Raman Scattering through a quantum-critical point

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Funding: National Science Foundation (US)
National Science and Engineering Research Council (Canada)
Thanks to: Paul Miller and Andrij Shvaika

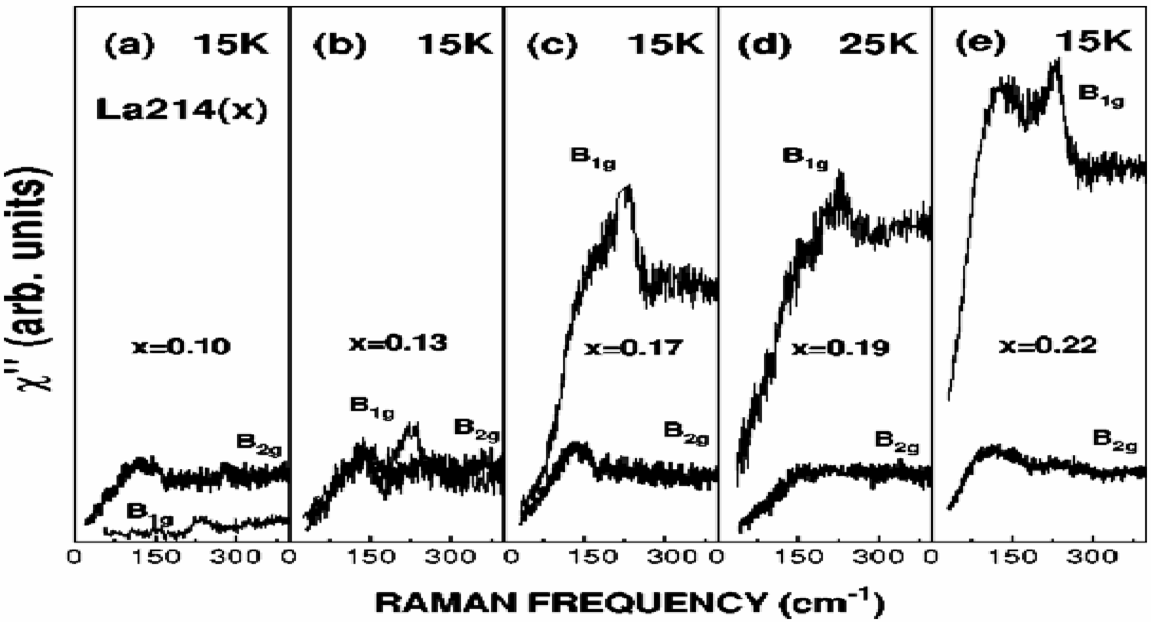
Raman scattering probes electronic excitations

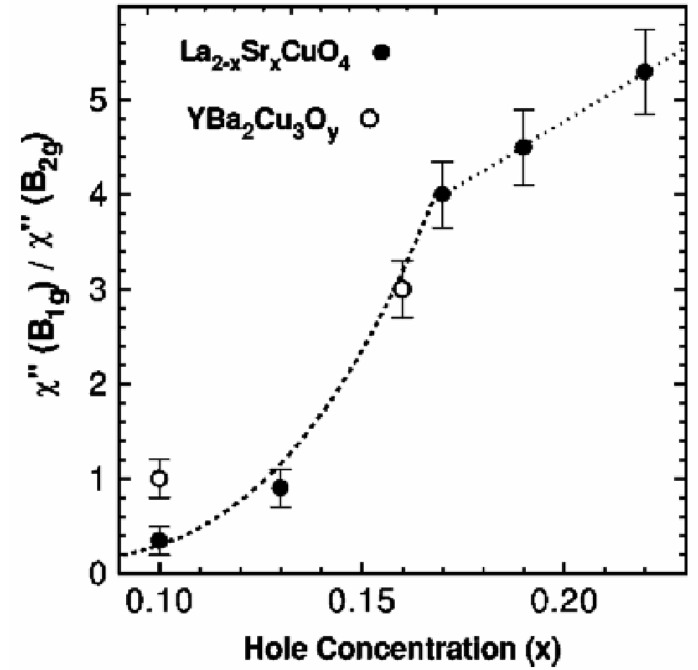
- Inelastic scattering of light with electron-hole excitations of the correlated many-body system.
- Use of polarizers for the incoming and reflected light allows one to **select different symmetries** of the electron-hole excitations.
- Signal depends on the Raman scattering amplitude $\boldsymbol{\gamma(k)}$. We consider three different symmetries here:
- A_{1g}: $\gamma(k) \sim \mathbf{C}+\cos(k_x a)+\cos(k_y a)$
- B_{1g}: $\gamma(k) \sim \cos(k_x a)-\cos(k_y a)$
- B_{2g}: $\gamma(k) \sim \sin(k_x a)\sin(k_y a)$

Review of Raman Data for the Cuprates

Normal state at low frequencies:

J. G. Naeini *et al*., PRB 1999

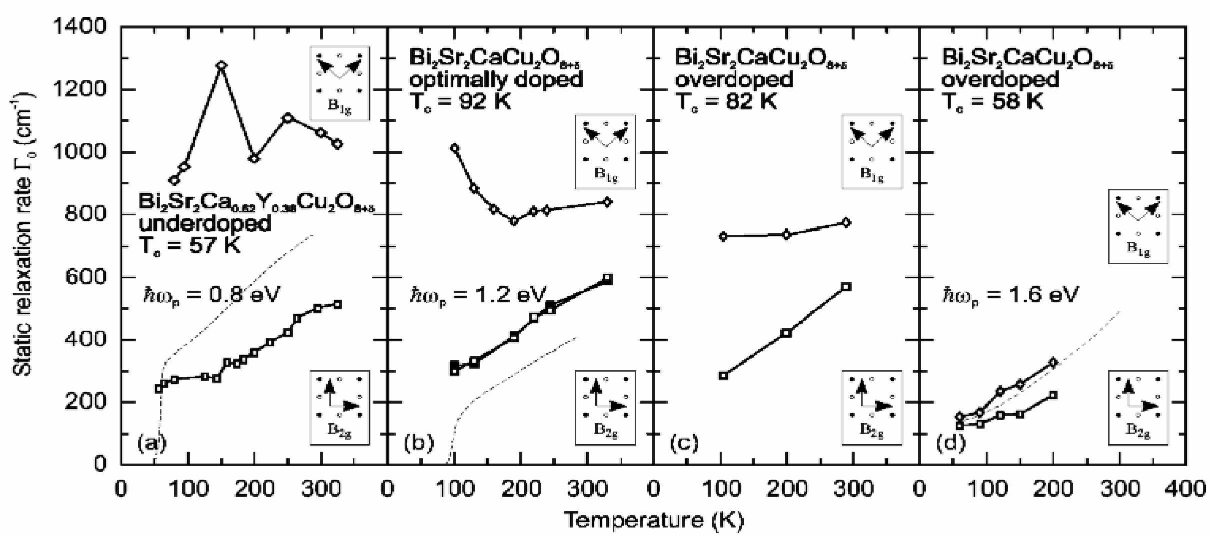




- B_{2g} - intensity largely **independent** of doping and temperature.
- B_{1g} - **loss** of low frequency spectral weight with underdoping.

Review of Raman Data for the Cuprates (ctd.)

M. Opel *et al.*, PRB 2000



Low-frequency Raman response measures the inverse of the quasiparticle lifetime (if qps exist) and can be used to measure the qp lifetime as a function of the symmetry of the excitations.

$$\chi^{//}(T >> \Omega \sim 0) \sim \Omega \langle Z^2_{\mathbf{k}}\, \gamma^2(\mathbf{k}) / \Gamma_{\mathbf{k}}(T) \rangle$$

$\Gamma_{\mathbf{k}}(T)$ qp scattering rate, $Z_{\mathbf{k}}$ qp residue, $\langle . \rangle$ average over Fermi surface.

Inverse of the Raman slope determines the T-dependence of the qp scattering rate.

