpha \langle \alpha|\alpha\rangle \langle \alpha|n\rangle \prod_{\gamma \neq \alpha} (1 + e^{\omega_\gamma}) \sum_{n_\alpha = 0,1} n_\alpha e^{n_\alpha \omega_\alpha} = \sum_\alpha \langle m|\alpha\rangle \langle \alpha|n\rangle \frac{\det(1 + e^Z)}{1 + e^{\omega_\alpha}} e^{\omega_\alpha} = \sum_\alpha \langle m| \frac{e^Z}{1 + e^Z} |\alpha\rangle \langle \alpha|n\rangle \det(1 + e^Z) = \langle m| \frac{e^Z}{1 + e^Z} |n\rangle \det(1 + e^Z)$

Functional determinant formalism
Model of weakly interacting quasiparticles can explain REXS data qualitatively when we include nonequilibrium dynamics of electrons in the presence of core hole potential. Implication for microscopic models of cuprates: long lived electron quasiparticles. Observed numerically in DMFT by Georges et al, PRL (2013)
Resonant Inelastic XRay Scattering (RIXS)
Dispersive spin excitations in highly overdoped cuprates

Le Tacon et al., PRB (2013)
see also Dean et al., PRL (2013)

Neutron scattering does not observe strong magnetic scattering in this frequency range. These materials should be good metals with suppressed magnetic fluctuations (also lower Tc)
Spin flip processes are possible due to spin-orbit of core level Polarized incoming beam can select either spin-flip or non-spin-flip
RIXS cross section

RIXS amplitude as Fourier transform of “history”

\[ I \propto \int_{-\infty}^{\infty} ds \int_{0}^{\infty} dt \int_{0}^{\infty} d\tau \, e^{i\omega(t-\tau)-i\Delta\omega-i\Gamma(t+\tau)} \sum_{mn} e^{i\mathbf{Q} \cdot (\mathbf{R}_m-\mathbf{R}_n)} \chi_{\rho\sigma\chi_{\mu\nu}} S^{mn}_{\rho\sigma\mu\nu} \]

\[ S^{mn}_{\rho\sigma\mu\nu} = \langle e^{iH_{\tau}d_{n\rho}e^{-iH_{\tau}}}d_{n\sigma}^\dagger e^{iH_{s}}d_{m\mu}e^{iH_{mt}}d_{m\nu}^\dagger e^{-iH(t+s)} \rangle. \]

\[ \chi_{\alpha\beta} \] Polarization dependent matrix element

Forward and backward “histories” (Keldysh like)
Dispersing peaks in RIXS from quasiparticle model

Green line – experiments on Tl-2201 by Le Tacon et al, PRB (2013)
Black line – quasiparticle model

\[(t_1, t_2, t_3, t_4) = (181, -75, -4, 10) \text{ meV}\]

\[U_c = 1.0 \text{ eV}\]
Difference in spin-flip and non-spin-flip cross sections

dots—experiments in Bi-2212
by Dean et al, PRL (2013)
lines—quasiparticle model

The core hole potential separates spin flip and non-spin flip lineshapes.
Attractive potential of the hole tends to keep the photoexcited electron bound near the hole site leading to elastic scattering. Pauli blocking prevents other electrons of the same spin from hopping into this site and filling the core hole, thereby robbing spectral weight from inelastic scattering. With sufficient energy the photoexcited electron may be dislodged, allowing inelastic scattering. Inelastic scattering with small energy transfer $\Delta \omega$ is suppressed relative to scattering at larger $\Delta \omega$.

In spin-flip scattering electrons are not Pauli blocked.

standard band structure parameters

$$(t_1, t_2, t_3, t_4) = (126, -36, 15, 1.5) \text{ meV}$$

$U_c = 1.0 \text{ eV}$
False-fiable prediction of quasiparticle model of RIXS

Dependence of scattering intensity on incoming photon energy. Optimally doped Bi-2201 for $Q = (\pi/a,0)$. Frequency $\omega_0$ corresponds to the absorption maximum.

The increase in $\Delta \omega$ with $\omega$ does not occur if the peak is due to collective mode. It is a signature of particle-hole continuum.
Model of weakly interacting quasiparticles can explain key features of RIXS when we include nonequilibrium dynamics of electrons in the presence of core hole potential. Remaining puzzle: continuity of spectra into Mott AF states.
Nonequilibrium dynamics of coherently split one dimensional condensates

Theory: K. Agarwalk, E. Dalla Torre, E. Demler
Experiments: Schmiedmayer’s group in TU Vienna
The Experiment - Apparatus

(a) side view

E
B
A
C

view from below

B
A
D

Rb atoms, $F = 2$, $m_F = 2$

atomchip.org – Jorg Schmiedmayer group at University of Vienna
Interference of 1D Bose Gases

\[ \alpha = \left| \int_{-l/2}^{l/2} \frac{dx}{l} e^{i\phi(x)} \right|^2 \]

\[ P(\alpha) : \]


atomchip.org – Jorg Schmiedmayer group at University of Vienna
Time evolution of the DF $P(\alpha)$

$$\alpha = \left| \int_{-l/2}^{l/2} \frac{dx}{l} e^{i\phi(x)} \right|^2$$

- time = 0
- time = 2.5
- time = 5
- $l/\xi_s = 20$
- $l/\xi_s = 30$
- $l/\xi_s = 40$

