What Happens Inside a Unit Cell Matters -Effects of Umklapp Processes on Correlated Materials

Wei-Cheng Lee
Department of Physics, Applied Physics, and Astronomy,
Binghamton University – SUNY

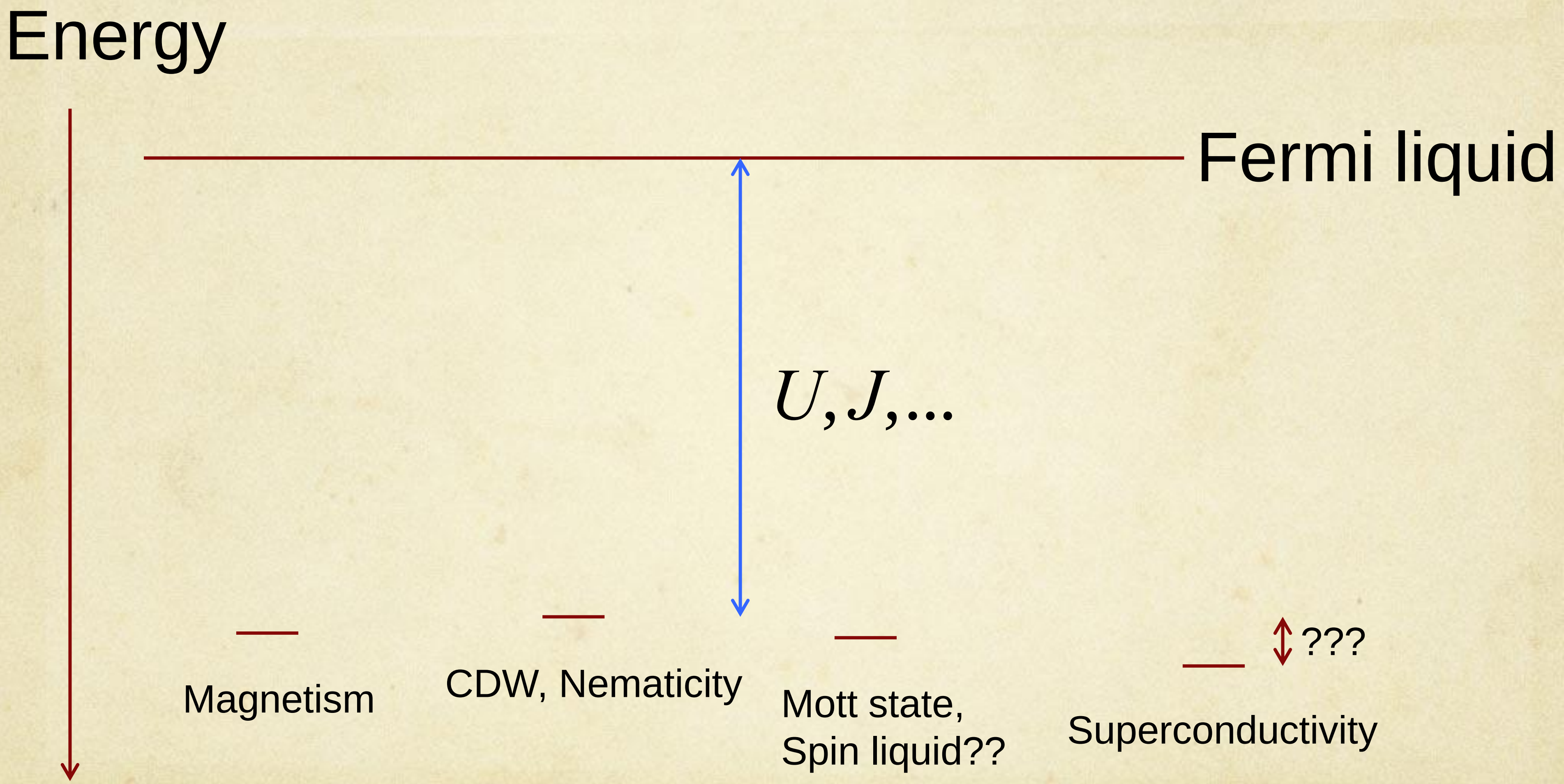
Almost always, the creative dedicated minority has made the world better.

- Martin Luther King, Jr.

Energy Scale (Per Site)

Local charge interaction	$U \sim 1-10eV$
Bandwidth	$W \sim 1-2eV$
Local spin interaction	$J \sim 100-400meV$
Superconducting gap	$D \sim 5-30meV$
Superconducting condensate energy	$<1meV$

Difference Matters



Is it enough to simply look at the interaction with largest energy scale?

Energetic Consideration

- Chester, Phys. Rev. **103**, 1693 (1956)

$$\langle \hat{H} \rangle = \langle \hat{K} \rangle + \langle \hat{V} \rangle = \frac{1}{2}\langle \hat{V} \rangle \ , \ \langle \hat{K} \rangle = -\frac{1}{2}\langle \hat{V} \rangle \ \text{(Virial Theorem)}$$

$$E_{cond} = \langle \hat{H} \rangle_N - \langle \hat{H} \rangle_S > 0 \Rightarrow \langle \hat{V} \rangle_s < \langle \hat{V} \rangle_N$$

- Leggett's extension:

$$\hat{V} = \frac{1}{2}\frac{1}{4\pi\varepsilon_0}\sum_{ij}\frac{e^2}{\varepsilon\left|\vec{r}_i - \vec{r}_j\right|} \ + \ \ldots \ , \quad \varepsilon = \text{dielectric constant renormalized by the ionic cores}$$

If ε is the only parameter that can change,

$$\frac{\partial E_{cond}}{\partial \varepsilon} = \left\langle \frac{\partial \hat{V}}{\partial \varepsilon} \right\rangle_N - \left\langle \frac{\partial \hat{V}}{\partial \varepsilon} \right\rangle_s = -\frac{1}{\varepsilon}\left(\langle \hat{V} \rangle_N - \langle \hat{V} \rangle_S\right)$$

$$\boxed{if \quad e = e_0 \qquad \left(\langle \hat{V} \rangle_N - \langle \hat{V} \rangle_S\right) > 0}$$

$$E_{cond} > 0, e < e_0$$

**Smaller ε (stronger Coulomb interactio
the stronger superconductivity!!!**

Short Range Coulomb Interaction (Majority)

Strongly correlated systems

Electrons need to rearrange themselves locally to compromise the short range interaction

‘Extended’ description, e.g., band structure description, is likely breaking down and new phases like AFM, CDW, Mottness, etc. can emerge.