Summary of Experimental Data in the Cuprates

- *Distinctly different behavior of dynamics of B_{1g} and B_{2g} Raman response.*

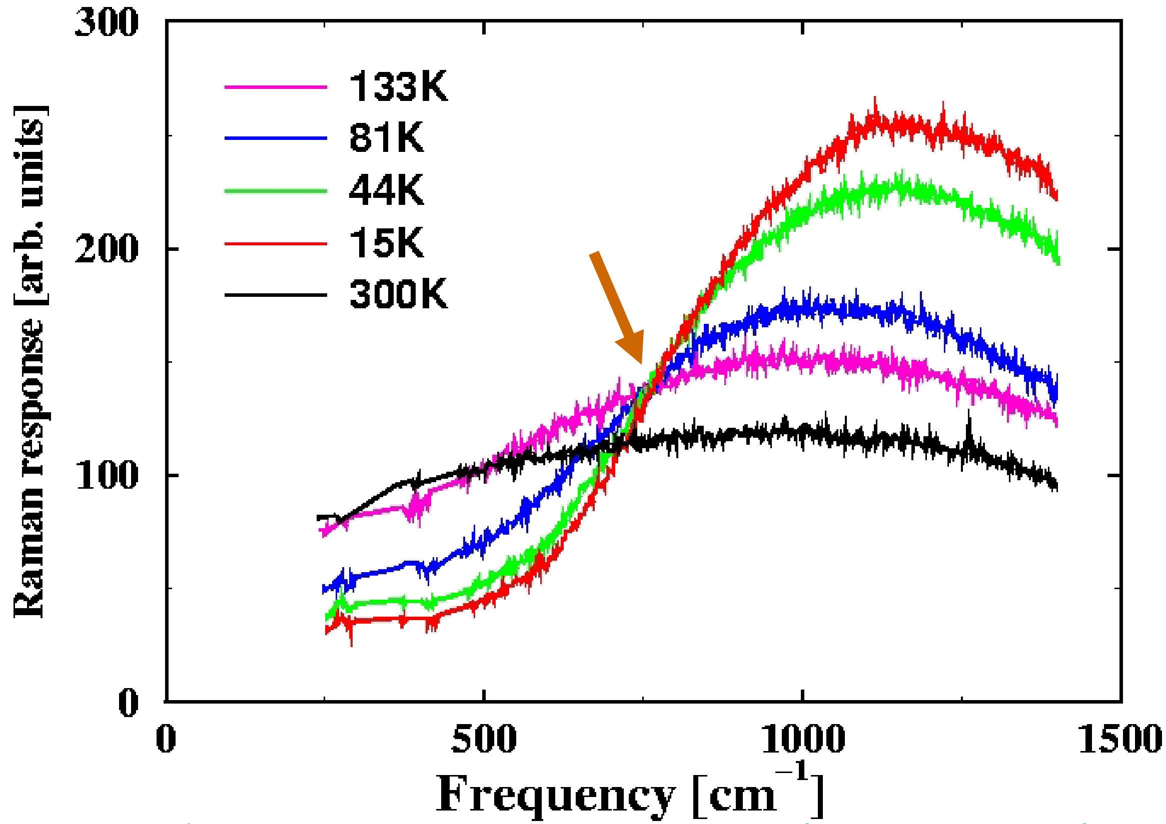
A_{1g}, B_{2g} :

- relatively **independent** of doping.
- follows transport in normal state.

B_{1g}:

- **strongly** doping dependent.
- spectral weight transfer to higher energies for low dopings shows a **gapped response** at different energy and temperature than B_{2g}.
- **Merges** with B_{2g} behavior for **overdoped** samples.

Experimental data for Kondo insulators



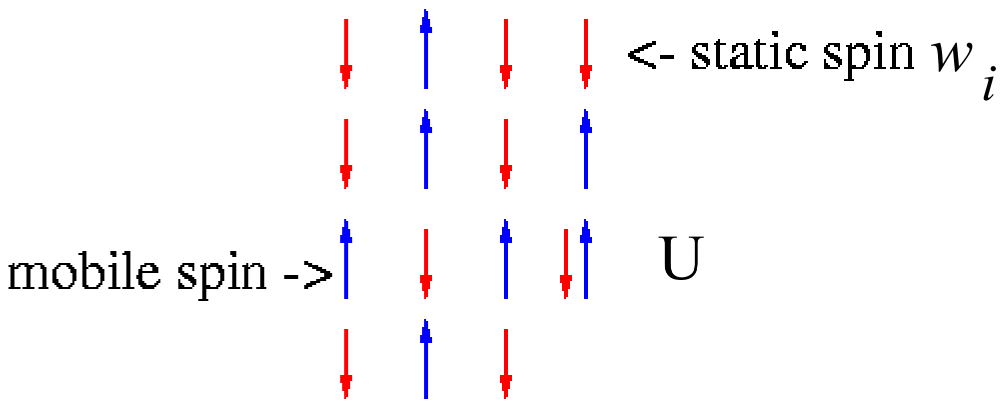
- *Nyhus et al, PRB 95* Raman scattering on FeSi. Note the appearance of the **isosbestic point** below about 150K.
- The low frequency spectral weight is **reduced** and the higher frequency weight is **enhanced** as the temperature is lowered.

Theories of Raman Scattering

- The **insulating limit** has been analyzed by Chubukov and Frenkel (PRL, 1995).
- The **antiferromagnetically correlated metal** has been described by Devereaux and Kampf (PRB, 1999).
- But no theory exists that can connect these two regimes and carry one through the **quantum critical point** of a metal-insulator transition.
- Experimental results exist for a variety of materials that pass through a **metal-insulator transition** as a function of doping.
- ***Here we show how one can solve for Raman scattering through a metal-insulator transition in both the Falicov-Kimball model and the Hubbard model***.

Spinless Falicov-Kimball Model

$$H = -\frac{t}{2\sqrt{d}}\sum_{<i,j>} c_i^\dagger c_j + E\sum_i w_i + U\sum_i c_i^\dagger c_i w_i$$



•**exactly solvable model** on a hypercubic lattice in infinite dimensions using dynamical mean field theory.

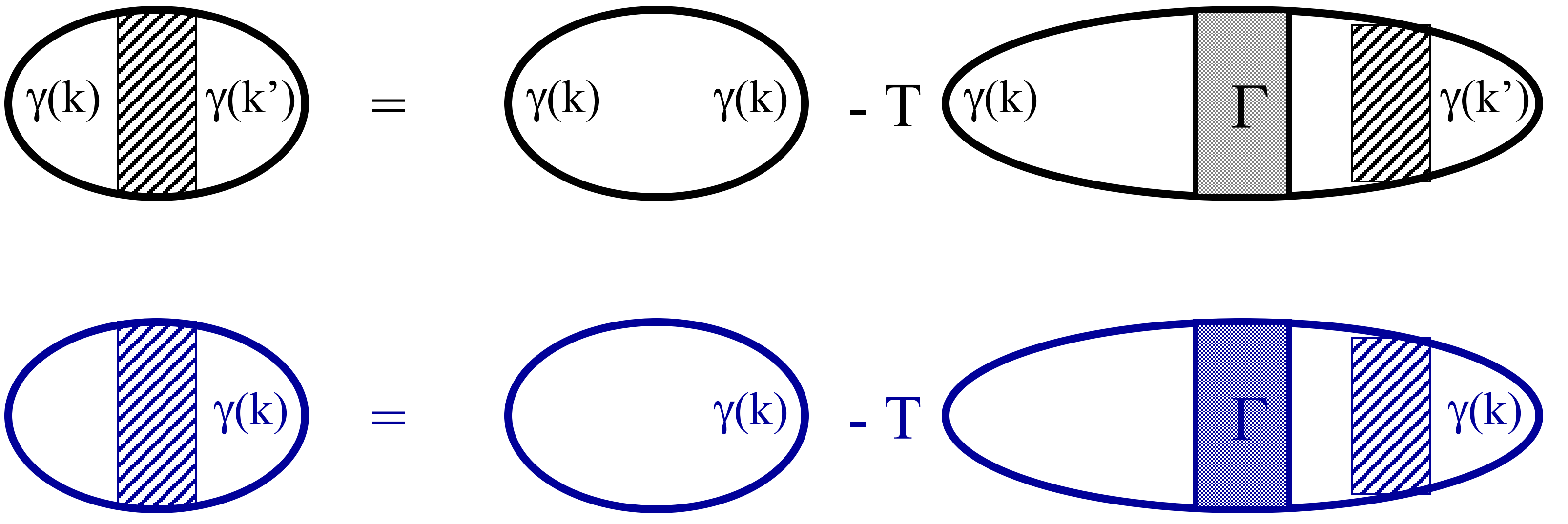
•possesses homogeneous, commensurate/incommensurate CDW phases, phase segregation, and **MI transitions**.

