

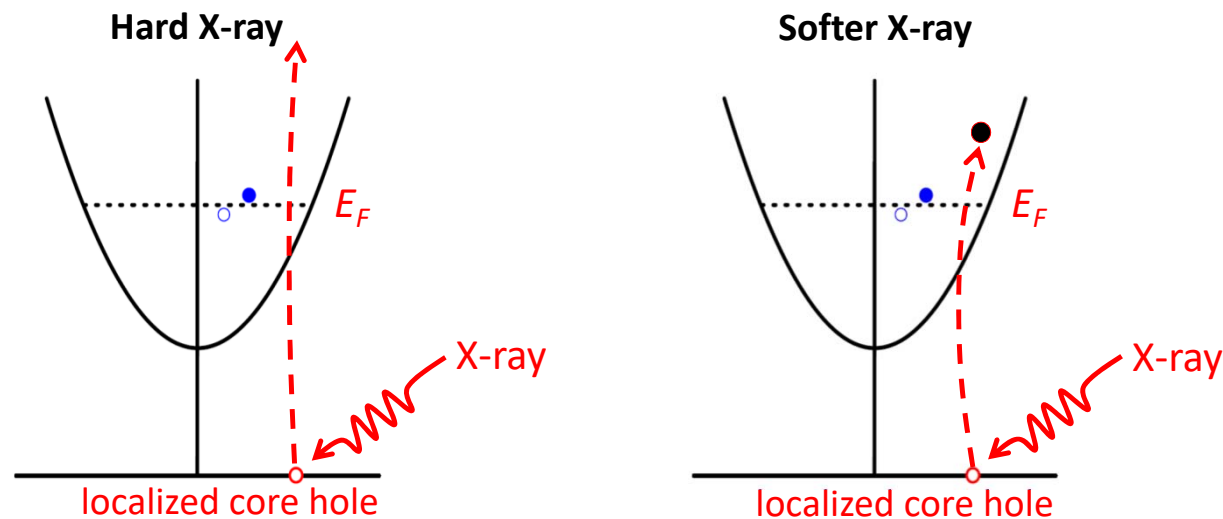
Orthogonality catastrophe in Coulomb systems

University of
Massachusetts
Amherst

Igor Tupitsyn and Nikolay Prokof'ev

SIMONS
FOUNDATION

A prototypical process leading to the Anderson orthogonality catastrophe problem is a sudden excitation of a core electron in an atom, as in the X-Ray absorption, leaving a hole in a deep core level:



Hard X-ray limit: electron leaves atom. **Softer X-ray limit:** electron remains in atom $\rightarrow$ RIXS, RSXS.

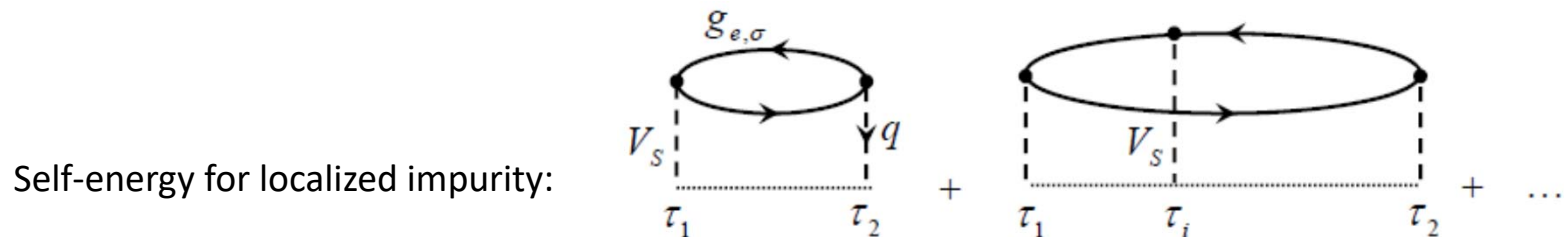
The localized core-hole acts in the same way as a heavy impurity in Anderson's formulation: its potential polarizes the surrounding vacuum by creating electron-hole pairs around the Fermi level. As predicted by Anderson, the overlap integral between the initial system's state, with no impurity, and the state with impurity decays. **Q: How it decays with time?**

CCQ - Flatiron Institute, 2019

Hard X-Ray limit: Orthogonality catastrophe

The standard approach to the solution (Nozieres and de Dominicis 1969) is based on two key assumptions:
(i) impurity potentials with finite cross-section and (ii) non-interacting fermions.