How can superconductivity, a delocalized state, comprise the short range interaction??

Savings of Short Range Part of Coulomb Energy (Large *q*)

- Coulomb Energy:

$$H_{Coul} = \frac{1}{2\Omega}\sum_{q\neq 0} U_q \hat{\rho}_q \hat{\rho}_{-q} \equiv \frac{1}{2\Omega}\sum_{q\neq 0} \hat{V}_q \quad , \quad \hat{\rho}_q = \sum_{k,\sigma} c^{+}_{k-q,\sigma} c_{k,\sigma}$$

$$U_q^{3D} = \frac{e^2}{\varepsilon_0 \varepsilon_\infty q^2} \quad , \quad U_q^{2D} = \frac{e^2}{2\varepsilon_0 \varepsilon_\infty q}$$

- Superconducting condensation energy in this region:

$$E_C(\delta\langle \hat{V}_q \rangle) = U_q \langle \hat{\rho}_q \hat{\rho}_{-q} \rangle_N - U_q \langle \hat{\rho}_q \hat{\rho}_{-q} \rangle_S \approx -U_q \sum_k \Delta^*_{k+\frac{q}{2}} \Delta_{k-\frac{q}{2}}$$

- Short Range Part of Coulomb Energy can be saved in superconducting state by sign-changing gap function (for example, d-wave in cuprates)

What about long-range Coulomb Energy? (Minority)

Some Arguments Against the Long Range Coulomb Energy

- Screening??
  - 3D → Yes, screening is effective.
  - 2D → Not necessary!!!

- Anderson's theory (Phys. Rev. 110, 827(1958), Phys. Rev. 112, 1900(1958))

	Stability of BCS state	f-sum rule
BCS Hamiltonian	○	⊘
+ long range Coulomb	?	○
Anderson's theory	○	○

No change in long range Coulomb energy because plasmon is immortal a

Anderson's Theory

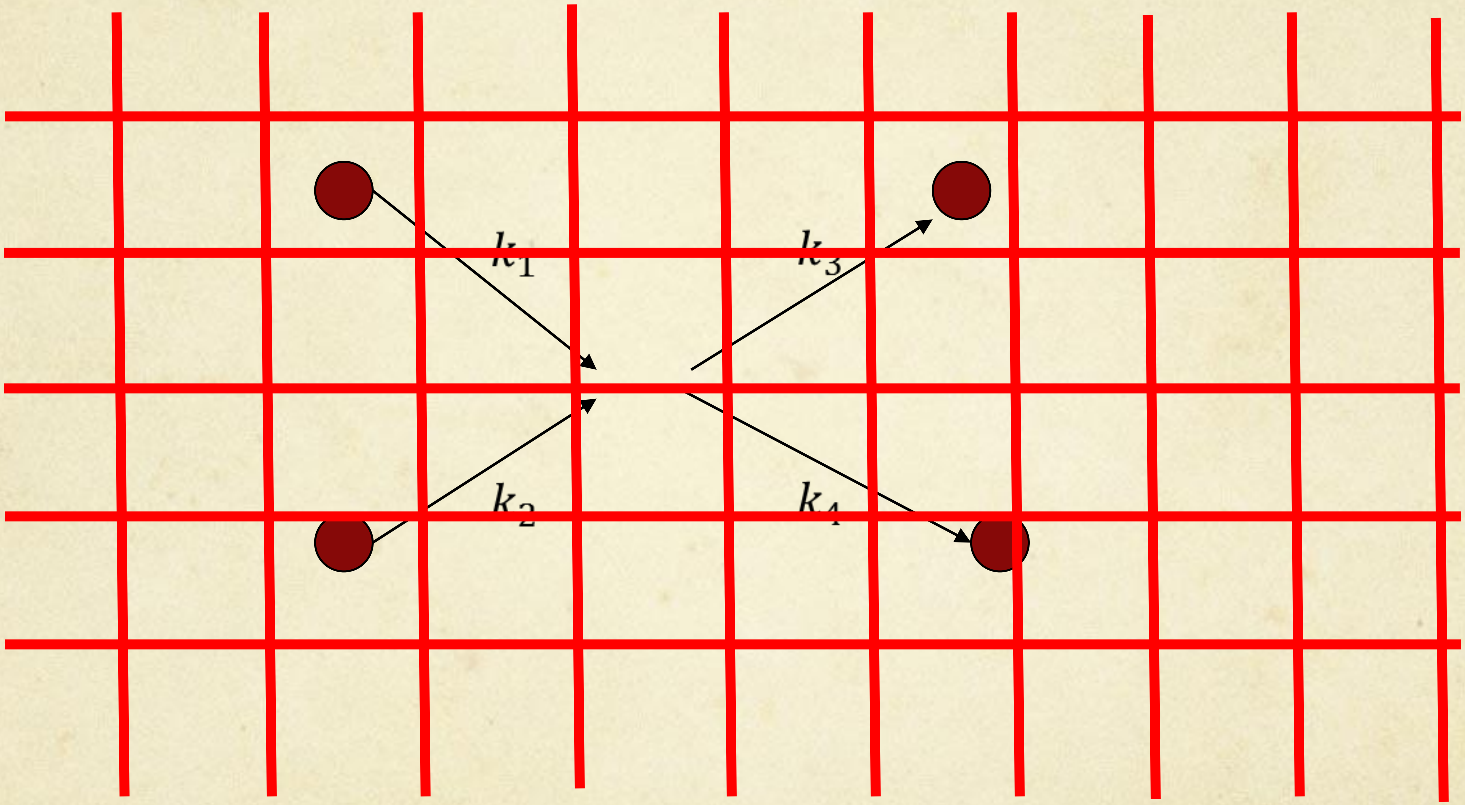
$$\left\langle \hat{V}_q \right\rangle = \frac{1}{2\pi} \int d\omega U_q \left\langle \widehat{\rho}_q(\omega) \widehat{\rho}_{-q}(\omega) \right\rangle = \frac{1}{2\pi} \int d\omega U_q \operatorname{Im} \chi\left(q, \omega\right)$$

at small q $\quad \operatorname{Im} \chi\left(q,\omega\right) \sim \pi\hbar\omega_p \delta(\omega - \omega_p)$

$$\left\langle \hat{V}_q \right\rangle = \frac{\hbar\omega_p}{2} + O(q^2)$$ **For any states**

