Inelastic x-ray scattering as a probe of electronic correlations

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We construct an exact dynamical mean field theory for nonresonant inelastic light scattering in the infinite-dimensional Falicov-Kimball model, which can be tuned through a quantum critical metal-insulator transition. Due to the projection of the polarization orientations onto different regions of the Brillouin zone and due to the transfer of energy and momentum from the light to the strongly correlated charge excitations, the nature of the dynamics can be naturally interpreted as strongly temperature-dependent low-energy particle-hole excitations and weakly temperature-dependent high-energy charge transfer excitations which depend delicately on the electronic correlations. These results can be used to give important information concerning the evolution of charge dynamics in different regions of the Brillouin zone.

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I. INTRODUCTION

Inelastic x-ray scattering (with meV accuracy over a spectral range of several eVs) has improved significantly over the past few years due to the increased photon flux of third generation synchrotron sources. The large cross-section of light-coupled probes (as compared to neutron scattering, for example) allows for a systematic study of the dispersive charge dynamics in a wide dynamical range (q, Ω) in solids and fluids. It has opened an additional window to study correlation effects on phonons, plasmons, quasiparticles, charge transfer excitations, and orbital excitations. One particular point of interest has been the study of the evolution of strongly correlated systems as some parameter of the system, such as the electron density, is varied by doping or pressure. While many single-particle properties have been studied via angle-resolved photoemission, important questions concerning the evolution of the unoccupied states are now directly accessible via inelastic x-ray scattering.

Recent experiments have focused on a number of correlated (Mott) insulators such as La$_2$CuO$_4$ and Sr$_2$CuO$_2$Cl$_2$, Ca$_2$CuO$_2$Cl$_2$, NaV$_2$O$_5$, Nd$_2$CuO$_4$, and the one-dimensional insulators Sr$_2$CuO$_3$ and Sr$_2$CuO$_2$Cl$_2$. The measurements have revealed dispersive high-energy and low-energy excitations which have been identified with a photon-induced charge transfer between different atomic orbitals, or with transitions from the lower to the upper Hubbard band across an effective q-dependent Mott gap.

More recent measurements have begun to appear in materials doped from their parent Mott insulating phases. However, the theoretical development of inelastic x-ray scattering in strongly correlated metals and insulators is just starting to form. Of particular interest is a determination of how the upper and lower Hubbard bands and consequently the Mott gap evolve with correlations. As experiments reach greater and greater resolution, it will shortly be possible to track the evolution of electronic correlations from strongly correlated insulators to strongly and then weakly correlated metals. The purpose of this contribution is to investigate such a theory for inelastic x-ray scattering. In particular, we develop an exact dynamical mean field theory for nonresonant inelastic light scattering in a system which can be tuned across the quantum critical point of a metal-insulator transition. We calculate the inelastic x-ray cross-section on both sides of the transition and near the critical point.

The outline of this manuscript is as follows: in Section II we develop the general formalism for nonresonant inelastic x-ray scattering and review simple physical ideas for weakly correlated metals. In Section III we present the specific formalism for calculating the x-ray response in the Falicov-Kimball model in the limit of large spatial dimensions, and in Section IV we present the numerical results. Lastly, we summarized our results and discuss them in light of recent measurements in Section V. This paper expands on results for the insulating phase to consider metals and materials close to the metal-insulator transition.

II. FORMALISM

A. Non-resonant response

Light can scatter off of many different excitations in a system, but here we focus on the inelastic scattering of x-rays from electrons. X-rays, unlike optical photons, can exchange both energy and momentum when they scatter with a solid. The scattering occurs as light creates charge fluctuations in different locations of the Brillouin zone (BZ). These charge fluctuations are classified as either isotropic charge fluctuations or anisotropic charge fluctuations.
fluctuations (which vanish when averaging their k-space variation over the BZ). The way in which the charge fluctuations are created is dictated by the polarization orientation of the incoming and outgoing photons set by the scattering geometry. These polarization orientations transform according to the operations of the point-group symmetry of the crystal, and therefore so must the charge fluctuations that they create. It is through this mechanism that the charge excitations in different regions of the BZ can be systematically selected and explored via inelastic light scattering.

These charge fluctuations relax by internal scattering processes, such as due to impurities or Coulomb scattering, and finally via the re-emission of photons; inelastic x-ray scattering probes these relaxation processes at different regions of the BZ and at different transferred energies. An important distinction between isotropic and anisotropic charge fluctuations is that the former are coupled to long-range Coulomb interactions while the latter are not. This has dramatic consequences on the polarization dependence of the observed spectra. We now elaborate upon this further.

We limit focus to the case of non-resonant x-ray scattering since resonant processes have not yet been treated exactly in any correlated itinerant model. The inelastic x-ray response is given generally by the inelastic density-density correlation function

\[ S(q, \omega) = -\frac{1}{2}[1 + n(\omega)]\chi''(q, \omega) \]  

formed with an “effective” density operator given by

\[ \tilde{\rho}(q) = \sum_{k, \sigma} \gamma_a(k) c_{\sigma}^\dagger(k + q/2) c_{\sigma}(k - q/2), \]

where \( n(\omega) \) is the Bose distribution function, and the double prime superscript denotes the imaginary part. We relate the inelastic light scattering vertex \( \gamma_a \) to the curvature of the energy band \( \epsilon(k) \) to the light polarizations through

\[ \gamma_a(k) = \sum_{\alpha, \beta} e_k^a \partial\epsilon/\partial k_{\alpha} \partial k_{\beta} e_k^i. \]