•***Raman response can be constructed formally exactly***.

Formal Solution for Raman Scattering Response
A_{1g} channel

- This channel has the **full symmetry** of the lattice
- The Raman response contains **resonant**, **mixed** and **nonresonant** terms. (We consider only the **nonresonant** terms here).
- The irreducible charge vertex for the Falicov-Kimball model is a **simple function** of the electronic self energy and Green's function (Shvaika, Physica C, 2000; Freericks and Miller, PRB, 2000). *This is **not** true for the Hubbard model*.
- The **nonresonant** Raman response can be determined **exactly** by properly solving the relevant Dyson equations.
- We illustrate how to solve this problem using Feynman diagrams.

Diagrams for the A_{1g} Raman response



$\gamma(k) = c - \varepsilon(k)$, Γ is local and has no k-dependence

Solving these coupled equations allows for the full nonresonant Raman response to be determined.

Formal Solution for Raman Scattering Response
B_{1g} channel

- This channel is **orthogonal** to the lattice.
- There are **no vertex corrections** (Khurana, PRL, 1990), so the Raman response is represented by the **bare bubble**.
- This response is **identical** to that of the optical conductivity multiplied by one factor of frequency (Shraiman and Shastry, PRL, 1990).
- **Mixed** and **resonant** Raman scattering are possible in this channel, but won’t be analyzed in detail here.

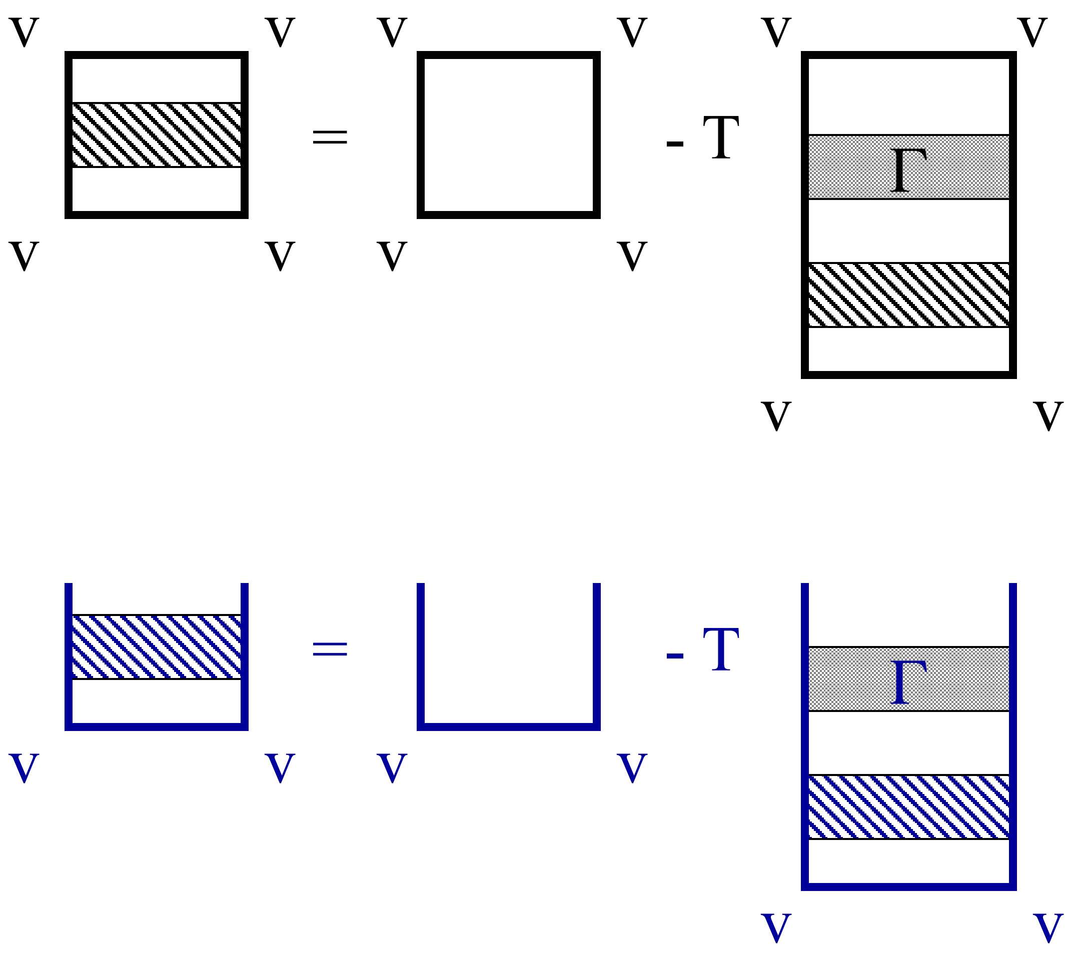
The nonresonant B_{1g} Raman response is closely related to the optical conductivity.

Formal Solution for Raman Scattering Response
B_{2g} channel

- The Raman scattering amplitude vanishes for nearest neighbor hopping on a hypercubic lattice, so there are **no nonresonant or mixed responses**.
- The square of the current operator does contain B_{2g} symmetry, so **pure resonant processes are possible**.
- **Vertex corrections** are needed, but are relatively simple to handle.
- We **illustrate** schematic diagrams on the next page, but present no results for this process here.

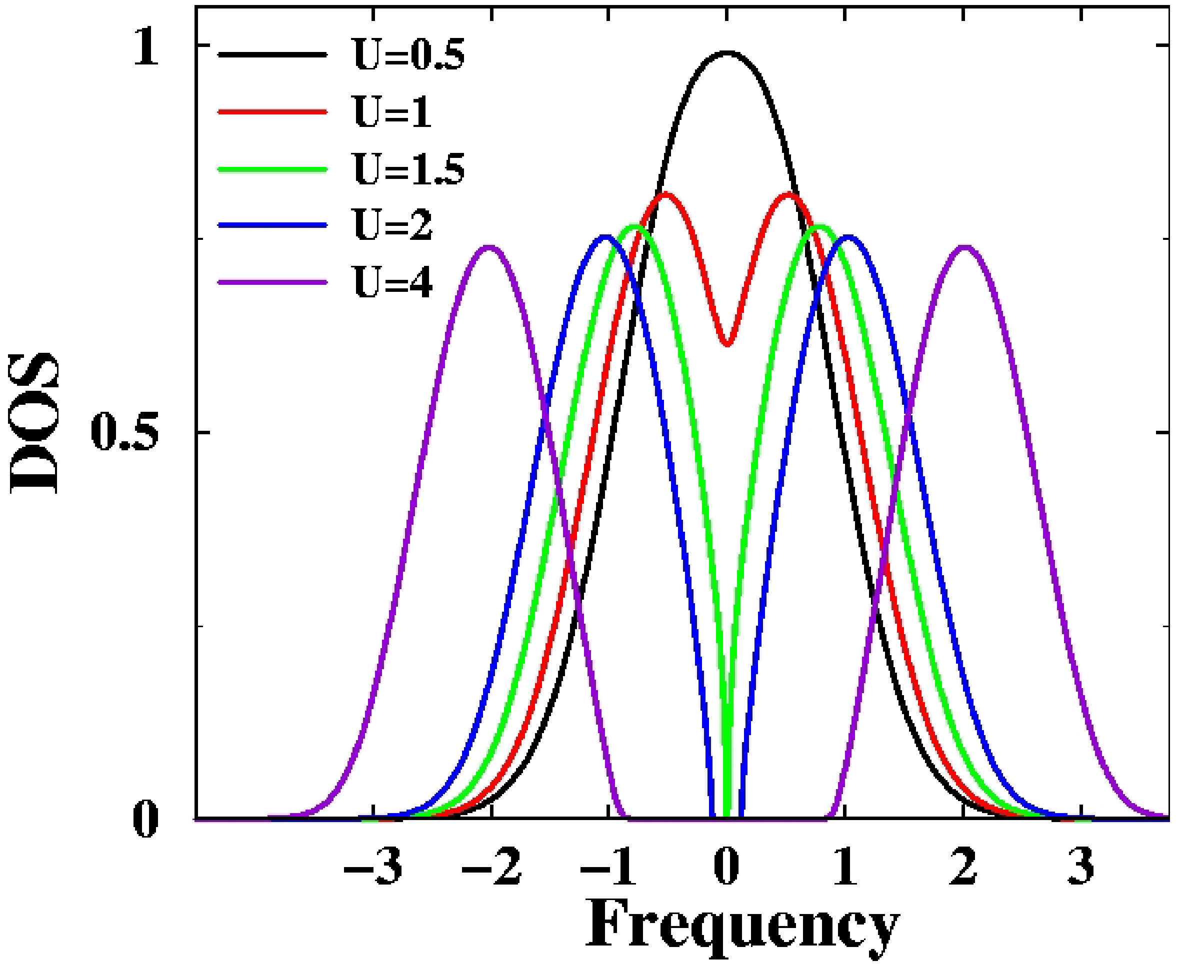
B_{2g} Raman scattering is purely resonant.