Scattering of non-interacting electrons and holes off the (short-range/contact) static impurity potential V_s :



$$I(t) = |\langle \Psi_f | \Psi_i \rangle|^2 \propto |t|^{-\gamma} \rightarrow 0; \quad \gamma = 2 \sum_l (2l+1) (\delta_l / \pi)^2 \quad (\delta_l \text{ is the scattering phase shift in the orbital channel } l).$$

γ is finite only if the scattering cross section is finite

Both approximations are highly inaccurate for problems involving charged particles in metals.

- (i) All interactions in metals are of the long-range Coulomb nature and Coulomb potential has infinite cross section;
- (ii) To screen impurity's potential one has to account for Coulomb interactions between the Fermi sea electrons.

Q. How the Orthogonality catastrophe scenario gets modified?

Outline

- Effect of dynamic screening of long-range Coulomb potential
- Plasmon effect
- Effect of finite impurity/hole mass

Orthogonality catastrophe in Coulomb systems

Dynamically screened long-range Coulomb potentials: Approach

One-loop diagrams are based on Taylor series expansion in powers of V_s . With integration/summation over all intermediate scattering events, one-loop contributions can be replaced with an equivalent bosonic propagator $\Phi(q, \tau_2 - \tau_1)$, leading to the hole/impurity Greens function in the form:

$$G(p, \tau) = \sum_{\text{topologies}} \left[\begin{array}{c} \text{Diagram with dashed arcs labeled } \Phi(q, \tau_2 - \tau_1) \text{ and } G_0 \\ \text{Diagram with dashed arcs labeled } \Phi(q, \tau_2 - \tau_1) \text{ and } G_0 \\ \text{Diagram with dashed arcs labeled } \Phi(q, \tau_2 - \tau_1) \text{ and } G_0 \end{array} \right] \Rightarrow$$

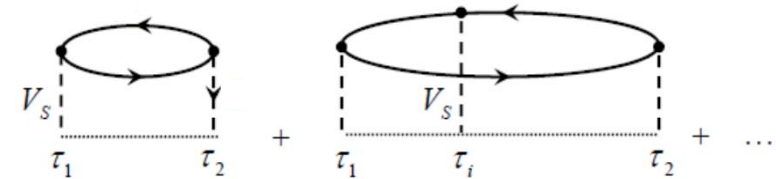
$$G_0(p, \tau) = e^{-(E-\mu)\tau}, \quad E = p^2/2M$$

Dynamic screening, perturbative r_s -- RPA ($V_C = 4\pi e^2/q^2$; $\Phi = W - V_C$):

$$\Phi(q, \tau_2 - \tau_1) = \begin{array}{c} \text{Diagram with } V_C \text{ and } \Pi \\ \text{Diagram with } V_C \text{ and } \Pi \\ \text{Diagram with } V_C \text{ and } \Pi \end{array} + \dots$$

$\Pi = G_e G_e$

Exact approach at perturbative values of Coulomb parameter r_s .



Obvious approach: polaron technique

$$G(p=0, \tau > 1/\varepsilon_F) = Z(\tau) e^{-(\varepsilon-\mu)\tau}$$

$$Z = |\langle \Psi_f | \Psi_i \rangle|^2$$

Localized impurity (infinite mass):

$$G(\tau) = \exp \left\{ - \int_0^\tau \int_0^{\tau_2} d\tau_1 d\tau_2 F(\tau_2 - \tau_1) \right\}$$

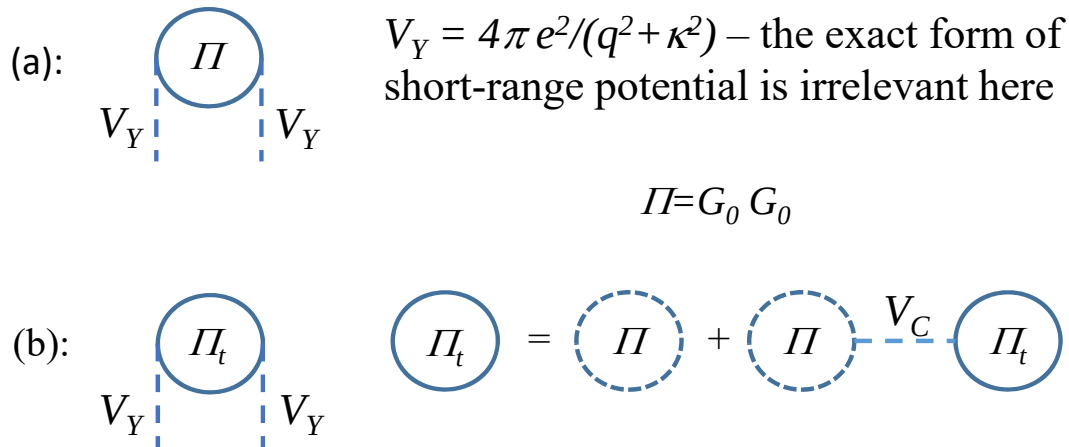
$$F(\tau_2 - \tau_1) = \int \frac{d\mathbf{q}}{(2\pi)^3} \Phi(\mathbf{q}, \tau_2 - \tau_1)$$