This holds in the limit of vanishing energy transfers, but can also be generalized in terms of Brillouin zone harmonics to other non-resonant cases. Here \( e_k^i \) denote the incident, scattered x-ray polarization vectors, respectively, and we have chosen units \( k_B = c = \hbar = 1 \) and have set the lattice constant equal to 1. We can classify the scattering amplitudes by their point group symmetry operations. It is customary to have \( A_{1g} \) denote the symmetry of the lattice (s-wave) and \( B_{1g} \) and \( B_{2g} \) denote two of the d-wave symmetries. For any dimension \( d > 1 \), if we choose \( e^i = (1, 1, 1, ...) \) and \( e^* = (1, -1, 1, -1, ...) \), then we have the \( B_{1g} \) sector, while \( e^i = e^* = (1, 1, 1, ...) \) projects out the \( A_{1g} \) sector since the \( B_{2g} \) component is identically zero for models with only nearest-neighbor hopping. Thus, we can cast the scattering amplitudes into a simple form: \( \gamma_{A_{1g}}(k) = -\epsilon(k) \) and \( \gamma_{B_{1g}}(k) = t^* \sum_{j=1}^{\infty} \cos k_j (1)^{j/\sqrt{d}} \), which recovers the \( d = 2 \) representations of the tetragonal point group symmetry operations commonly used in CuO\(_2\) systems. We note that if we take the pure charge vertex for \( A_{1g} \), \( \gamma_{A_{1g}} = 1 \), then \( S(q, \omega) \propto Im \left\{ \frac{1}{\gamma(q, \omega)} \right\} \) with \( \epsilon \) the dielectric function.

### B. Weakly correlated electrons

It is useful to review the nonresonant response for weakly correlated metals to determine where we expect to see the role of correlations emerge. For non-interacting electrons the effective density response is given in terms of a generalized Lindhard function which incorporates the symmetry dependence of the light scattering amplitudes \( \gamma \) in the Lindhard kernel. In particular, in the limit \( q \to 0 \) there is no low energy inelastic light scattering (for three-dimensions) as there is no phase space to create electron-hole pairs and the only excitation is the high-energy collective plasmon. This is analogous to the situation of the charge susceptibility, which vanishes at a finite frequency when \( q = 0 \) because the total charge of the system commutes with the Hamiltonian. For finite \( q \), the particle-hole continuum gives low-energy scattering up to a frequency \( \nu \approx q \) with \( \nu \approx \nu \) the Fermi velocity. When scattering off an impurity potential \( V_{k, k'} \) is added, this sharp cut-off is smeared, and scattering occurs over a wide range of transferred frequencies. The density response at small \( q \) is given by an effective density-density Kubo formula:

\[ \chi''_{LL}(q, \Omega) = N_F \frac{\Omega \tau^{-1}_L}{\Omega^2 + \tau^{-2}_L}, \]

with \( N_F \) the density of states at the Fermi level and \( \tau^{-1}_L \) the relaxation rate for density fluctuations having a symmetry selected by light orientations labelled by \( L \) (\( L \) denotes an irreducible representation of the point group of the crystal, such as \( A_{1g} \) or \( B_{1g} \) for a tetragonal crystal; we use \( L = 0 \) to denote the \( A_{1g} \) sector). Expanding the impurity potential in terms of a complete set of basis functions \( \phi_L(k) \) yields

\[ | V_{k, k'} |^2 = \sum_L \phi_L^*(k') \Gamma_L \phi_L(k). \]

The width and location of the peak of the response is given by \( \tau^{-1}_L = \tau^{-1}_{L=0} - \tau^{-1}_L + D q^2 \), where \( \tau^{-1}_L = 2\pi N_F \Gamma_L \) is the scattering rate that preserves charge fluctuations having symmetry \( L \), and \( D \) is the diffusion constant related to the resistivity \( \rho \) by an Einstein relation, \( D^{-1} = 2e^2 N_F \rho \). Here we have assumed that the impurity potential is rotationally invariant and largely independent of momentum transfer. Thus in this case, phase space is already created by the impurity scattering potential for
anisotropic \((L \neq 0)\) density fluctuations coupled to the x-rays. However, isotropic density fluctuations \((L = 0)\) are governed by the continuity equation and must vanish at \(q=0\) even in the presence of an impurity potential. Therefore, for \(L \neq 0\) channels \((B_{1g})\) the x-ray response has a Lorenzian lineshape with a peak position and width which grows as \(q^2\) for momentum transfers away from the zone center \(q = 0\), while for \(L = 0\) \((A_{1g})\), there is only low energy scattering for finite \(q\) due to particle number conservation.

### III. FORMALISM WITH CORRELATIONS

Coulomb interactions create phase-space for particle-hole excitations and lead to inelastic scattering even at \(q=0\) for channels not having the underlying symmetry of the lattice. The scattering can be enhanced when the momentum structure of the Coulomb interaction is considered further. For example, in a material having a nested or slightly nested Fermi surface (FS) at some points in the BZ, the resulting response would be enhanced for polarization orientations which highlight the nested or nearly nested regions of the FS. In the case of antiferromagnetic interactions which are strong for momentum transfers of \((\pi, \pi)\) the response is appreciably modified for the \(B_{1g}\) channel in two-dimensional tetragonal systems. The dispersion of these excitations can then be tracked as a function of light momentum transfers \(q\) just as they can via neutron scattering. Thus, in principle, inelastic x-ray scattering systematically tracks the role of correlations and the accompanying FS instabilities by exploring the polarization dependence and momentum transfer dependence of the resulting spectra.