No superconducting condensate energy can be obtained fron

Unconventional Superconductors are mostly built on 2D Lattice!!!



$$k_1 + k_2 + k_3 + k_4 = \boldsymbol{nK}$$

(another minority)

Role of Umklapp Scattering I → Sum Rule Analysis

- Rigorous sum rules for density-density response function:

$$J_{-1} \equiv \frac{2}{\pi}\int_0^\infty d\omega \frac{\operatorname{Im}\chi(q,\omega)}{\omega} = \chi(q,\omega=0) \quad \text{KK relation}$$

$$J_1 \equiv \frac{2}{\pi}\int_0^\infty d\omega\omega \operatorname{Im}\chi(q,\omega) = \frac{nq^2}{m} \quad \text{f - sum rule}$$

$$J_3 \equiv \frac{2}{\pi}\int_0^\infty d\omega\omega^3 \operatorname{Im}\chi(q,\omega) = \quad q^4 \frac{n^2}{m^2}\left\langle V_q \right\rangle + o(q^4)$$

- Applying Cauchy-Schwartz inequalities places limits on the Coulomb Energy at small q

$$\frac{\hbar\omega_p}{2} + o(q^2) \geq \left\langle V_q \right\rangle \geq \frac{\hbar\omega_p}{2} + o(q^2)$$

M. Turlakov and A.J. Leggett, Phys. Rev. B 67, 044517 (2003)

Proc. Natl. Acad. Sci. USA
Vol. 96, pp. 8365–8372, July 1999
Physics

This contribution is part of a special series of Inaugural Articles by members of the National Academy of Sciences elected April 29, 1997.

A "midinfrared" scenario for cuprate superconductivity

A. J. LEGGETT[a]

Department of Physics, University of Illinois, 1110 West Green Street, Urbana, IL 61801, and Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106

$\Delta\langle V_q\rangle$ *is comparable to superconducting condensate energy*!!!

Take Away Message – Two Minorities Make A Difference?

Without periodic potential, plasmon mode is IMMORTAL at small q.

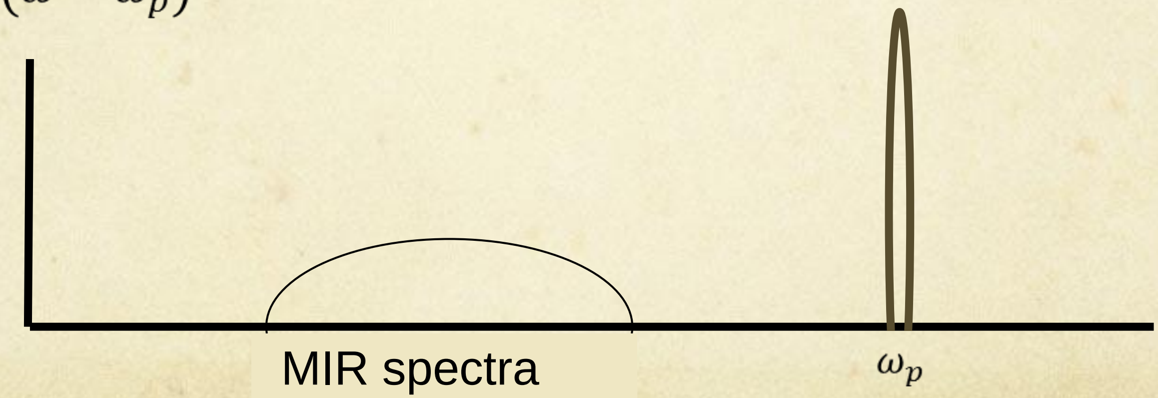
$$Im\chi(q,\omega)\sim\delta(\omega-\omega_p) \qquad \Delta\left\langle \hat{V}_q \right\rangle = 0 + O(q^2)$$

With periodic potential (Umklapp scattering), plasmon mode is no longer IMMORTAL at small q.

$$J_1 \equiv \frac{2}{\pi}\int_0^\infty d\omega\,\omega\,\mathrm{Im}\,\chi(q,\omega) = \frac{nq^2}{m} \quad \text{f-sum rule}$$

$$Im\chi(q,\omega) \neq \delta(\omega-\omega_p)$$

$$=$$



$$\left\langle \hat{V}_q \right\rangle = \frac{1}{2\pi} U_q \int d\omega\,\mathrm{Im}\,\chi\left(q,\omega\right)$$

Could be reduced if the spectrum in MIR is red

Microscopic theory of the density-density correlation function with Umklapp process