Orthogonality catastrophe in Coulomb systems

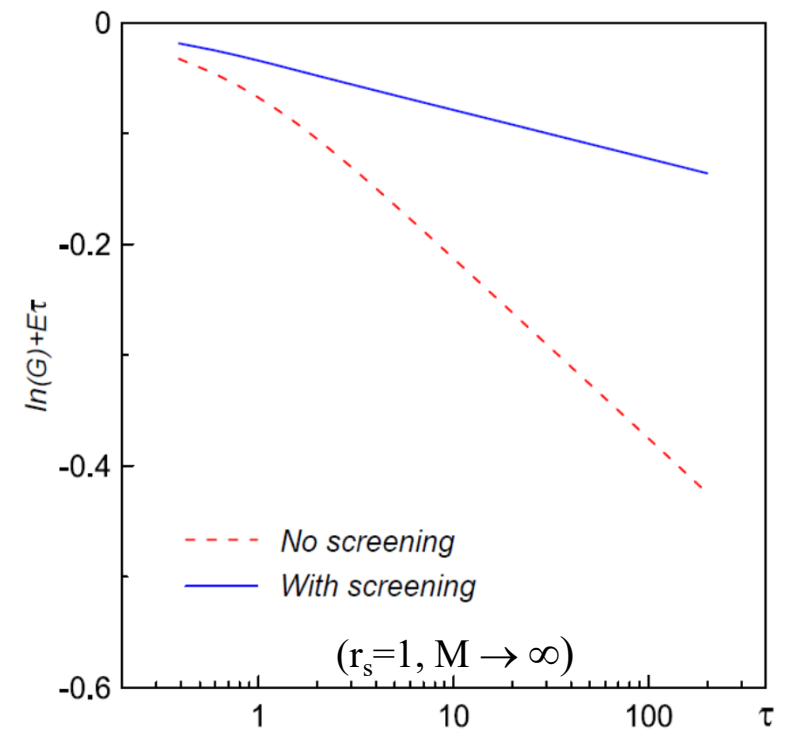
Effect of dynamic screening of long-range Coulomb potentials on OC

Q. To what degree the OC is modified by dynamic screening effects in metallic system?

Two versions of $\Phi(q, \tau_2 - \tau_1)$ – with (a) and without (b) screening:



Power-law decay of $Z(\tau)$ at $\tau \gg 1/\varepsilon$ remains, but dynamic screening leads to much weaker decay than in the non-interacting Fermi-sea case.



This clearly demonstrates that residual interactions between quasiparticles in the metallic Fermi-liquid regime cannot be neglected.

Orthogonality catastrophe in Coulomb systems

Plasmon effect

Screening of the Coulomb potential leads to collective (gapped) plasmon excitations at small momenta. Correspondingly, $\Phi(\mathbf{q}, \tau_2 - \tau_1)$ features a plasmon pole. The plasmon pole approximation satisfies two limiting cases:

(1) at $\omega=0$ and small momentum potential has Yukawa form and

$$\varepsilon^{-1} - 1 = -\frac{\kappa^2}{q^2 + \kappa^2}$$

(2) at $q=0$ and small frequency dielectric function features a zero at ω_p ;

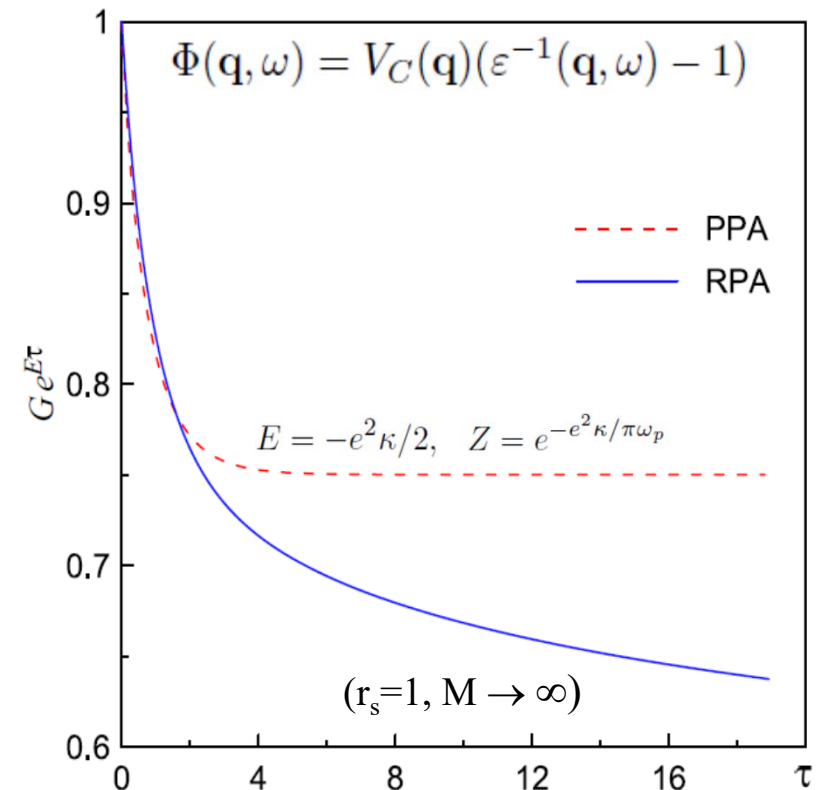
$$\varepsilon^{-1} - 1 = \frac{\omega_p^2}{\omega^2 - \omega_p^2}$$