In this paper, we are interested in carrying out calculations in which electronic correlations can be handled exactly in a system which can be tuned through a quantum critical point. The Falicov-Kimball model, which has been used to describe a variety of phenomenon in binary alloys, rare-earth compounds, and intermediate-valence materials, contains itinerant band electrons and localized electrons, in which the band electrons can hop with amplitude \(t^*/2\sqrt{d}\) between nearest neighbors on a \(d\)-dimensional hypercubic lattice and interact via a screened Coulomb interaction \(U\) with the localized electrons:

\[
H = -\frac{t^*}{2\sqrt{d}} \sum_{\langle i,j \rangle} c_i^\dagger c_j + E_f \sum_i w_i - \mu \sum_i c_i^\dagger c_i + U \sum_i c_i^\dagger c_i w_i,
\]

where \(c_i^\dagger\), \(c_i\) is the spinless conduction electron creation (annihilation) operator at site \(i\) and \(w_i = 0\) or 1 is a classical variable for the localized electron number at site \(i\), 
\(E_f\) and \(\mu\) control the filling of the localized and conduction electrons, respectively. We restrict consideration to half filling \(\langle c_i^\dagger c_i \rangle = \langle w_i \rangle = 1/2\).

In this model, at half-filling, the system possesses a non-Fermi liquid metallic ground state for \(U < U_c\) and an insulating state for \(U > U_c\). The single particle density of states (DOS) at the Fermi level (FL) vanishes at the critical \(U_c \approx 1.5t^*\) and the self energy develops a pole. As \(U\) approaches \(U_c\), from below, a pseudogap develops near the FL and for \(U > U_c\), the DOS evolves into lower and upper Hubbard bands separated at the band centers by \(U\). However, the DOS is independent of temperature (aside from a trivial shift due to the temperature dependence of the chemical potential, if applicable) and thus it is not possible to determine the particle dynamics from the single-particle properties alone.

The many-body problem is solved by first recognizing that the self energy and relevant irreducible vertex functions are local and then mapping the local objects of the lattice problem onto an effective atomic problem in a time-dependent dynamical field \(\lambda\). In this procedure, we are interested in calculating the local Green’s function, which is defined by

\[
G(\tau) = -\text{Tr}_{c\bar{f}} \langle \tau \rangle \langle \epsilon - \beta H(c) c^\dagger(0) S(\lambda) \rangle / Z(\lambda)
\]

for imaginary times \(\tau\). Here Tr, denotes the trace over conduction and localized electrons and \(\mathcal{T}\) denotes the time ordering operator. The partition function is

\[
Z(\lambda) = \text{Tr}_{c\bar{f}} \langle \exp[-\beta H] S(\lambda) \rangle \text{ with the evolution operator } S \text{ defined by}
\]

\[
S(\lambda) = \exp \left[-\int_0^\beta d\tau \int_0^\beta d\tau' c^\dagger(\tau)c(\tau') \lambda(\tau, \tau') c(\tau') \right].
\]

In these equations the Hamiltonian is the atomic Hamiltonian, which has \(t^* = 0\) and all time dependence is with respect to this atomic Hamiltonian.

In order to determine the Green’s function anywhere in the complex plane, we follow the iterative algorithm of Jarrell: (i) begin with the self energy \(\Sigma\) set equal to zero; (ii) determine the local lattice Green’s function from the Hilbert transform

\[
G(z) = \int d\epsilon \rho(\epsilon) \frac{1}{z + \mu - \Sigma(z) - \epsilon}
\]

with \(\rho(\epsilon)\) the noninteracting DOS (a Gaussian here); (iii) extract the effective medium \(G_0\) from \(G^{-1}(z) + \Sigma(z) = G_0^{-1}(z)\); (iv) calculate the new Green’s function from \(G(z) = (1 - w_1)G_0(z) + w_1/[G_0^{-1}(z) - U]\); (v) and extract the new self energy from \(\Sigma(z) = G_0^{-1}(z) - G^{-1}(z)\). Steps (ii) through (v) are repeated until the iterations converge. Sometimes we need to perform weighted averages of the iterations to attain convergence. We usually work with solutions that are converged to at least one part in \(10^8\). Using this algorithm, we can determine the Green’s function and self energy either along the imaginary axis, or along the real axis. These solutions are then employed to calculate the inelastic light scattering response functions.

The inelastic light scattering is calculated by evaluating the density-density correlation function defined in Eq. (1). The Bethe-Salpeter equation for the susceptibility is shown schematically in Fig. 1. Note that there
are two coupled equations, which differ by the number of factors of the inelastic light scattering vertex that are present. The solid lines denote dressed Green’s functions in momentum space, and the symbol Γ denotes the local irreducible charge vertex. The calculation of the relevant momentum summations implied in Fig. 1 is nontrivial. The starting point is to determine the direction in momentum space that the transferred momentum \( q \) lies. In this contribution we consider two different directions: (i) the zone diagonal, where \( q = (q, q, q, ..., q) \) and (ii) a generalized “zone boundary”, where \( q = (0, q, 0, q, 0, q, ..., 0, q) \) or \( q = (q, π, q, π, q, π, ..., q, π) \); in all cases we vary \( 0 \leq q \leq π \). We choose to call the wavevector in (ii) the zone-boundary because it reduces to the two-dimensional zone boundary when \( d = 2 \) and it is a nontrivial generalization in the infinite dimensional limit. If, on the other hand, we examined the true infinite-dimensional zone boundary, where only one dimension has a nonzero wavevector component, then that zone boundary maps onto the zone center wavevector (since only one of the \( d \)-components is nonzero), and there is no dispersion. From now on we will refer to the generalized zone-boundary direction as the zone-boundary direction.