Diagrams for the B_{2g} Raman response



- In these diagrams, the vertex v is the **velocity operator** v(k)=dε(k)/dk dotted into the photon polarization.
- These **coupled** Dyson equations must be solved together in order to get the resonant Raman response.

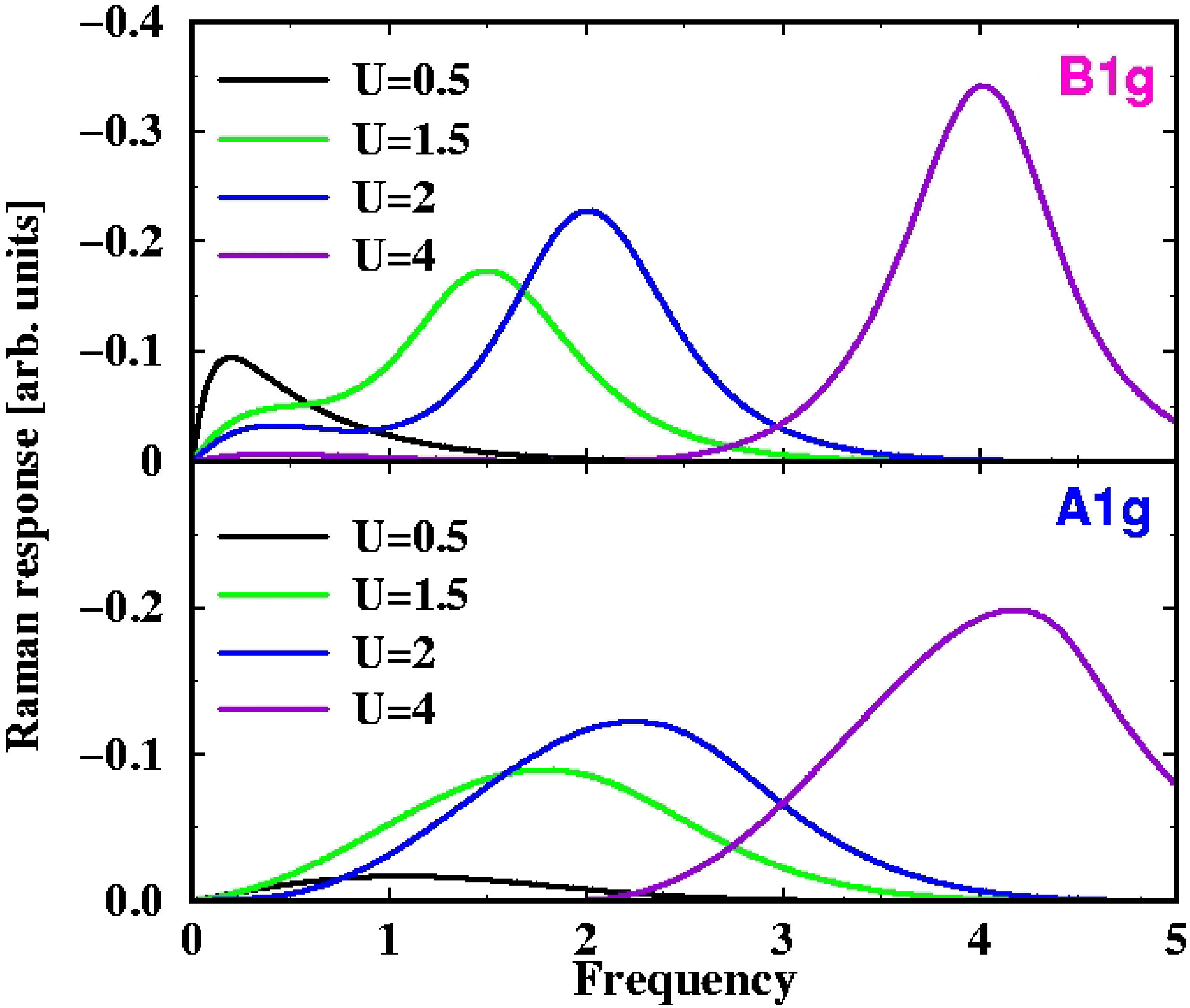
Metal-Insulator transition



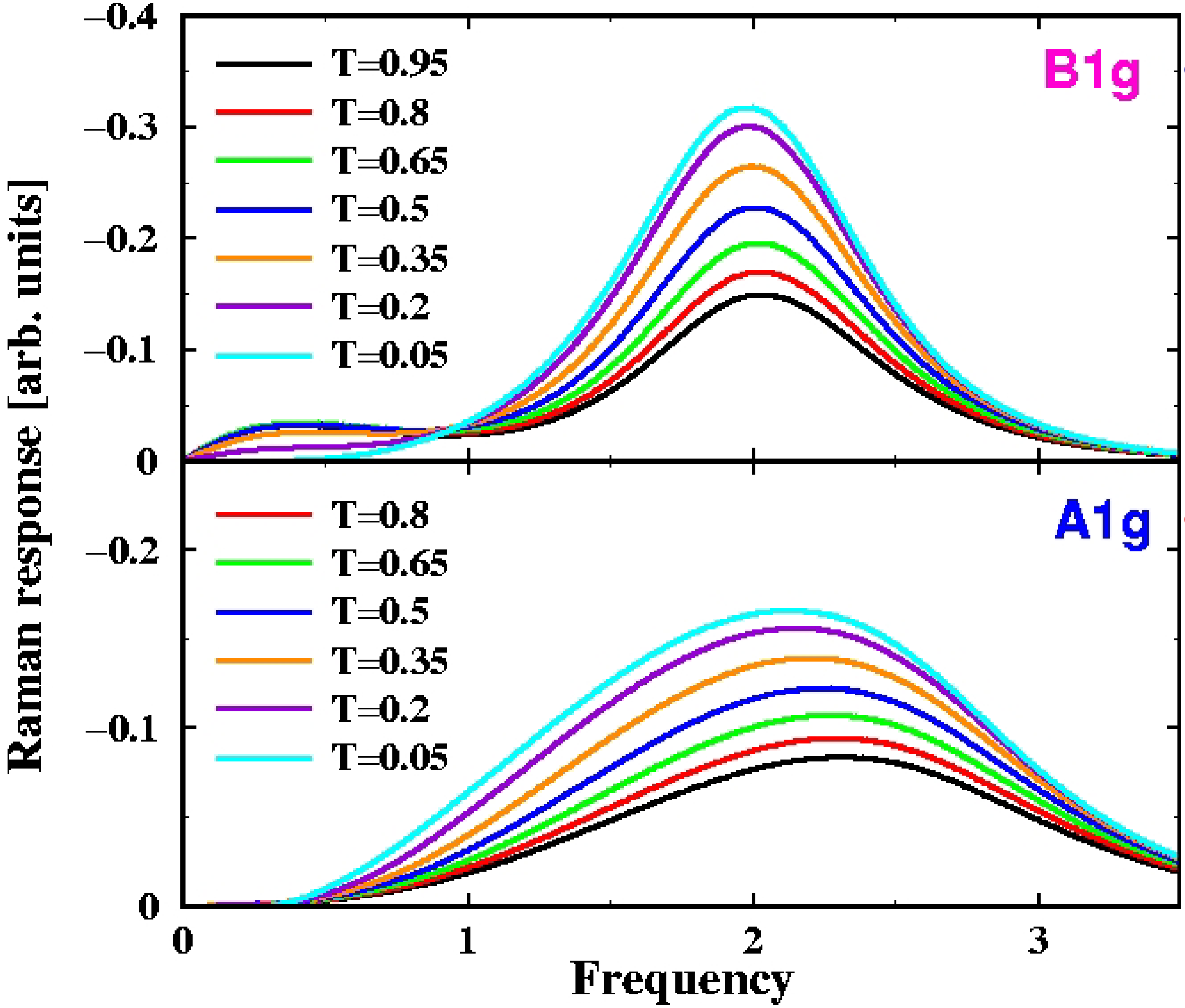
- **Correlation-induced** gap drives the single-particle DOS to zero at U=1.5
- Interacting DOS is **independent of T** in DMFT (Van Dongen, PRB, 1992)
- **Examine Raman response through the quantum phase transition**.