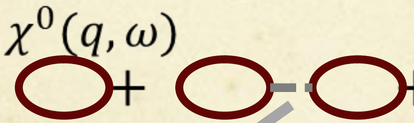
Warm Up – Plasmon Excitation in Fermi Liquid

$$\chi(q, t - t') = -i\langle T_t\, \rho_q(t)\rho_q^+(t')\rangle$$

$$\rho_q = \sum_{k,\sigma} c^+_{k+q,\sigma} c_{k,\sigma}$$

Random phase approximation (RPA)

$$\chi^{RPA}(q,\omega) =$$



$$+ \cdots = \frac{\chi^0(q,\omega)}{1 - v_q \chi^0(q,\omega)}$$

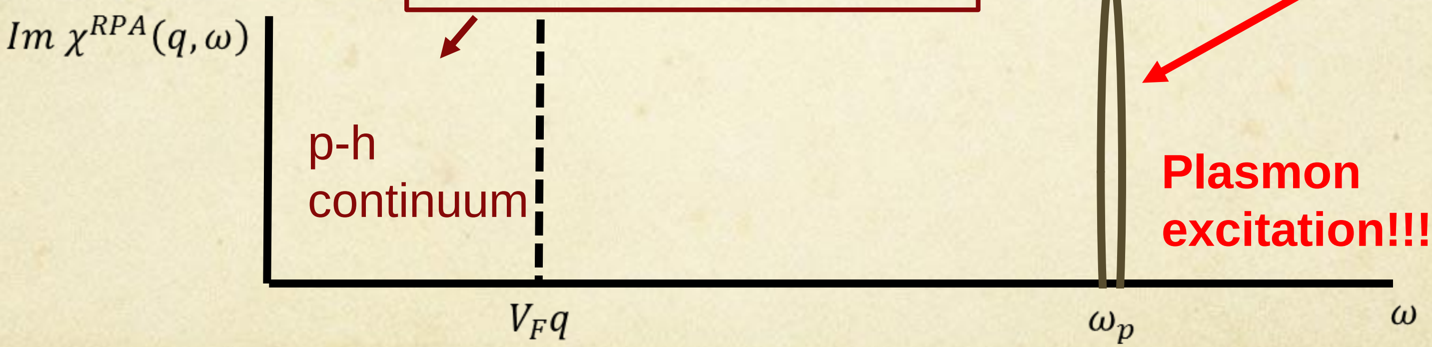
$$v_q = \frac{e^2}{4\pi\epsilon q}\ (2D)$$

Warm Up – Plasmon Excitation in Fermi Liquid

$$\chi^0(q,\omega) = \sum_k \frac{n_F(E(k+q)-\mu) - n_F(E(k)-\mu)}{\omega + E(k) - E(k+q)}$$

$$\chi^{RPA}(q,\omega) = \frac{\chi^0(q,\omega)}{1 - v_q\chi^0(q,\omega)}$$

$$Im\,\chi^{RPA}(q,\omega) = \boxed{Re\left(\frac{1}{1-v_q\chi^0(q,\omega)}\right) Im\chi^0(q,\omega)} + \boxed{Re\chi^0(q,\omega) Im\left(\frac{1}{1-v_q\chi^0(q,\omega)}\right)}$$



Periodic Potential

$$H = \sum_{k\sigma} \frac{\hbar^2 k^2}{2m} c_{k\sigma}^{+} c_{k\sigma} + \sum_{q} V_q \rho_q \rho_{-q} + \sum_{K} \sum_{k\sigma} U_K c_{k\sigma}^{+} c_{k+K\sigma} + h.c.$$

$$\chi^0(q,\omega) = \sum_{k} \frac{n_F(E(k+q)-\mu) - n_F(E(k)-\mu)}{\omega + E(k) - E(k+q)}$$

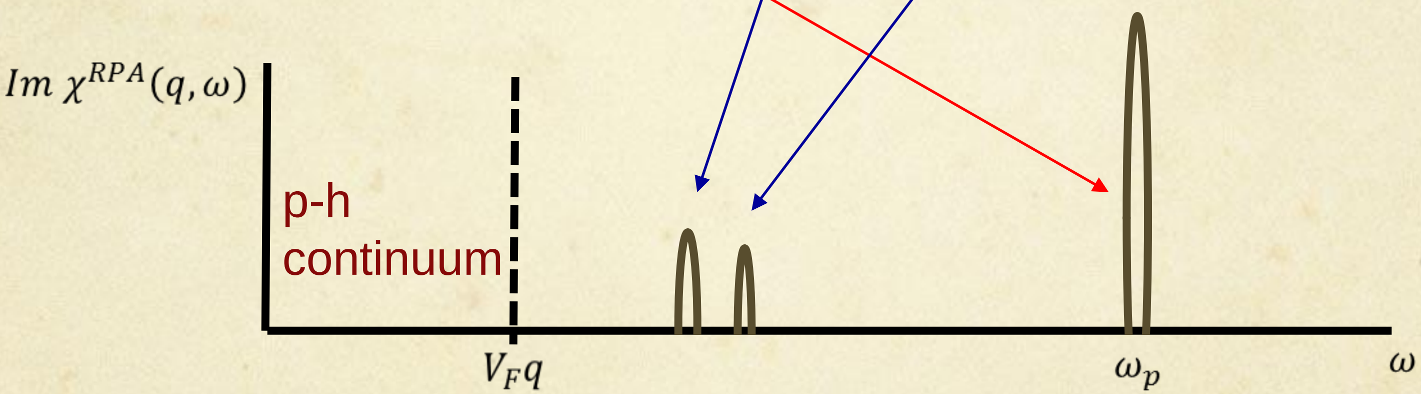
$$\chi^{RPA}(q,\omega) = \frac{\chi^0(q,\omega)}{1 - v_q \chi^0(q,\omega)}$$

$E(k+K) = E(k) \rightarrow \ \chi^0(q+K,\omega), \chi^0(q,\omega)$ both have p-h continuum ~ q

$\chi(q+nK, q+mK, \omega) \neq 0 \rightarrow Umklapp\ scattering$!!!