When evaluating the density-density correlation function, we will need to evaluate momentum summations of the form:

\[
\sum_\mathbf{k} \sum_\mathbf{j} \cos(k_j + \frac{q_j}{2})
\]

for the \( A_{1g} \) sector and

\[
\sum_\mathbf{k} \sum_{j} \cos(k_j + \frac{q_j}{2})
\]

for the \( B_{1g} \) sector. In the above equations, \( z \) denotes a number in the complex plane. The summation can be evaluated by first rewriting each momentum-dependent Green’s function as an integral of an exponential function

\[
\frac{1}{z + \mu - \Sigma(z) - \epsilon(k)} = -i \int_0^\infty d\lambda e^{i\lambda[z + \mu - \Sigma(z) - \epsilon(k)]},
\]

and then expanding each band-structure energy in terms of the summation over each component of the wavevector. Then the integral over momentum factorizes into an infinite product of one-dimensional integrals. Each integral need be expanded just to the order of \( 1/d \), and the resulting terms can be exponentiated into a form that has a Gaussian dependence on \( \lambda \). The Gaussian integral can then be evaluated directly. When we do this, we find that the relevant bare susceptibilities have all of their \( q \)-dependence summarized in the form of two scalar parameters

\[
X = \lim_{d \to \infty} \frac{1}{d} \sum_{j=1}^{d} \cos q_j
\]

and

\[
X'_{A_{1g}} = \lim_{d \to \infty} \frac{1}{d} \sum_{j=1}^{d} \cos \frac{q_j}{2}
\]

\[
X'_{B_{1g}} = \lim_{d \to \infty} \frac{1}{d} \sum_{j=1}^{d} (-1)^j \cos \frac{q_j}{2}.
\]

In situations where the summation in Eqs. (11) or (12) vanish, then the response function is not renormalized by the irreducible charge vertex, and it can be expressed solely in terms of the bare response function (this phenomenon was first seen for the optical conductivity). This never occurs for the \( A_{1g} \) channel, but it does for the \( B_{1g} \) channel when \( q \) lies on the zone diagonal. In all other cases, the response function is renormalized by the irreducible charge vertex which takes the form

\[
\Gamma(i\omega_m, i\omega_n; i\nu_l \neq 0) = \delta_{mn} \frac{1}{T} \frac{\Sigma_m - \Sigma_{m+l}}{G_m - G_{m+l}}.
\]

on the imaginary axis [\( i\omega_m = i\pi T(2m + 1) \) is the Fermionic Matsubara frequency and \( i\nu_l = 2i\pi Tl \) is the bosonic Matsubara frequency]. Here \( \Sigma_m = \Sigma(i\omega_m) \) is the local self energy on the imaginary axis and \( G_m = G(i\omega_m) \)
is the local Green’s function on the imaginary axis. These vertex corrections are particularly crucial for the $A_{1g}$ symmetry in order to satisfy Ward identities and particle-number conservation. Note that the vertex corrections enter for the different symmetry channels away from the zone diagonal because at a finite momentum transfer, the different symmetry representations generically mix together.

The strategy for determining the final forms for the response functions on the real axis is to first calculate the response functions on the imaginary axis, then replace Matsubara frequency summations by contour integrals that surround the poles of the Fermi-Dirac distribution function $f(\omega) = 1/[1 + \exp(\beta \omega)]$ with $\beta = 1/T$. Then the contours are deformed to be parallel to the real axis, and terms that depend on the Bosonic Matsubara frequency as $f(\omega + i\eta)$ are replaced by $f(\omega)$. Finally, we analytically continue the Bosonic Matsubara frequency to the real axis. This procedure was carried out in detail for the Raman response, and will not be repeated here.

The final formulas for the response functions are complicated integrals of functions that depend on one of six different bare susceptibilities are