Nonresonant Raman Response (Constant T)

- The A_{1g} response is suppressed at low frequencies, but the B_{1g} response displays low-frequency spectral weight as one passes through the **metal-insulator transition**.
- Note the **charge transfer peaks** for large U.



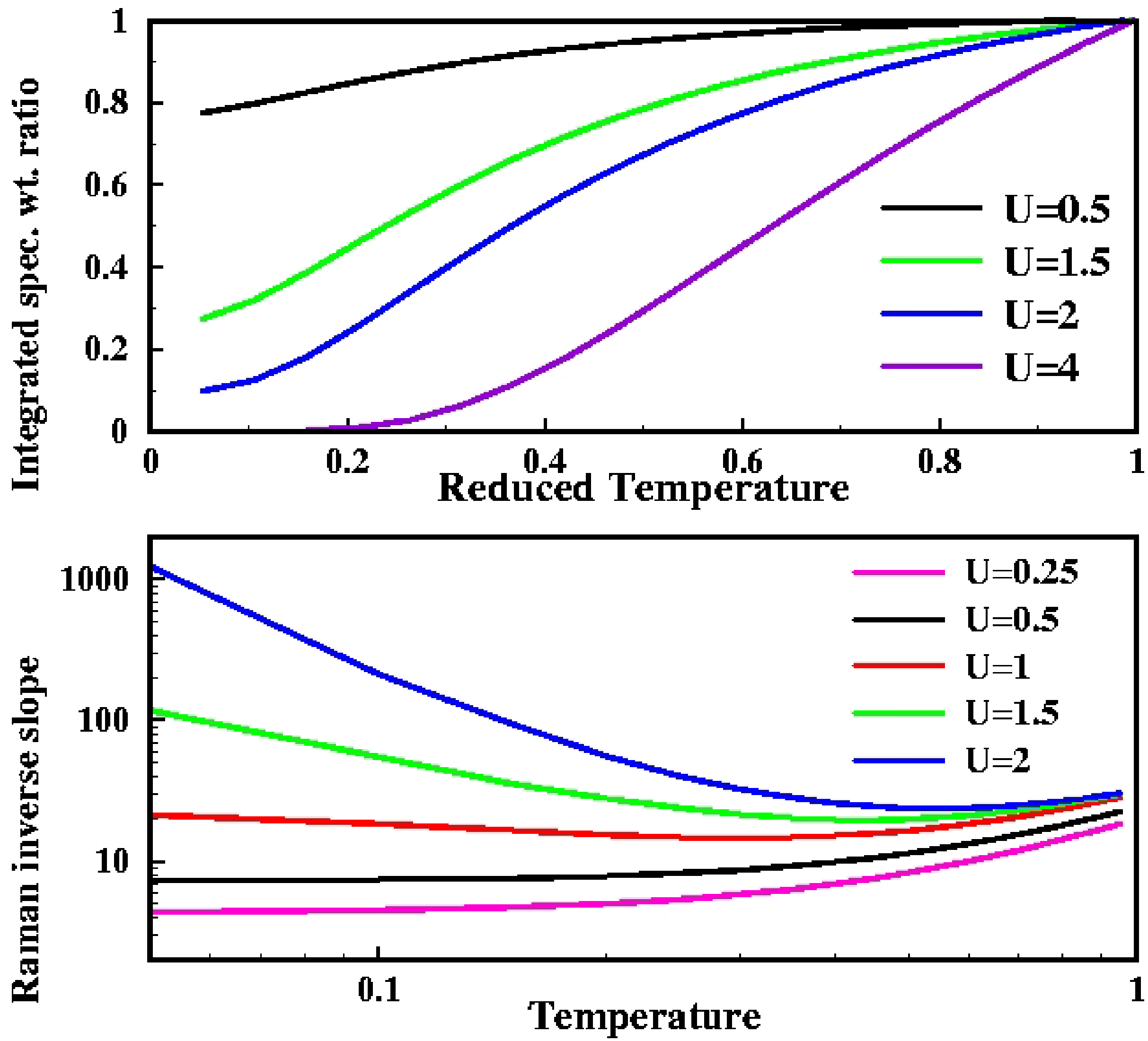
Nonresonant Raman Response (U=2)



- The low-frequency B_{1g} response develops at a low temperature over a **wide frequency range** of O(1).
- An **isosbestic point** divides where spectral weight increases or decreases as T is lowered (B_{1g}).

Spectral weight and Inverse Raman Slope

- The B_{1g} Raman response is **sharply depleted** at low-T.
- The inverse Raman slope changes from **nearly constant** uncorrelated metallic behavior to a **rising** pseudogap or insulating behavior as the correlations increase.

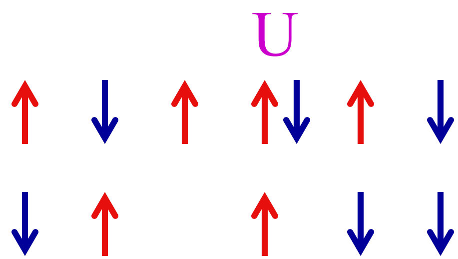


Summary (Falicov-Kimball model)

- Theoretical results are **qualitatively similar** to experimental results measured in correlated systems.
- The nonresonant B_{1g} channel displays (i) an **isosbestic point** that divides the regions where the Raman response increase or decrease as T is lowered; (ii) a **sharp depletion of spectral weight** in the low-frequency region as T is reduced; and (iii) the temperature where low-frequency spectral features appear is **much lower than the range** in frequency over which those features appear.
- Results for the Raman scattering are **model independent** on the insulating side of the MIT.
- Vertex corrections **suppress all nontrivial behavior** for the A_{1g} channel.