- time = 7.5
- time = 10
- time = 12.5
Sudden Splitting and Prethermalization

\[ l / \xi_s = 30 \]

\[ k_B T_{\text{eff}} = \mu / 2 = g\rho / 2 \]


M. Gring et al. 2012 Science
So far, we cooled into 7.5 Hz trap, or split very slow in the beginning (large $t_1$)!
Different splitting

Fast first segment of the ramp

\[ \langle e^{i\phi(z_1)} e^{-i\phi(z_2)} \rangle \]
Correlations at $x, -x$ arise from population difference of Symm./Asymm modes.

$$\phi \sim \int \frac{dk}{k} \left[ \cos(kx)a_k^S + \sin(kx)a_k^A + \text{h.c.} \right]$$

$$\langle (\phi(x_1) - \phi(x_2))^2 \rangle = \int \frac{dk}{k} \left( 1 - \cos(k(x_1 - x_2)) \right) (N_k^S + N_k^A + 1)$$
$$+ \int \frac{dk}{2k} \left( \cos(2kx_1) + \cos(2kx_2) - 2\cos(k(x_1 + x_2)) \right) (N_k^S - N_k^A)$$
Different splitting

Fast first segment of the ramp

Correlations of $z = -z'$, stronger population of even modes

$$\beta_{2m} = k_B \left( T_{\text{eff}} + \Delta T \right)^{-1}$$
$$\beta_{2m+1} = k_B \left( T_{\text{eff}} - \Delta T \right)^{-1}$$

GGE !

Here: $\Delta T = 0.6 \, T_{\text{eff}}$
Changing the speed of the ramp changes the temperatures
Generalization of quench models

Fully utilizing the conformal symmetry of the post-quench Hamiltonian to solve a case of more general quench space-time trajectory.
Dynamics of the relative phase

\[
H(t) = \int dx \left( 2gn^2 + \frac{\rho}{4m} (\partial_x \phi)^2 + m_0^2(x, t) \phi^2 \right)
\]

\[
m_0^2 = 2g\rho^2 \left( 1 - \Theta(x + v_s t) \right) \left( \Theta(x - v_s t) \right)
\]

System initially in the ground state of:

\[
H(-\infty) = \int dx \left[ 2gn^2 \frac{\rho}{4m} (\partial_x \phi)^2 + 2g\rho^2 \phi^2 \right]
\]

\[\phi = \phi_L - \phi_R\]
Symmetric/Anti-symmetric Hamiltonians

\[ H_{S/A} = \int_{0}^{L/2} dx \, g n_{S/A}^2 + \frac{\rho}{2m} (\partial_x \phi_{S/A})^2 + m^2(x, t) \phi_{S/A}^2 \]

\[ m^2 = 4g\rho^2 \left(1 - \Theta(x + v_s t)\right) \]

\[ \phi(x > 0) = \phi_S(x) + \phi_A(x) \]
\[ \phi(x < 0) = \phi_S(|x|) - \phi_A(|x|) \]

\[ \phi_A(0) = 0 \]
\[ \partial_x \phi_S(0) = 0 \]

\[ \partial_x \phi_{S/A}(x = L/2) = 0 \]
Life in the Lorentz Boosted Frame

\[ t' = \gamma u_s (t + u_s x) \]
\[ x' = \gamma u_s (x + u_s t) \]
\[ u_s = c^2 / v_s \]

\[ 1 - \Theta(x + v_s t) = \Theta(-t') \]

Quench is instantaneous.
Calculations and Simulations for a finite size system: Boundary Conditions

- B. C.
- Splitter

Massless Dynamics

$x = u_s t$

$x = L/2$

$x = 0$

$t' = L / (2 \gamma_s)$

$x'$

$t'$
At the right boundary both fields have

\[ \phi_A(x = 0) = 0 \rightarrow \phi_A(x' = u_s t') = 0 \]

\[ \partial_x \phi_S(x = 0) = 0 \rightarrow (\partial'_x + u_s \partial'_t)\phi_S(x' = u_s t') = 0 \]

\[ \partial_x \phi_{S/A}(x = L/2) = 0 \]
What are the linearly independent solutions?

\[ t' < 0 \]

\[ v_{k}^{\pm,(1)} = B_{k} \left( e^{-ikx - i\omega_{k}'t} \pm e^{i\xi(k)x - i\omega_{f}(k)t} \right) ; k > 0 \]

\[ v_{k}^{\pm,(2)} = C_{k} \left( e^{ikx - i\omega_{k}'t} \pm e^{i\eta(k)x - i\omega_{g}(k)t} \right) ; 0 < k < k_{0} \]

\[ k = m \frac{u_{s}}{\sqrt{1 - u_{s}^{2}}} \]

\[ \omega_{k}' = \sqrt{(ck)^{2} + m^{2}} \]

We need 2 sets of modes!