\begin{align}
\chi_0(\omega; X, \nu) &= - \int_{-\infty}^{\infty} d\rho(\epsilon) \frac{1}{\omega + \mu - \Sigma(\omega) - \epsilon} \frac{1}{\sqrt{1 - X^2}} F_\infty \left( \frac{\omega + \nu + \mu - \Sigma(\omega + \nu) - X \epsilon}{\sqrt{1 - X^2}} \right), \\
\tilde{\chi}_0(\omega; X, \nu) &= - \int_{-\infty}^{\infty} d\rho(\epsilon) \frac{1}{\omega + \mu - \Sigma^*(\omega) - \epsilon} \frac{1}{\sqrt{1 - X^2}} F_\infty \left( \frac{\omega + \nu + \mu - \Sigma(\omega + \nu) - X \epsilon}{\sqrt{1 - X^2}} \right), \\
\chi'_0(\omega; X, \nu) &= \frac{X'}{2} \int_{-\infty}^{\infty} d\rho(\epsilon) \left\{ \frac{1}{\sqrt{1 - X^2}} F_\infty \left( \frac{\omega + \nu + \mu - \Sigma(\omega + \nu) - X \epsilon}{\sqrt{1 - X^2}} \right) \right. \\
&\quad \left. \frac{1}{\omega + \mu - \Sigma^*(\omega) - \epsilon} \right\} \frac{1}{\sqrt{1 - X^2}} F_\infty \left( \frac{\omega + \nu + \mu - \Sigma(\omega + \nu) - X \epsilon}{\sqrt{1 - X^2}} \right), \\
\tilde{\chi}'_0(\omega; X, \nu) &= \frac{X'}{2} \int_{-\infty}^{\infty} d\rho(\epsilon) \left\{ \frac{1}{\sqrt{1 - X^2}} F_\infty \left( \frac{\omega + \nu + \mu - \Sigma(\omega + \nu) - X \epsilon}{\sqrt{1 - X^2}} \right) \right. \\
&\quad \left. \frac{1}{\omega + \mu - \Sigma^*(\omega) - \epsilon} \right\} \frac{1}{\sqrt{1 - X^2}} F_\infty \left( \frac{\omega + \nu + \mu - \Sigma(\omega + \nu) - X \epsilon}{\sqrt{1 - X^2}} \right), \\
\bar{\chi}_0(\omega; X, \nu) &= \frac{1}{2} \chi_0(\omega; X, \nu) - \frac{X'^2}{2} \int_{-\infty}^{\infty} d\rho(\epsilon) \left\{ \frac{1}{\sqrt{1 - X^2}} F_\infty \left( \frac{\omega + \nu + \mu - \Sigma(\omega + \nu) - X \epsilon}{\sqrt{1 - X^2}} \right) \right. \\
&\quad \left. \frac{1}{|\omega + \mu - \Sigma^*(\omega) - \epsilon|^3} \right\} \frac{1}{\sqrt{1 - X^2}} F_\infty \left( \frac{\omega + \nu + \mu - \Sigma(\omega + \nu) - X \epsilon}{\sqrt{1 - X^2}} \right), \\
\bar{\tilde{\chi}}_0(\omega; X, \nu) &= \frac{1}{2} \tilde{\chi}_0(\omega; X, \nu) - \frac{X'^2}{2} \int_{-\infty}^{\infty} d\rho(\epsilon) \left\{ \frac{1}{\sqrt{1 - X^2}} F_\infty \left( \frac{\omega + \nu + \mu - \Sigma(\omega + \nu) - X \epsilon}{\sqrt{1 - X^2}} \right) \right. \\
&\quad \left. \frac{1}{|\omega + \mu - \Sigma^*(\omega) - \epsilon|^3} \right\} \frac{1}{\sqrt{1 - X^2}} F_\infty \left( \frac{\omega + \nu + \mu - \Sigma(\omega + \nu) - X \epsilon}{\sqrt{1 - X^2}} \right),
\end{align}
In these equations, $F_\infty(z) = \int d\rho(\epsilon)/(z - \epsilon)$, is the Hilbert transform of the noninteracting DOS $[\rho(\epsilon) = \exp(-\epsilon^2)/\sqrt{\pi}]$. The $A_{1g}$ and $B_{1g}$ responses both can be written as

$$
\chi(q, \nu) = \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \left\{ f(\omega) \bar{\chi}_0(\omega; X, \nu) + \frac{\Sigma(\omega) - \Sigma(\omega + \nu)}{\Sigma(\omega) - \Sigma(\omega + \nu + \nu)} \chi_0(\omega; X, \nu) \bar{\chi}_0(\omega; X, \nu) - \chi_0^2(\omega; X, \nu) \right\} 
- f(\omega + \nu) \left\{ \bar{\chi}_0(\omega; X, \nu) + \frac{\Sigma(\omega) - \Sigma(\omega + \nu)}{\Sigma(\omega) - \Sigma(\omega + \nu + \nu)} \chi_0(\omega; X, \nu) \bar{\chi}_0(\omega; X, \nu) - \chi_0^2(\omega; X, \nu) \right\} 
- [f(\omega) - f(\omega + \nu)] \left\{ \bar{\chi}_0(\omega; X, \nu) - [f(\omega) - f(\omega + \nu)] \chi_0(\omega; X, \nu) \right\} \right\} (22)
$$

In the case of the $A_{1g}$ response on the zone diagonal $q = (q, q, ..., q)$, we have $X = \cos q$ and $X' = \cos \frac{q}{2} = \sqrt{1 + X}/2$. In these equations, the $A_{1g}$ response on the zone edge we have $X = (1 + \cos q)/2$ and $X' = (1 + \cos \frac{q}{2})/2 = (1 + \sqrt{X}/2$ for $q = (0, 0, 0, ..., 0)$ and $X = (\cos q - 1)/2$ and $X' = \cos \frac{q}{2} = \sqrt{1 + X}/2$ for $q = (q, q, q, ..., q, \pi)$. In the case of the $B_{1g}$ response on the zone diagonal, we have $X = (1 + \cos q)/2$ and $X' = -(1 + \cos \frac{q}{2})/2 = -(1 + \sqrt{X})/2$ for $q = (0, 0, 0, ..., 0)$ and $X = (\cos q - 1)/2$ and $X' = \cos \frac{q}{2} = -\sqrt{1 + X}/2$ for $q = (q, q, q, ..., q, \pi)$. The case of the $B_{1g}$ response on the zone diagonal is much simpler, because it does not have any renormalizations due to the charge vertex and doesn’t depend on $X'$. It becomes

$$
\chi_{B_{1g}}(q, \nu) = \frac{i}{4\pi} \int_{-\infty}^{\infty} d\omega \left\{ f(\omega) \chi_0(\omega; X, \nu) - f(\omega + \nu) \right\} \chi_0(\omega; X, \nu) \right\} \right\} (23)
$$