Hubbard Model

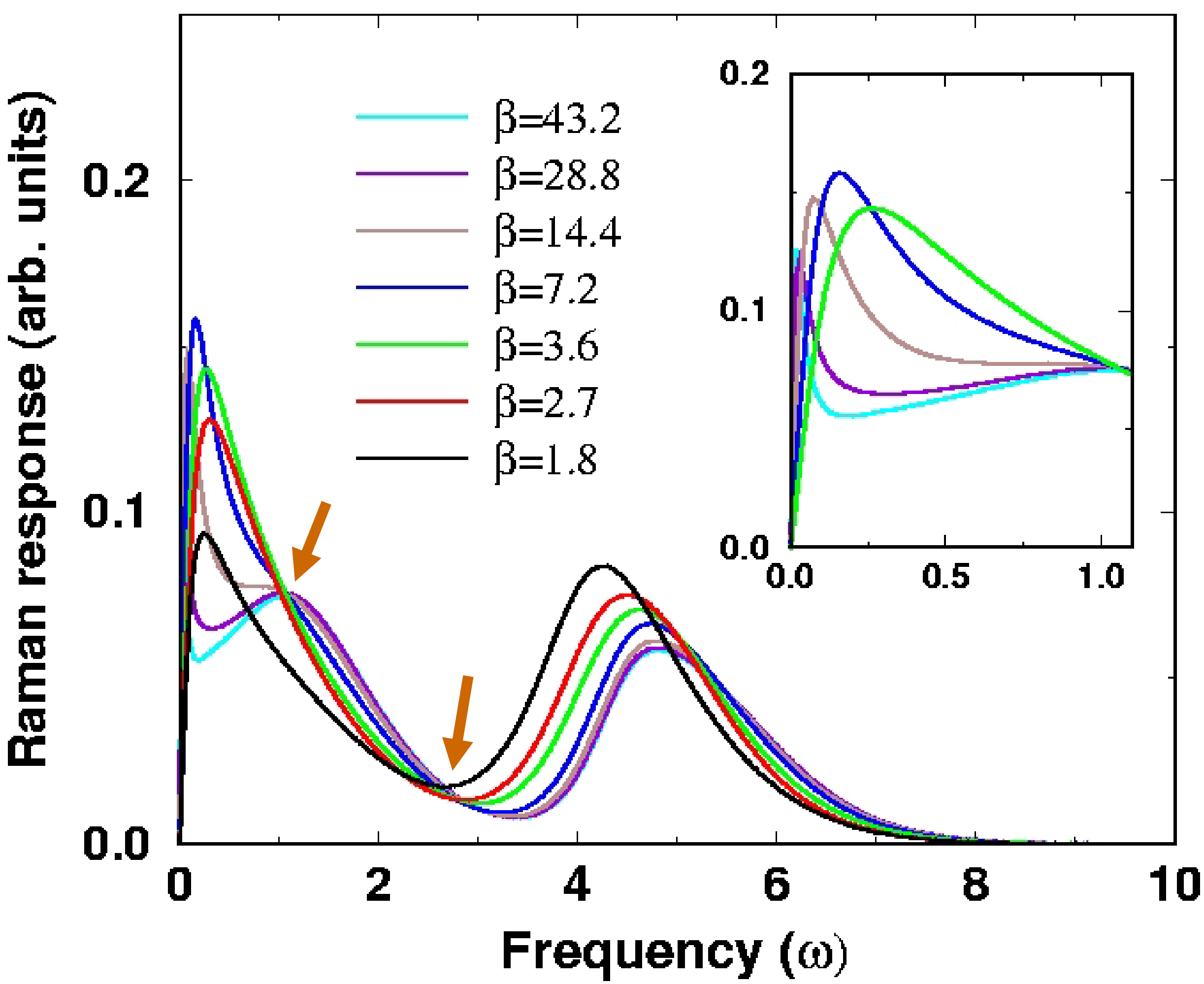
$$H = -\frac{t}{2\sqrt{d}} \sum c^{*}_{i\sigma} c_{j\sigma} + U \sum n_{i\uparrow} n_{i\downarrow}$$



Both electrons are now **mobile**

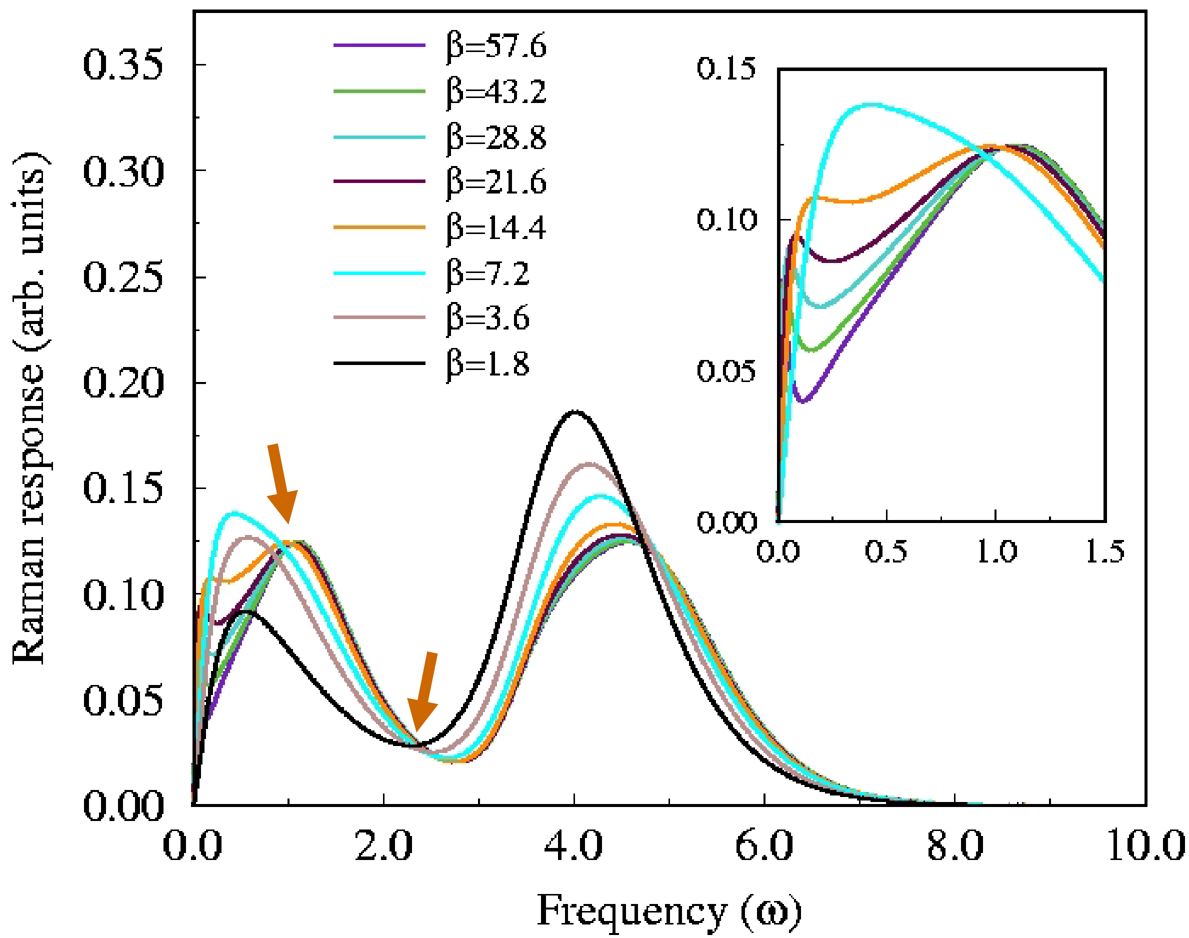
- **Exactly solvable** model on a hypercubic lattice in infinite dimensions using dynamical mean field theory (but requires quantum Monte Carlo and maximum entropy analytic continuation).
- The irreducible charge vertex is problematic to calculate because it possesses too large a dynamic range for the max-ent techniques.
- ***Hence, the Raman response can be constructed formally exactly for the nonresonant B_{1g} channel only.***

Nonresonant B_{1g} Raman scattering (n=0.55)