Simple guess: Take two massive modes, and add them up in the right way so that the boundary conditions are satisfied.
Life in the Lorentz Boosted Frame

\[ t' > 0 \]

Still, moving BC

\[ u_s < c \]

\[ \phi_A(x = 0) = 0 \rightarrow \phi_A(x' = u_st') = 0 \]

\[ \partial_x \phi_S(x = 0) = 0 \rightarrow (\partial'_x + u_s \partial'_t)\phi_S(x' = u_st') = 0 \]

\[ \partial_x \phi_{S/A}(x = L/2) = 0 \]

Massless Dynamics

\[ \frac{L}{2\gamma_s} \]
What are the linearly independent solutions?

\[ t' > 0 \]

\[ u_k^{\pm} = A_k \left( e^{-ikv} \pm e^{-i\eta kv} \right) \quad k > 0 \]

\[ \eta = \frac{1 + u_s}{1 - u_s} \quad \text{like classical doppler shift} \]

\[ A_k = \frac{1}{\sqrt{4\pi k}} \]

\[ u = (t' - x') \quad v = (t' + x') \]

Simple guess: Take two massless modes, and add them up in the right way so that the boundary conditions are satisfied.
Quantization of momentum

• While the modes $v_{k}^{\pm,(n)}$, $u_{k}^{\pm}$ are complicated combinations of waves with different frequencies, in the lab frame, they are a single frequency in time.

\[ u_{k}^{\pm} = \frac{1}{\sqrt{2L(\eta_{R}k)}} \cos / \sin (\eta_{R}kx)e^{-i\eta_{R}kt} \]

\[ v_{k}^{\pm,(1)} = B_{k}(L) \cos / \sin (\gamma_{s}(k + u_{s}\omega_{k}^{'}))x e^{-\gamma_{s}(\omega_{k}^{'}+u_{s}k)t} \]

\[ v_{k}^{\pm,(2)} = C_{k}(L) \cos / \sin (\gamma_{s}(-k + u_{s}\omega_{k}^{'}))x e^{-\gamma_{s}(\omega_{k}^{'}-u_{s}k)t} \]

Quantization of $k$ comes from

\[ \partial_{x}\phi_{S/A}(x = L/2) = 0 \]
Quench in the boosted frame

• Assume initially \((t' < 0)\), the system resides in the ground state of the modes \(v_k^{+/-, (1)/(2)}\).

• Re-express old solutions in terms of new ones.

\[
\phi(x', t') = \sum_{\epsilon = \pm} \left( \sum_{k > 0} \left( b_k^{\epsilon,(1)} v_k^{\epsilon,(1)}(x', t') + b_k^{\epsilon,(1)\dagger} v_k^{\epsilon,(1)*}(x', t') \right) + \right.

\left. \sum_{k < k_0} \left( b_k^{\epsilon,(2)} v_k^{\epsilon,(2)}(x', t') + b_k^{\epsilon,(2)\dagger} v_k^{\epsilon,(2)*}(x', t') \right) \right)
\]

\[
\phi(x', t') = \sum_{\epsilon = \pm} \sum_k \left( a_k u_k^{\epsilon}(x', t') + a_k^{\epsilon\dagger} u_k^{\epsilon*}(x', t') \right).
\]
Quench in the boosted frame

\[ a_k^\pm = \sum_{n=1,2} \sum_{k'} (\alpha_{kk'}^\pm (n) b_{k'}^\pm (n) + \beta_{kk'}^\pm (n) b_{k'}^\pm (n) ) \]

\[ \beta_{kk'}^\pm (n) = -(u_k^\pm, v_{k'}^\pm (n)) \]

\[ \alpha_{kk'}^\pm (n) = (u_k^\pm, v_{k'}^\pm (n)^*) \]

\[ (u_1, u_2) = -ic \int_{x'=u_s, t'=0} dx' (u_1 \partial_t u_2^* - u_2^* \partial_t u_1) \]

\[ N_k^S = \sum_{k'} |\beta_{k,k'}^+ (1)|^2 + \sum_{k'<k_0} |\beta_{k,k'}^+ (2)|^2 \]

\[ N_k^A = \sum_{k'} |\beta_{k,k'}^- (1)|^2 + \sum_{k'<k_0} |\beta_{k,k'}^- (2)|^2 \]
Structure of correlations right after the splitting process is completed.

Faster splitting yields stronger cross correlations.
Chiral prethermalization

Faster splitting yields stronger cross correlations

1.5 ms  2.5 ms  3 ms  5 ms  7 ms

$\Delta T (T_{\text{eff}})$

$\text{time}$

$\text{splitting time } t_1 (\text{ms})$
Theory already needs to address interesting puzzles of quantum dynamics

Role of non-equilibrium processes in resonant XRay

Chiral prethermalization in non-uniformly split condensates