At half filling, the x-ray response function has an extra symmetry $\chi(q, \nu) = \chi^*(q, -\nu)$ for both the $A_{1g}$ and $B_{1g}$ channels. This symmetry is straightforward, but tedious to prove. First note that at half filling we have $G(-\omega) = G^*(\omega)$ and $\Sigma(-\omega) = 2\mu - \Sigma^*(\omega)$. Using these results, one can directly show the following six identities: $\chi_0(\omega; X, \nu) = \chi_0^*(-\omega - \nu; X, \nu)$; $\chi_0(\omega; X, \nu) = \chi_0^*(-\omega - \nu; X, \nu)$; $\chi_0(\omega; X, \nu) = -\chi_0^*(-\omega - \nu; X, \nu)$; $\chi_0(\omega; X, \nu) = -\chi_0^*(-\omega - \nu; X, \nu)$; $\chi_0(\omega; X, \nu) = \chi_0^*(-\omega - \nu; X, \nu)$; and $\bar{\chi}_0(\omega; X, \nu) = \bar{\chi}_0^*(\omega + \nu; X, \nu)$. Now if we substitute $\omega \rightarrow -\omega$ in the integral similar to Eq. (22) for $\chi(q, \nu)$, replace $f(-\omega)$ by $1 - f(\omega)$, and employ the above identities for the different $\chi_0$’s, then the integral for $\chi(q, \nu)$ can be shown to be equal to $\chi^*(q, \nu)$ plus the imaginary part of an integral equal to the first term in Eq. (22) without the $f(\omega)$ factor. But one can see that the resulting integral is real, which proves the symmetry for the response function. A similar argument shows the bare bubble for the $B_{1g}$ response on the zone diagonal also satisfies $\chi(q, -\nu) = \chi^*(q, \nu)$.

There is a special point in momentum space, where the response functions become simple again. This occurs at the $(\pi, \pi, ..., \pi)$ point, where $X = -1$ and $X' = 0$. In this case, $\chi_0 = 0$ and $\bar{\chi}_0$ is proportional to $\chi_0$, so the Bethe-Salpeter equation factorizes, and the susceptibility in Eq. (22) becomes proportional to the bare susceptibility for any symmetry. Hence the $A_{1g}$ response and the $B_{1g}$ response are identical at that point in the BZ. In fact, this result implies that polarized measurements at the zone corner point can immediately show the effects of nonlocal charge fluctuations on the inelastic x-ray response functions, since any deviation of the $A_{1g}$ signal from the $B_{1g}$ signal arises from effects of nonlocal charge fluctuations.

We feel this may be one of the cleanest experimental tests for the importance of nonlocal charge fluctuations in a correlated many-body system.

Finally, a careful examination of Eqs. (16–22) shows that the response function depends only on $X'$ and $X''$. Since the only difference for the $A_{1g}$ and $B_{1g}$ responses along the zone edge (for $1 \leq X' \leq 0$) is a sign change in $X'$, the x-ray scattering is identical for the $A_{1g}$ and $B_{1g}$ channels along the zone edge for $-1 \leq X < 0$. It might be difficult to locate the relevant path in the BZ that would show this behavior in two or three dimensions, so examining the zone corner for the effects of nonlocal charge fluctuations still remains the best bet.

IV. RESULTS

A. Correlated metal

With the summary of what we expect for weakly correlated metals in mind, we present the results for $U = t'/2$ at different temperatures in Figs. 2 and 3 for $B_{1g}$ and $A_{1g}$ inelastic x-ray scattering, respectively, as a function of transferred energy for different momentum transfers throughout the BZ measured by the momentum-space parameter $X$. Panel (a) for Figs. 2 and 3 refers to scattering along the zone diagonal $X = \cos q$ for the zone-diagonal wavevector $q = (q, q, q, ..., q, q)$ and panel (b) refers to scattering along the generalized zone edge [here we have $q = (q, 0, q, 0, ..., q, 0)$ for $1 \geq X = (1 + \cos q)/2 \geq 0$ and $q = (\pi, q, \pi, ..., \pi, q)$ for $0 \geq X = -(1 + \cos q)/2 \geq -1$]. The curves have been shifted vertically for clarity. The lowest set of curves $X = 1$
corresponds to Raman scattering with optical photons.30

For the $B_{1g}$ channel (Fig. 2), a well defined low energy Fermi-like coherence peak (below $U = 0.5t^*$) moves to higher energies and broadens as one moves away from the zone center ($X = 1$), as would be expected of Landau damping via particle-hole creation at larger $q$. (recall the Falicov-Kimball model is not a Fermi liquid for small enough $U$, but can be viewed as a “dirty” Fermi liquid for small enough $U$). In addition, the peak sharpens with decreasing temperature as the channels for Landau damping are lost. No particular signature can be seen at the energy transfer of $U$ since it falls within the lifetime of the Fermi-like coherence peak, and thus the role of electronic correlations, while present, are obscured by the larger Landau damping.