PPA:

$$\Phi(\mathbf{q}, \omega) = \frac{4\pi e^2}{q^2} \frac{\omega_p^2}{\omega^2 - \omega_p^2(1 + q^2/\kappa^2)}$$

PPA accounts only for gapped (plasmon) modes and eliminates OC. RPA accounts for both gapped and gapless (electron-hole pairs) modes and preserves OC since the power-law decay originates from gapless low-energy excitations.

In proper treatment plasmons essentially reduce but do not eliminate the power-law in time decay of $Z(t)$.



Orthogonality catastrophe in Coulomb systems

OC in metals and effect of finite impurity mass

Full $\Phi(q, \tau_2 - \tau_1)$ case: Dynamically screened Coulomb potentials

Infinite M:

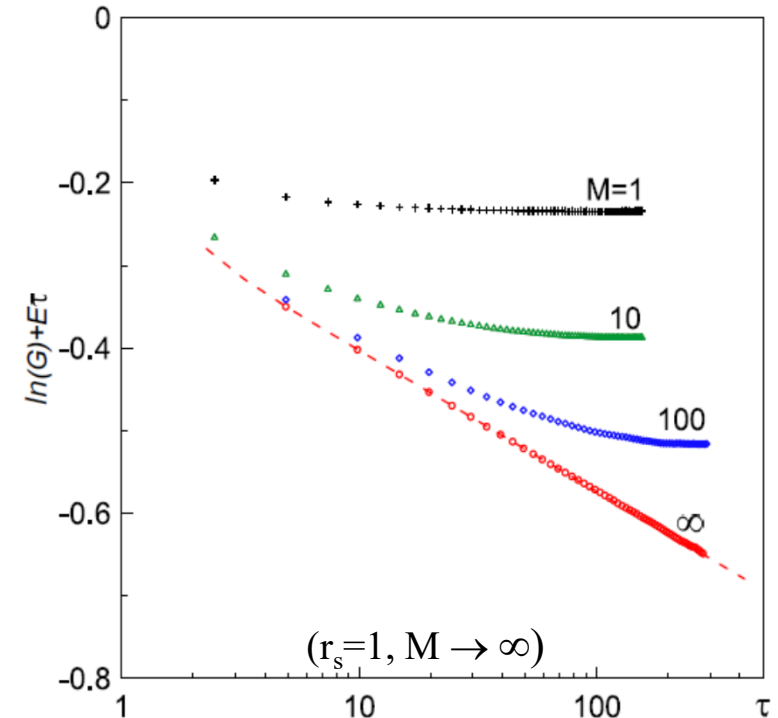
$$G(\tau) = \exp \left\{ - \int_0^\tau \int_0^{\tau_2} d\tau_1 d\tau_2 F(\tau_2 - \tau_1) \right\}$$

$$F(\tau_2 - \tau_1) = \int \frac{d\mathbf{q}}{(2\pi)^3} \Phi(\mathbf{q}, \tau_2 - \tau_1)$$

Finite M:

Polaron Diagrammatic Monte Carlo

Recoil effects for finite mass eliminate OC for light particles and shrinks the domain of power-law decay for heavier ones.



Conclusions: (i) In Coulomb systems the OC retains its universal power-law form, but exponent γ is very sensitive to screening effects. (ii) For dynamically screened Coulomb potential the value of γ is larger than that for often used static Yukawa potential in non-interacting case. (iii) For short-range potentials screening dramatically decrease γ .

[I. Tupitsyn and N. Prokof'ev, Phys. Rev. B 99, 245122, (2019)]