Generalized RPA with Umklapp Processes

$$\hat{\chi}^{-1} = \begin{bmatrix} \chi^0(q,q,\omega) & \chi^0(q+K,q,\omega) & \cdots \\ \chi^0(q,q+K,\omega) & \chi^0(q+K,q+K,\omega) & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}^{-1} - \hat{V}$$

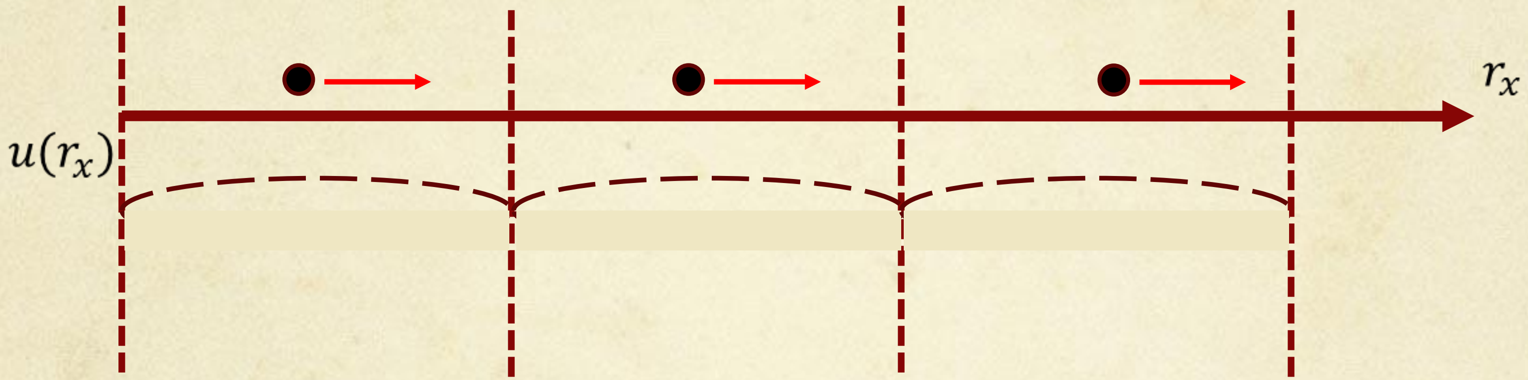


New spectral weight in Mid Infrared region appears due to the Umklapp process!!!

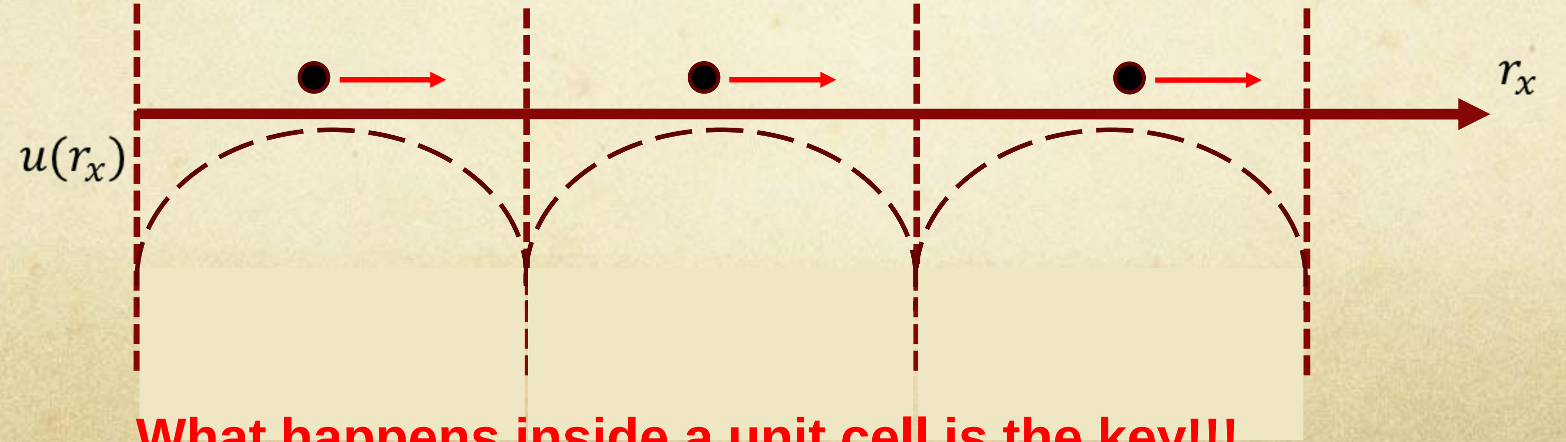
Why Plasmon Loses Spectral Weight?