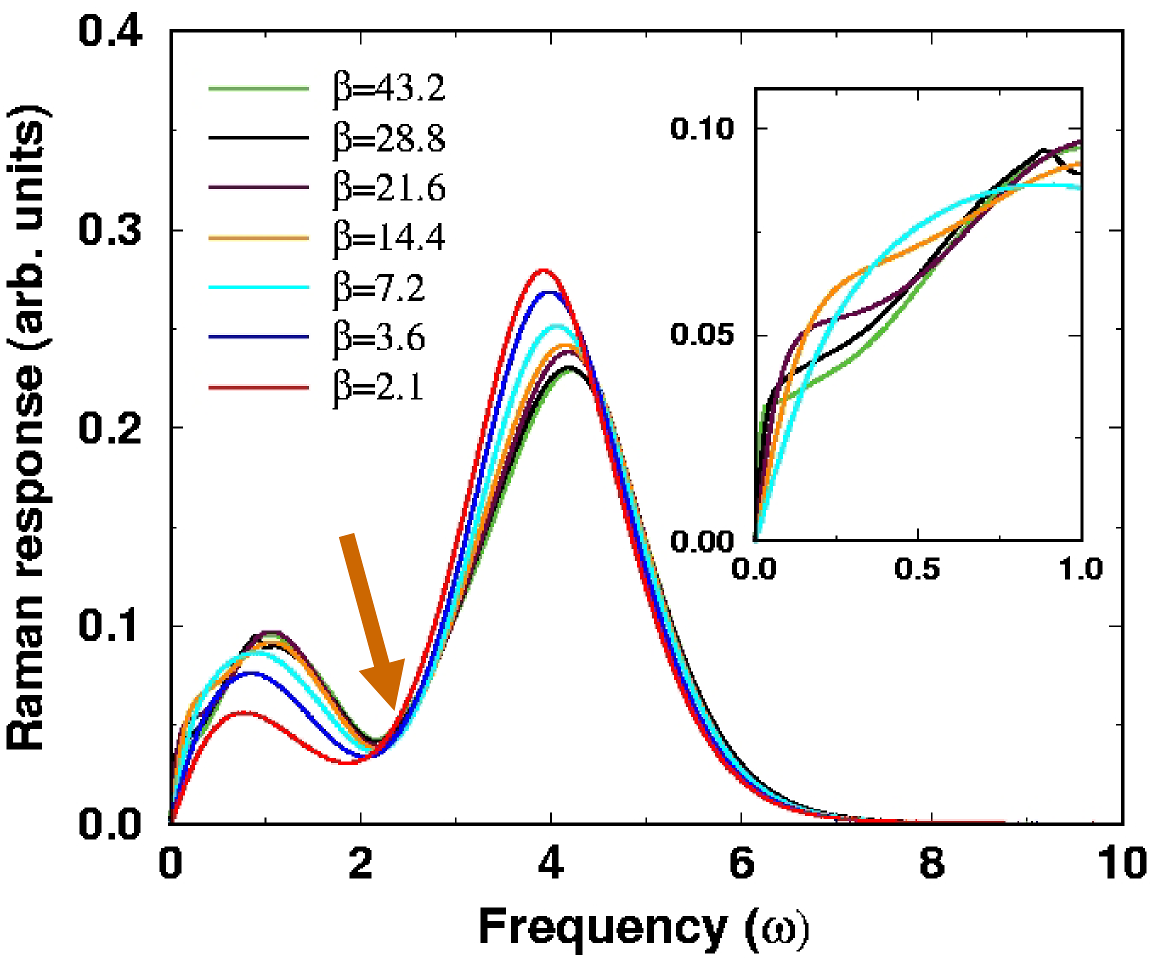
- As the temperature is lowered, we see the characteristic form of a Fermi-liquid develop at low frequencies (note the **sharp narrow peak** at low frequency).
- Note **two isosbestic points** and the charge-transfer peak indicating it is correlated.

Nonresonant B_{1g} Raman scattering (n=0.7545)



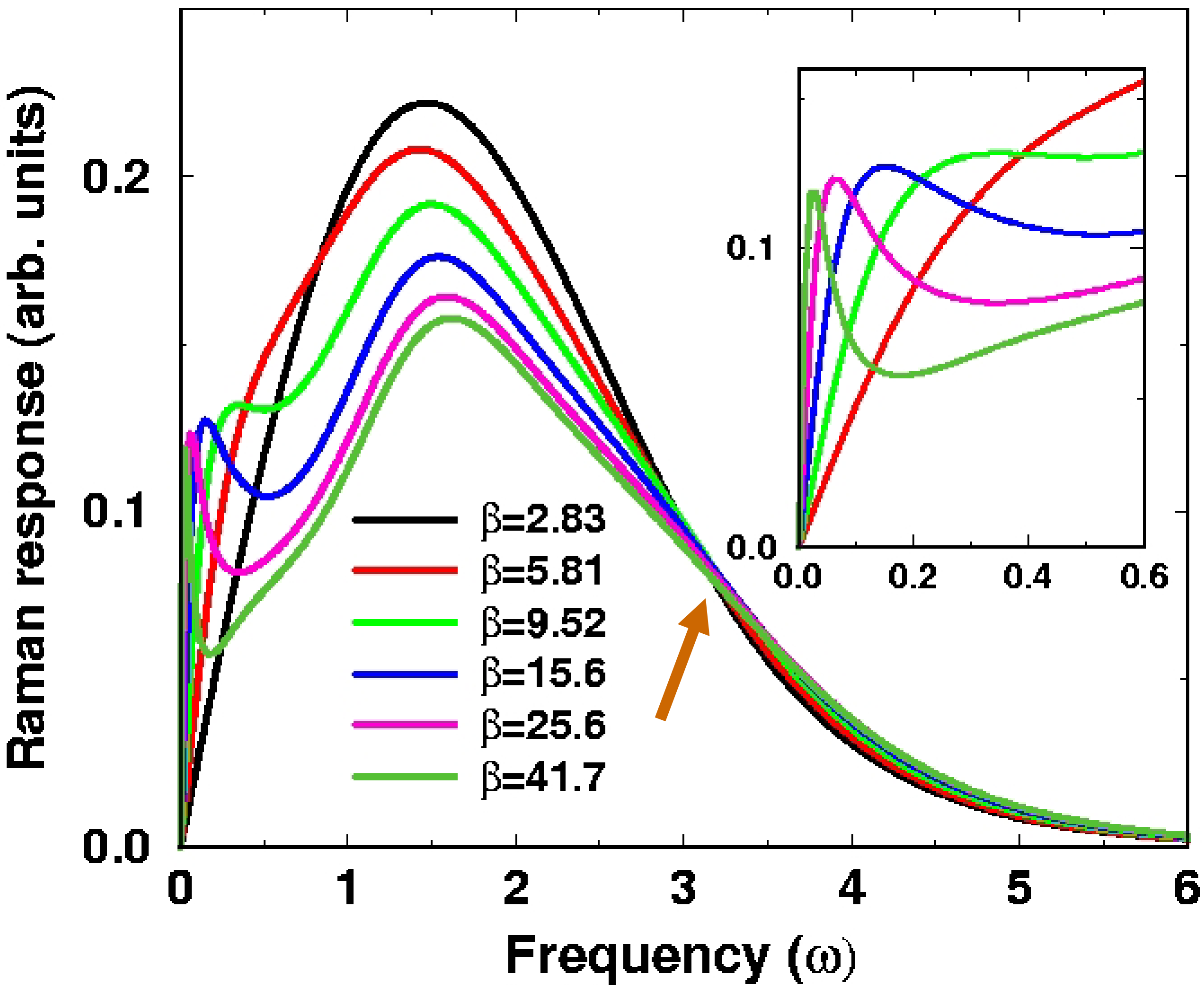
- There is a **second** low frequency isosbestic point at low temperature.
- The Fermi-liquid shape still forms at low T, but has **less weight**.
- The charge transfer peak is **reduced** while the mid-IR peak remains **constant** as T is lowered.

Nonresonant B_{1g} Raman scattering (n=0.9072)