In Fig. 3 we plot the position and width of the low energy peak for the $B_{1g}$ channel for momentum transfers along the BZ diagonal. The peak moves to higher frequencies from $\sim 0.25t^*$ for small momentum transfers $X < 1$ and reaches a maximum $\sim t^*$ for momentum transfers slightly greater than $(\pi/2, \pi/2, \cdots)$ before softening as the BZ corner $(\pi, \pi, \cdots)$ is approached. In fact, the peak position is comparable to $U$ for large momentum transfers in all directions. The width of the peak grows continually with increasing $q$ as more and more phase-space is created by which charge excitations may relax. The width initially grows like $q^2$ for momentum transfers away from the BZ center and then slows its growth rate farther from the zone center (recall that $X = \cos \theta$ so an initial $q^2$ dependence translates into a linear dependence on $X$).

An important difference is that the $A_{1g}$ results have no low-energy spectral weight for $q = 0$ as a result of particle-number conservation. In a model with long-range Coulomb interactions, the only excitation would be a high energy plasmon which is soft for uncharged systems but is pushed up to higher energies via the Higgs mechanism by the Coulomb interaction. In our short-range model, a mild peak occurs on the energy scale of both $U$ and the bandwidth at the zone center (we cannot differentiate which one dominates). The vertex corrections do not completely remove low energy scattering for any finite value of $q$, and the low energy spectral weight grows for increasing $q$ either along the zone diagonal or zone edge. For large $q$, the $A_{1g}$ spectra have a temperature dependence similar to the $B_{1g}$ response, dominated by particle-hole excitations. In fact, the $A_{1g}$ and $B_{1g}$ responses are identical at the $(\pi, \pi, \cdots)$ point $X = -1$ due to the local approximation. Any variation in the signal at the zone corner in different symmetry channels is due to nonlocal many-body correlations.

For low $q$ however (such as $X = 0.5$), the temperature dependence is nonmonotonic due to a competition between increased vertex corrections, which deplete spectral weight, and decreased particle-hole damping, which aggregates spectral weight into the Fermi-like coherence peak as the temperature is reduced. It is important to note that for an unpolarized (partially polarized) measurement, the x-ray response is a (weighted) superposition of the $B_{1g}$ and $A_{1g}$ spectra. However, the spectra at small $q$ in a metal would largely have contributions from the $B_{1g}$ channel due to the significant phase space reduction in the $A_{1g}$ channel.

B. Near Critical dynamics

Now we turn to our results for a near critical value of $U = 1.5t^* \approx U_c$ where the density of states vanishes at the Fermi level and the system undergoes a metal-
insulator transition (our choice for $U$ lies just on the insulating side of the metal-insulator transition). We plot in Figs. 3 and 4 the results for the $B_{1g}$ and $A_{1g}$ channels, respectively, for the same temperature ranges as in the previous plots. The effect of electronic correlations is clearly visible. For both the $B_{1g}$ and the $A_{1g}$ spectra, two peaks become discernable at small $\mathbf{q}$: the low energy peak (similar to the one seen for smaller values of $U$), and a non-dispersive high-energy peak (at an energy of roughly $U$ corresponding to transitions between the lower and upper Hubbard band). Indeed the results at large $\mathbf{q}$ are more similar to the small $U$ results since the Landau damping pushes the low frequency peak into the high frequency peak and further smears both peaks. Again, the low energy peak is removed near the zone center for the $A_{1g}$ channel, but in this case the charge-transfer peak (at a frequency near $U$) remains.

It is important to note that even though the system is near critical, low energy spectral weight is visible, particularly in the $B_{1g}$ channel. We focus now on the spectral weight in this region as a function of temperature, shown in Fig. 4. In this low frequency region one can clearly see for the $B_{1g}$ channel that the low energy spectral weight increases with increasing temperature throughout the BZ. This is most clearly seen at $\mathbf{q} = 0$. For the $A_{1g}$ channel the same behavior is masked by the role of vertex corrections which reduce the spectral weight for momentum transfers near the BZ center. Nevertheless, the growth of intensity with increasing temperature is clearly seen in both channels. The growth is particularly clear at low frequency transfers and for increasing transfers the effect vanishes and crosses over at larger frequencies to a region where spectral weight depletes as temperature is increased. The point separating these regions occurs at a crude isosbestic point near $\sim 0.5t^*$, where the spectra are roughly independent of temperature. The isosbestic point becomes less well-defined for momentum transfers away from the zone center, and therefore it is most clearly observable in Raman measurements in the $B_{1g}$ channel. As the temperature is increased further, the isosbestic behavior disappears.

C. Insulator

Turning to the insulating phase, our results for $U = 2t^*$ for the $B_{1g}$ and $A_{1g}$ channel are shown in Figs. 5 and 6, respectively. Clearly two features can be resolved in both the $B_{1g}$ and $A_{1g}$ channel: a small, dispersive low-energy peak for frequencies $\sim t^*$ and a large, dispersionless charge-transfer peak $\sim U$ well separated from the low-energy peak. Here we see more clearly the develop-
FIG. 7: Detail of the low energy inelastic x-ray scattering response $U = 1.5t^*$ along the zone diagonal for (a) the $B_{1g}$ channel and (b) the $A_{1g}$ channel for the temperatures shown in Figs. 8 and 9.

FIG. 8: Inelastic x-ray scattering response $U = 2t^*$ in the $B_{1g}$ channel along (a) the BZ diagonal and (b) along the zone edge. The solid, dotted, short-dashed and long-dashed curves correspond to temperatures $T = 0.1, 0.25, 0.5, 1.0$, respectively.