$$\psi_{nk}(r) = e^{ikr} u_n(r)$$

(a) No Umklapp process

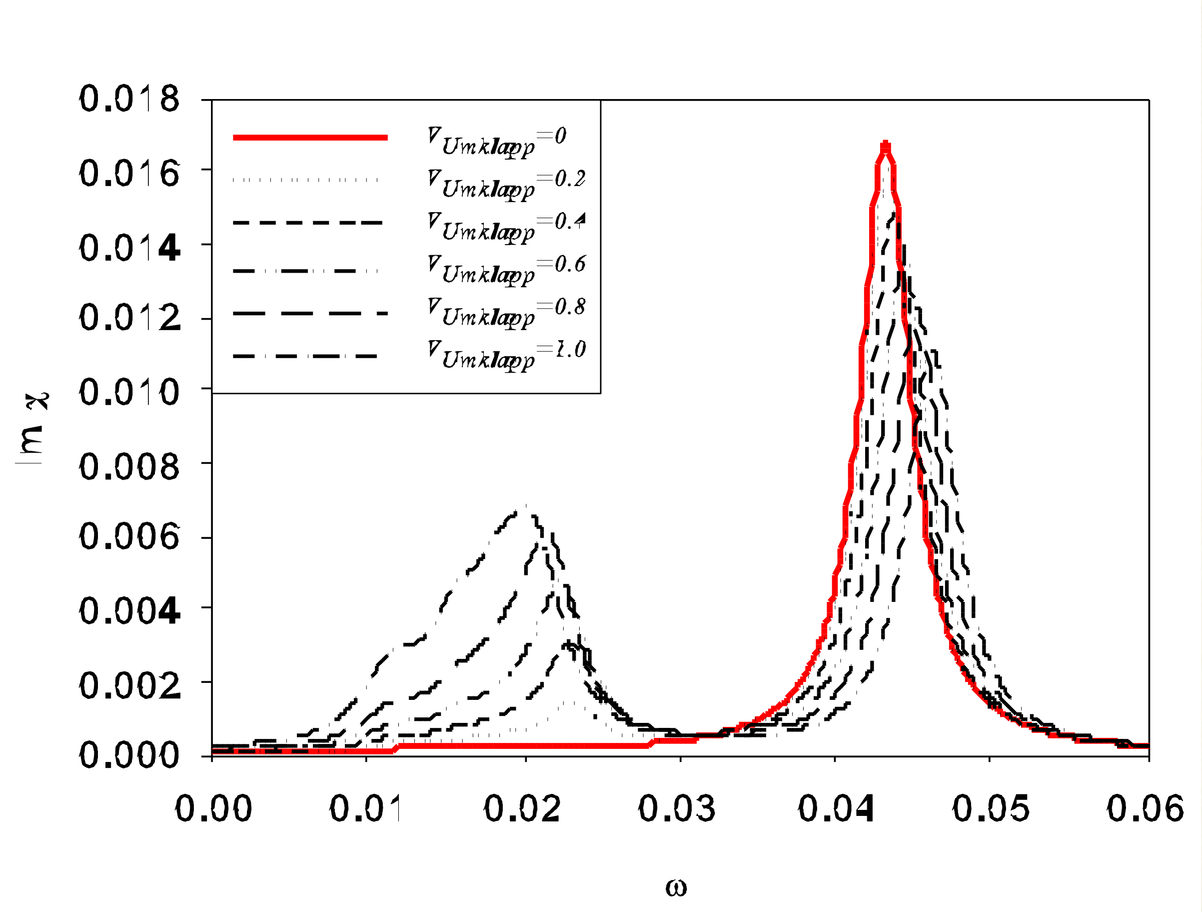


(b) With Umklapp process



What happens inside a unit cell is the key!!!

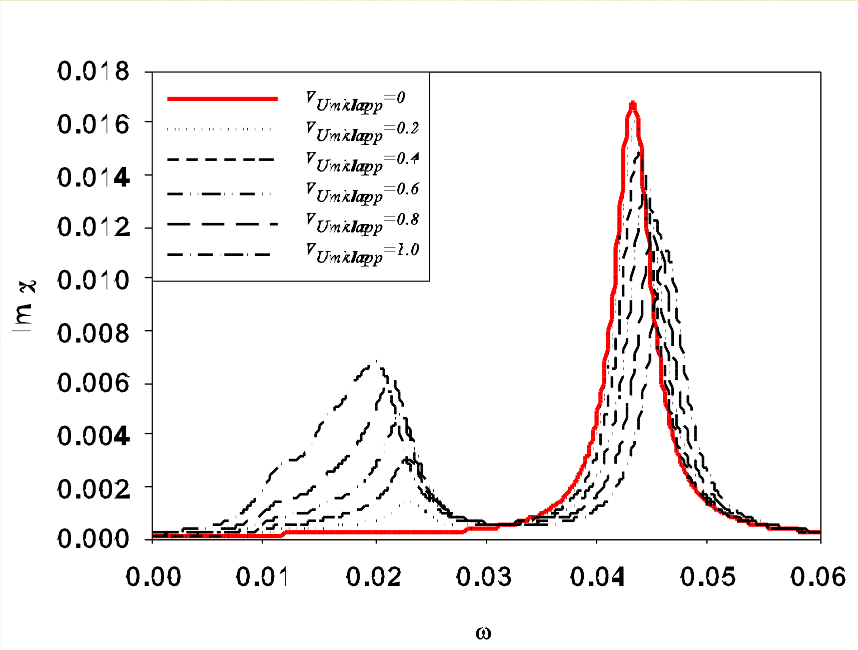
Calculations



To obtain a truly broad spectrum, we need to go beyond RPA. Solving quantum Boltzmann equations can do the trick.

Why Superconductivity Can Take Advantage?

Because it is not local and gapped, it has much less Umklapp scattering!!!



Umklapp scattering → Mid Infrared peaks →increase long-ranged Coulomb energy

Superconductivity suppresses Umklapp scattering → Mid Infrared peaks reduced→ long-ranged Coulomb energy decreased!!!