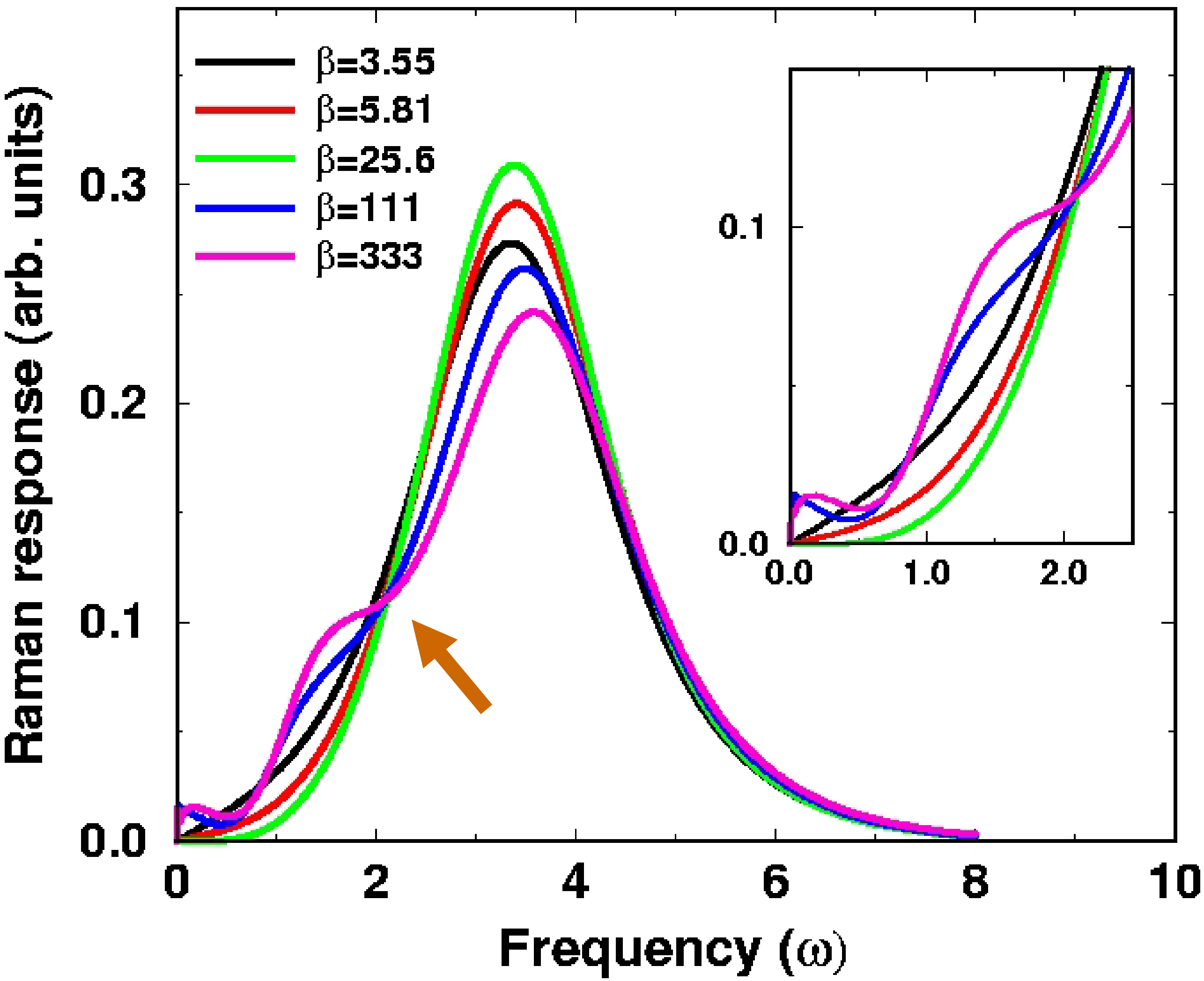
- Here the development of the Fermi-liquid peak occurs at such low temperature that is can **no longer be seen** in the Raman data.
- There is a **depletion** of low energy spectral weight and an **enhancement** at higher energies, but not as significant a change as seen in experiments or in the FK model.

Nonresonant B_{1g} Raman scattering (n=1,U=2.1)



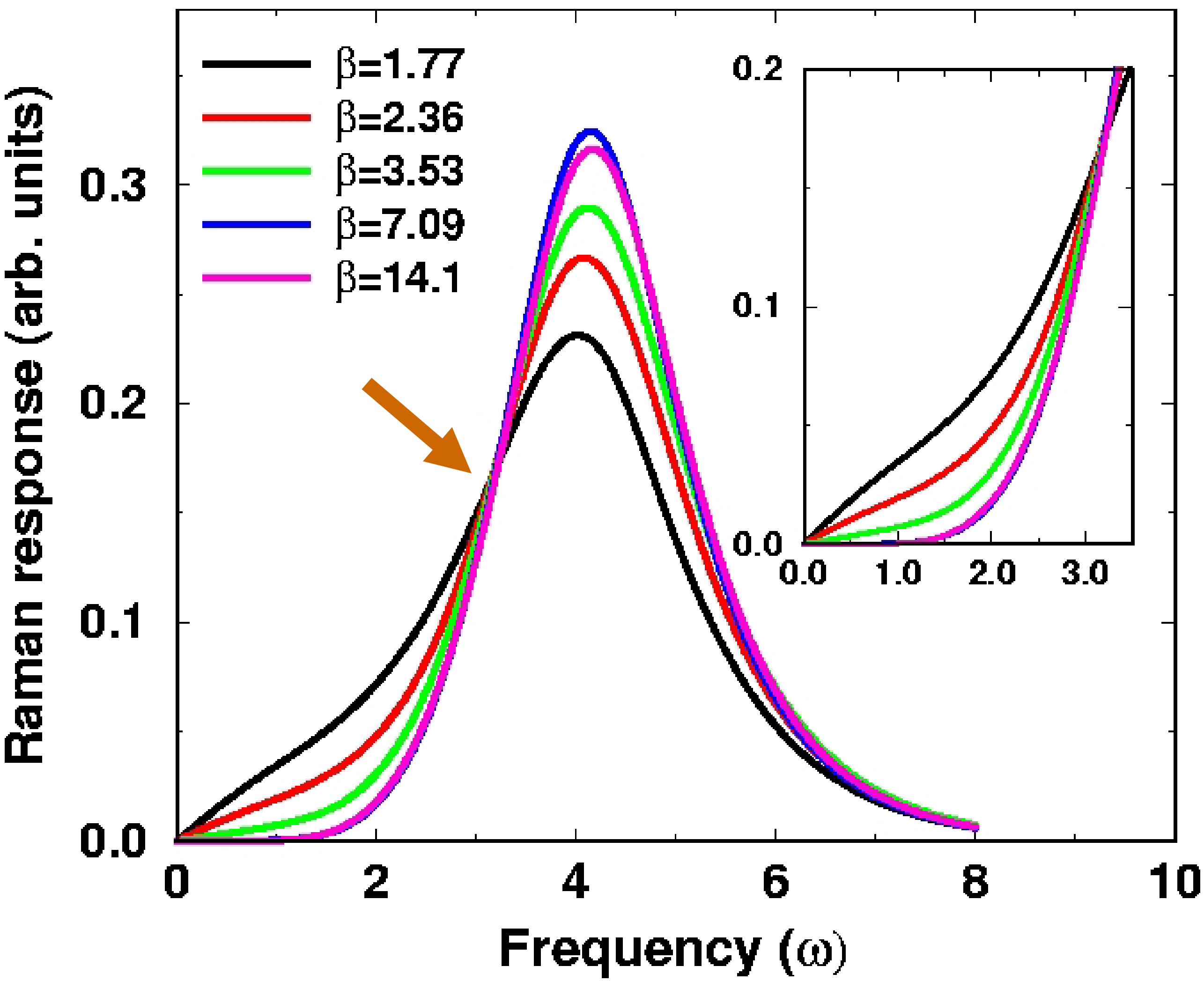
- Note the charge transfer peak as well as the Fermi liquid peak at low energy. As T goes to zero, the Fermi peak sharpens and moves to lower energy, as expected.
- There is **no low energy and low-T isosbestic point** as seen in the doped case.

Nonresonant B_{1g} Raman scattering (n=1,U=3.5)



- This is quite anomalous. A MIT occurs as a function of T. Note the appearance of the low-T isosbestic point.
- The low energy Raman response has rich behavior, with a number of low energy pekas developing at low-T, but **the low energy weight increases as T decreases here**.

Nonresonant B_{1g} Raman scattering (n=1,U=4.2)



- Here we see the expected **universal behavior** for the insulator---the low-energy spectral weight is **depleted** as T goes to zero and an **isosbestic point** appears.
- The temperature dependence here is over a **wider range** than for the FK model due to the **T-dependence** of the interacting DOS.

Summary Hubbard model

- The Fermi-liquid behavior introduces new features to the B_{1g} Raman response: there is a **second low-energy isosbestic** point which occurs only at low temperatures and there is a characteristic **Drude like feature** that develops at the lowest frequencies (with a width that decreases like T^2) for the doped cases.
- At half filling, new behavior occurs on the metallic side of the MIT, where the **low-energy spectral weight increases** as T decreases and where additional structure is seen.
- In the insulating phase we see the expected **universal behavior**, but the temperature dependence is slower here, because the interacting DOS is also T-dependant.

Conclusions

- Showed how an exact solution for **nonresonant** Raman scattering can be constructed for a system that passes through a metal-insulator transition. The solution displayed both an **isosbestic point** and a **rapid increase in low-frequency spectral weight** near the quantum-critical point.
- Results are **model independent** on the insulating side of the metal-insulator transition.
- Found the presence of low temperature Fermi-liquid behavior generically introduced a **second low frequency** and **low temperature isosbestic point** as well as **an even lower frequency Drude peak**.
- Illustrated how **resonant** Raman scattering can also be solved in the Falicov-Kimball model (but presented no results).