FIG. 9: Inelastic x-ray scattering response $U = 2t^*$ in the $A_{1g}$ channel along (a) the BZ diagonal and (b) along the zone edge. The solid, dotted, short-dashed and long-dashed curves correspond to temperatures $T = 0.1, 0.25, 0.5, 1.0$, respectively.

of the correlations. In contrast, the low-energy feature is a consequence of thermally generated double occupancies which open a low-energy band (up to energies $\sim t^*$) able to scatter x-rays. The low energy peak disperses due to Landau damping by the thermally generated excitations, created in greater numbers at larger $q$. These excitations are frozen out for decreasing temperature and the low-energy intensity disappears. Only scattering across the Mott gap remains at an energy transfer of $U$. The charge-transfer peak for all $q$ broadens for increasing temperature while the low-energy peak gains intensity from zero as temperature is increased, particularly in the $B_{1g}$ channel. As a consequence, both $B_{1g}$ and $A_{1g}$ possess a non-dispersive isosbestic point—a frequency at which the spectra are temperature independent—around $\nu \sim U/2$. This result agrees with our previous results for $U = 4$ in which the two peaks are further separated and the isosbestic point is more clearly observed.

We note that even in the insulating case there is no spectral weight at small energy transfers for the $A_{1g}$ channel. Thus we note that regardless of the strength of the correlations, the Raman response ($q=0$) and the inelastic x-ray response at small $q$ should be dominated by the $B_{1g}$ response. This can be an important diagnostic tool for investigating the nature of charge dynamics in different regions of the BZ due to the projection of the $B_{1g}$ scattering amplitude form factors compared to $A_{1g}$.

V. SUMMARY AND DISCUSSION

In summary, we have constructed a formally exact theory for non-resonant x-ray scattering in a system which can be tuned across a quantum metal-insulator transition. We focused on the polarization and momentum...
transfer dependence of the resulting spectra as a way of discerning the role of electron correlations. In particular, the way in which spectral weight is transferred over different frequency regions as a function of temperature can shed important light on the strength of the electronic correlations, and the momentum dependence of the observed spectra can be used to determine “hot regions” on the FS. In general, the temperature and polarization dependence of the spectrum would assist in an interpretation of observed peaks in the x-ray spectrum of correlated insulators for example.

In addition we have pointed out a number of features which reflect the nature of the electronic correlations. One important finding concerns the polarization dependence of the results for momentum transfers at the BZ corner ($\pi, \pi, ... \pi$). In a theory in which the correlations are purely local we find that the response function should be identical at this point for both $A_{1g}$ and $B_{1g}$ scattering geometries and that any differences can be attributed to the importance of non-local correlations (indeed, they are identical for $-1 \leq X \leq 0$ along the generalized zone boundary). In addition we have pointed out that for low $q$ the full response is dominated by the $B_{1g}$ channel which projects out particle-hole excitations. Thus in this limit, the excitations can be directly probed and tracked as a function of temperature.

There is currently limited experimental data concerning the polarization and/or temperature dependence of the observed spectra in either correlated metals or insulators and thus many of our predictions remain open to experimental verification. At this stage current experiments have focused on collective excitations such as the plasmons or excitons or excitations across a Mott gap in correlated insulators. Our theory would predict several new effects which could serve as a fingerprint of the role of electronic correlations in both correlated metals and insulators by a systematic study of the dependence on temperature and polarization orientations. In particular one could use x-ray scattering to elucidate electron dynamics near and through a quantum critical metal-insulator transition.

Our theory does not address the role of resonant scattering and the connection to multiband systems. To capture resonance effects, detailed information is needed about the energy separation of the various bands as well as the matrix elements which couple the valence and conduction bands via light scattering. For a Mott insulator this would include resonant transitions between the upper and lower Hubbard bands as well as between excitons. Recently this has been addressed via exact diagonalization studies and a spin-polaron approach, and its formulation for the Falicov-Kimball model is currently under investigation by us. A more realistic theory for resonant inelastic x-ray scattering should also include resonant transitions in which the deep core hole (created by the incident x-ray) decays via Auger processes and must also include the strong perturbing effect of the core hole on any intermediate states (such as band states or collective modes of the system such as plasmons or magnons) accessible to scattering transitions.

We have also chosen to focus on the paramagnetic metal to paramagnetic insulator transition. The Falicov-Kimball model however possesses phases containing charge order and phase separation. It would be extremely useful to examine the excitations in the ordered phases via light scattering in this model. More generally, dynamical mean field theory can be used to address the excitations in the ordered phase of this model as well as the Hubbard model.

We close with a discussion of the applicability of our results for the limit of large dimensions to finite dimensional systems. One important consequence of lower dimensions would be that the self energy and irreducible vertex function will not be strictly local and the momentum dependence may crucially alter not only the formalism but also the spectral evolution of the response as correlations are changed via doping. Particularly the spectra might show dispersive features which are much more complex than the ones we observed in these calculations. We again note that the inelastic x-ray spectra for momentum transfers at the BZ corner would be very useful to quantify the importance of these non-local correlations. One should note, however, that the “roughness” of the Fermi surface actually simplifies as the dimensionality is lowered, so the infinite-$d$ results already include many complex geometrical effects of the infinite-dimensional hypercubic Fermi surface.

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