Predictions

As getting into the superconducting state,

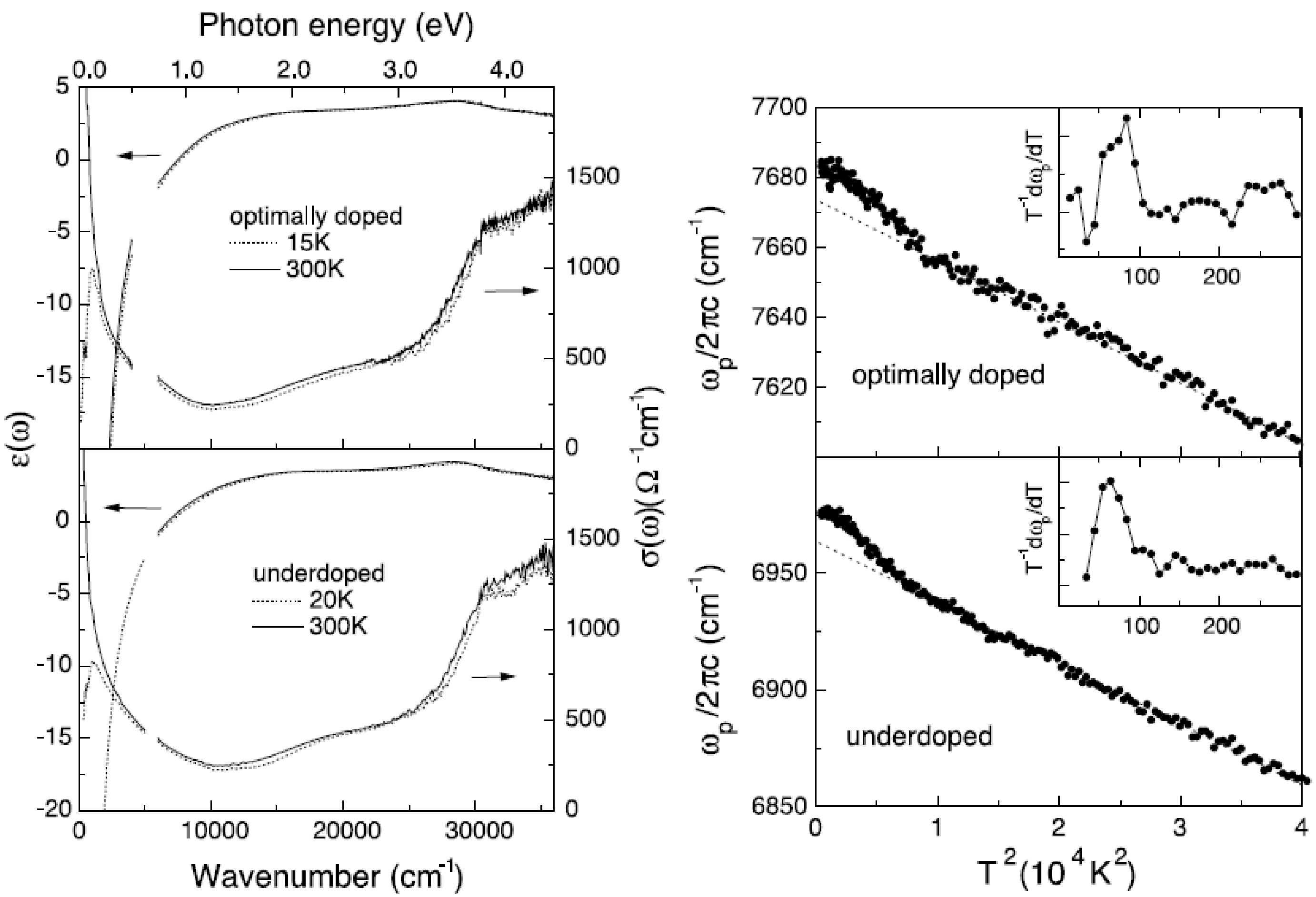
Broad spectrum in MIR region $\downarrow$

Plasmon frequency $\downarrow$

Can be verified ideally by EELS, or indirectly by optical conductivity!!!

Experimental Observation in Cuprates

Fig. 1 (left). Dielectric function $\varepsilon(\omega)$ and optical conductivity $\sigma(\omega)$ of optimally doped (top) and underdoped (bottom) $Bi_2Sr_2CaCu_2O_{8-\delta}$ versus photon energy in the superconducting state and at 300 K. **Fig. 2 (right).** Temperature dependence of the screened plasma frequency ω_p for optimally doped (top) and underdoped (bottom) $Bi_2Sr_2CaCu_2O_{8-\delta}$. **(Insets)** Derivatives $T^{-1}d\omega_p/dT$.



Mole graaf, et. al., Science **295**, 2239 (2002)

