Inelastic X-ray scattering from valence electrons near absorption edges of FeTe and TiSe$_2$

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(Dated: July 4, 2014)

We study resonant inelastic x-ray scattering (RIXS) peaks corresponding to low energy particle-hole excited states of metallic FeTe and semi-metallic TiSe$_2$ for photon incident energy tuned near the $L_3$ absorption edge of Fe and Ti respectively. We show that the cross section amplitudes are well described within a renormalization group theory where the effect of the core electrons is captured by effective dielectric functions expressed in terms of the the atomic scattering parameters $f_1$ of Fe and Ti. This method can be used to extract the dynamical structure factor from experimental RIXS spectra in metallic systems.

PACS numbers: 78.70.Ck,71.15.Qe,71.15.Mb

I. INTRODUCTION

Inelastic x-ray scattering (IXS) probes charge and spin electronic excitations in condensed matter but the corresponding cross section is generally small, especially at incident energy tuned slightly lower than the absorption threshold.

In order to explore the scattering of nearly-free electrons by a photon tuned near the binding energy of a core level, we have introduced a scheme based on the renormalization group (RG) theory able to cast the complicated RIXS problem to a much simpler IXS problem in an effective medium described by an effective dielectric function $\epsilon$, which integrates out the effect of the core electrons. In the RG approach, a differential equation describing the evolution of the coupling constant with screening yields the renormalization factor $\eta$ for the effective Thomson cross section in the polarizable medium. This method effectively allows one to calculate the incident photon energy dependence of the RIXS cross section in the case of a metallic system. Recently, Haverkort has shown that effective models based on the absorption spectra can give a good description of RIXS, although his approach was applied to spin excitations in strongly correlated systems rather than charge excitation in metallic systems as in the present case.

The present work studies high resolution measurements near the Fe $L_3$ edge of Fe$_{1.087}$Te and the Ti $L_3$ edge of TiSe$_2$ by considering low energy particle-hole scattering peaks as a function of incident photon energy. Previous RIXS studies at the $L_3$ edge of Cu and Ni performed at lower resolution have neglected momentum conservation. Based on the changes in intensity of these peaks, we show that the resonant scattering cross section can be described via a renormalization factor $\eta$ multiplying the non-resonant IXS cross section. In principle, the knowledge of the dynamical structure factor permits us to extract band structure information from measured dispersing electron-hole excitations. It also allows reconstructions of the density propagator of a system, which yields the time dependent linear response of the system to a point perturbation. Therefore, momentum dependent...
RIXS can become a unique window for visualizing the dynamics of weakly bound electrons in condensed matter.

An outline of this paper is as follows. Section II summarizes our model. In Sec. III, we present the methods for the electronic structure calculations and for the RIXS experiments. The results of the calculations are presented and compared with experimental results in Sec. IV, and the conclusions are given in Sec. V.

II. MODEL

In our model, the low-energy-loss scattering leads to particle-hole excited states of the valence electron system described by the double differential scattering cross-section, which is the product of the effective Thomson scattering cross section $d\sigma_{Th}/d\Omega$ and of the dynamical structure factor $S(q, \omega)$:

$$\frac{d^2 \sigma}{d\Omega d\omega} = \frac{d\sigma_{Th}^*}{d\Omega} S(q, \omega). \quad (1)$$

For particle-hole excitations the dynamical structure factor is given by:

$$S(q, \omega) = \int_{-\omega}^{0} dE \int \frac{d^3 p}{(2\pi)^3} A(p, E) A(p + q, E + \omega), \quad (2)$$

where $(q, \omega)$ are the momentum and energy transfer and $A(p, E) = (1/\pi) \text{Im}[G(p, E)]$ is the imaginary part of the electron Greens function $G(p, E)$. The spectral function $A(p, E)$ can be also expressed in terms of the Dyson orbitals $g_{\nu}$ as follows:

$$A(p, \omega) = \sum_{\nu} |g_{\nu}(p)|^2 A_{\nu}(\omega), \quad (3)$$

and

$$A_{\nu}(\omega) = \frac{\gamma}{\pi[(\omega - \epsilon_{\nu})^2 + \gamma^2]}, \quad (4)$$

where $\epsilon_{\nu}$ is the excitation energy of the Dyson orbital $g_{\nu}(r)$ and $\gamma$ is an inverse lifetime. In the present case, the Dyson orbitals are given by Bloch wave functions, where $\nu = (k, n)$ is given by the Bloch wave vector $k$ and by the energy band index $n$. Therefore one can write

$$g_{k, n}(r) = \exp(i k \cdot r) \sum_{G} C_{G}^{k, n} \exp(-i G \cdot r), \quad (5)$$

whose momentum density is

$$|g_{k, n}(p)|^2 = \sum_{G} \delta(p-k+G) |C_{G}^{k, n}|^2. \quad (6)$$

The Fourier coefficients $C_{G}^{k, n}$ of the periodic part of $g_{k, n}(r)$ are labeled by the reciprocal vectors $G$. Therefore, the spectral functions enforce the energy conservation near the Fermi level and the momentum conservation in the first Brillouin zone.