Experimental Observations in Iron Pnictides

ARTICLE

Received 15 Sep 2010 | Accepted 2 Feb 2011 | Published 1 Mar 2011

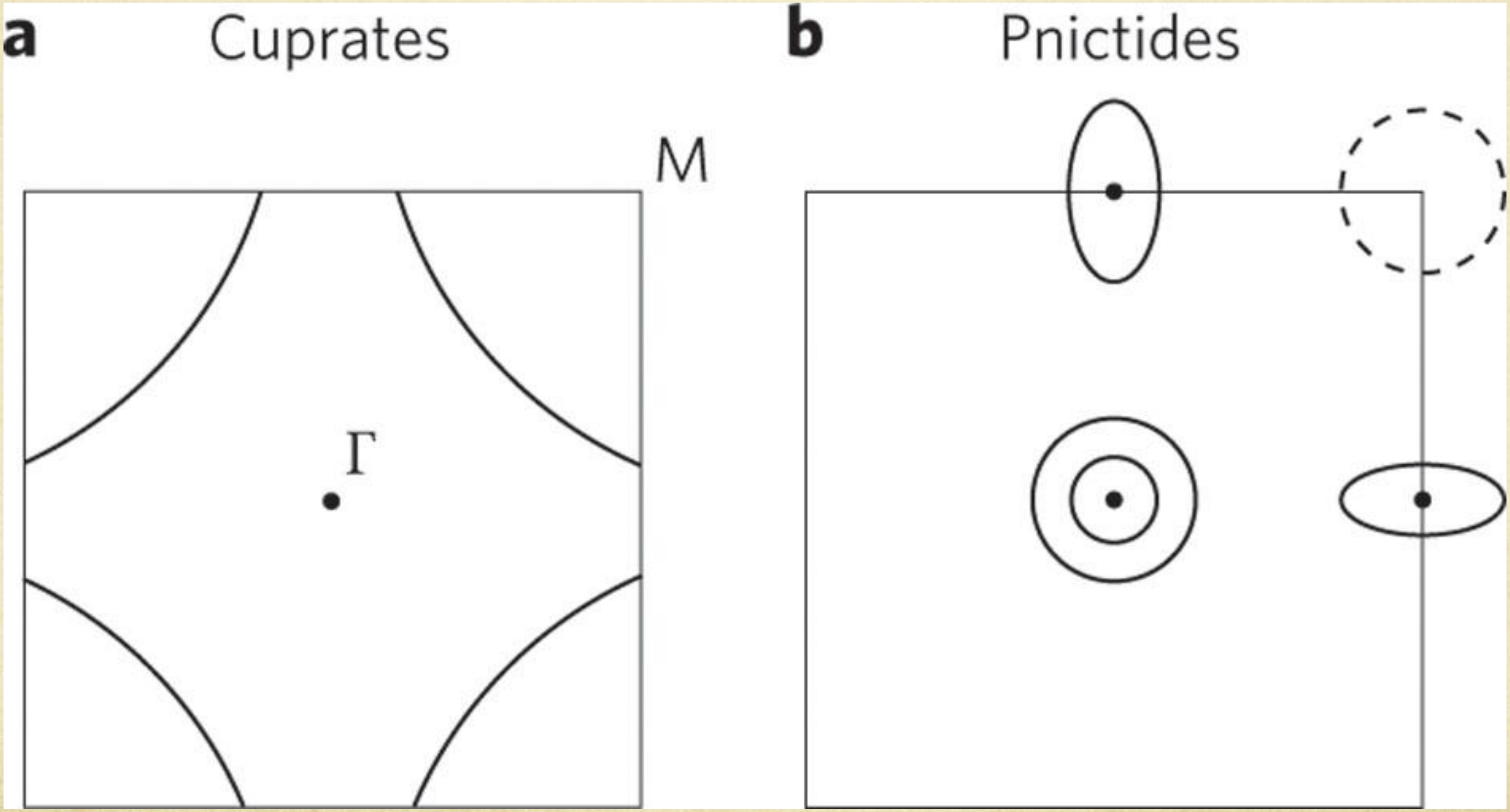
DOI: 10.1038/ncomms1223

Superconductivity-induced optical anomaly in an iron arsenide

A. Charnukha[1], P. Popovich[1], Y. Matiks[1], D. L. Sun[1], C. T. Lin[1], A. N. Yaresko[1], B. Keimer[1] & A. V. Boris[1,2]

One of the central tenets of conventional theories of superconductivity, including most models proposed for the recently discovered iron-pnictide superconductors, is the notion that only electronic excitations with energies comparable to the superconducting energy gap are affected by the transition. Here, we report the results of a comprehensive spectroscopic ellipsometry study of a high-quality crystal of superconducting $Ba_{0.68}K_{0.32}Fe_2As_2$ that challenges this notion. We observe a superconductivity-induced suppression of an absorption band at an energy of 2.5 eV, two orders of magnitude above the superconducting gap energy $2\Delta \approx 20$ meV. On the basis of density functional calculations, this band can be assigned to transitions from As-p to Fe-d orbitals crossing the Fermi level. We identify a related effect at the spin-density wave transition in parent compounds of the 122 family. This suggests that As-p states deep below the Fermi level contribute to the formation of the superconducting and spin-density wave states in the iron arsenides.

Fermi Surface Consideration



Umklapp scattering also affects pairing interaction

PHYSICAL REVIEW B, VOLUME 63, 035109

Breakdown of the Landau-Fermi liquid in two dimensions due to umklapp scattering

C. Honerkamp,[1] M. Salmhofer,[2] N. Furukawa,[1,3] and T. M. Rice[1]
[1]*Theoretische Physik, ETH-Hönggerberg, CH-8093 Zürich, Switzerland*
[2]*Mathematik, ETH Zentrum, CH-8092 Zürich, Switzerland*
[3]*Department of Physics, Aoyama Gakuin University, Setagaya, Tokyo 157-8572, Japan**
(Received 23 December 1999; published 2 January 2001)

We study the renormalization-group (RG) flow of interactions in the two-dimensional t-t' Hubbard model near half-filling in an N-patch representation of the whole Fermi surface. Starting from weak to intermediate couplings the flows are to strong coupling, with different characters depending on the choice of parameters. In a large parameter region elastic umklapp scatterings drive an instability which on parts of the Fermi surface exhibits the key signatures of an insulating spin liquid (ISL), as proposed by Furukawa, Rice, and Salmhofer [Phys. Rev. Lett. **81**, 3195 (1998)] rather than a conventional symmetry-broken state. The ISL is characterized by both strong d-wave pairing and antiferromagnetic correlations; however, it is insulating due to the vanishing local charge compressibility and a spin liquid because of the spin gap arising from the pairing correlations. We find that the unusual RG flow, which we interpret in terms of an ISL, is a consequence of a Fermi surface close to the saddle points at the Brillouin-zone boundaries which provides an intrinsic and mutually reinforcing coupling between pairing and umklapp channels.

Optical Conductivity s and DC Resistivity

	Fermi liquid	Non-Fermi liquid
Electron self-energy	$S \sim aT^2 + bw^2$	$S \sim aT^a + bw^a$
Momentum relaxing mechanism	Impurity, Umklapp	Impurity, Umklapp
		??????
	$DC \sim T^2$	$DC \sim T^a$
	$s \sim a'T^2 + b'w^2$	$s \sim a'T^a + b'w^a$

Published for SISSA by Springer

Received: June 12, 2012
Accepted: July 16, 2012
Published: July 27, 2012

Optical conductivity with holographic lattices

Gary T. Horowitz,[a] Jorge E. Santos[a] and David Tong[b]

[a] *Department of Physics, UCSB, Santa Barbara, CA 93106, U.S.A.*
[b] *DAMTP, University of Cambridge, Cambridge, CB3 0WA, U.K.*

E-mail: gary@physics.ucsb.edu, jss55@physics.ucsb.ed, d.tong@damtp.cam.ac.uk

Abstract: We add a gravitational background lattice to the simplest holographic model of matter at finite density and calculate the optical conductivity. With the lattice, the zero frequency delta function found in previous calculations (resulting from translation invariance) is broadened and the DC conductivity is finite. The optical conductivity exhibits a Drude peak with a cross-over to power-law behavior at higher frequencies. Surprisingly, these results bear a strong resemblance to the properties of some of the cuprates.

Keywords: AdS-CFT Correspondence, Holography and condensed matter physics (AdS/CMT)

ArXiv ePrint: 1204.0519

Final Remarks

Why Umklapp process is important in correlated materials?

- All correlated materials are crystalline
- Momentum relaxing mechanism is crucial for optical conductivity and DC resistivity.
- Long-range Coulomb energy is allowed to be variant.

Why superconductivity is so competitive?

- Short-range Coulomb energy saved by sign-changing gap
- Long-range Coulomb energy saved by reducing Umklapp process regardless gap symmetry

Much more efforts should be spent on changes due to superconductivity on optical conductivity, electron energy loss spectroscopy (EELS) (Peter Abbamonte at UIUC)!!!