Because of the proximity of the $L_3$ absorption threshold, the incoming photon generates a set of virtual intermediate states involving a $2p$ core hole and a corresponding electron excited in a $3d$ state which can be described by an effective dielectric function $\epsilon$ experienced by the valence electrons. When the scattering process is completed, it leaves behind low-lying valence excited states conserving energy and crystal momentum and the Thomson cross section $\sigma_{Th}$ of this resonant scattering is increased by the factor $\eta$ compared to the non resonant cross section. The solution of the renormalization group equation gives

$$\eta = \exp\left(\frac{2}{3\alpha}(\epsilon/\epsilon_0 - 1)\right), \quad (7)$$

where $\alpha$ is the fine structure constant, $\epsilon$ is the real part of an effective dielectric function for the valence electrons as a function of energy $\omega$ and $\epsilon_0$ is the dielectric constant in vacuum. One can connect $\epsilon$ to the atomic scattering parameter $f_1$ through the formula

$$\frac{\epsilon}{\epsilon_0} = 1 - (\frac{\omega_p}{\omega})^2 f_1, \quad (8)$$

where $\omega_p$ is the plasma frequency for the valence electron gas at the Fermi level, which can be written as

$$\omega_p = 47.1 \ r_s^{-3/2} \text{ eV}, \quad (9)$$

where $r_s$ is the radius containing a valence electron. The parameter $f_1$ is related to the absorption coefficient $\mu(E)$ via the Kramers-Kröning transform:

$$f_1(E) = Z + 2 \frac{\omega_p^2}{E^2} \int_0^\infty \frac{\mu(\omega)}{E^2 - \omega^2} d\omega, \quad (10)$$

where $Z$ is the atomic charge. The cross section enhancement occurs only if $f_1$ is negative. The parameter $f_1$ can be also determined by reflectivity experiments. The enhancement term is therefore given by

$$\eta = \exp(-\frac{2}{3\alpha}(\frac{\omega_p}{\omega})^2 f_1), \quad (11)$$

and it can be expanded in a power series of the parameter $f_1$ which contains a Lorentz oscillator for the core $2p$ electrons appearing also in the KH treatment of RIXS.

III. COMPUTATIONAL AND EXPERIMENTAL METHODS

We have calculated $f_1$ from first-principles using the program FDMNES within the Time Dependent Density Functional Theory (TDDFT). First, we have performed local density approximation self-consistent calculations for FeTe and TiSe$_2$, and then we computed $f_1$ at the Fe $L_3$ edge and at the Ti $L_3$ edge using TDDFT. The calculations for Ti are performed for the $L_3$ and the $L_2$ edges since the $L_2$ edge influences the $f_1$ value near the...
$L_3$ edge. The influence of the $L_2$ edge can be neglected in Fe since the separation between the $L_2$ and the $L_3$ edge is larger in this case. The crystal structure of FeTe is tetragonal with point group $P4/nmm$ and lattice constants $a = b = 3.8215$ Å, $c = 6.2695$ Å while the crystal structure of TiSe$_2$ has a point group $P-3m1$ with lattice constants $a = b = 3.54$ Å and $c = 6.008$ Å.

The experimental RIXS spectra considered in this paper were taken at the ADDRESS beam line$^{32}$ of the Swiss Light Source, Paul Scherrer Institut, using the SAXES spectrometer$^{33}$. A scattering angle of 130° was used, and the samples were measured at an incidence angle of 65°, using $\sigma$-polarized light. At the Ti $L_3$ edge, the combined energy resolution was 90 meV. TiSe$_2$ samples were measured at 16K. At the Fe $L_3$ edge, the combined energy resolution was 73 meV. The FeTe samples were measured near 20K. Our results showing the inelastic peak height dependence on the incident photon energy were obtained by integrating the RIXS intensity between 0.1 and 4.0 eV energy loss for FeTe and between 0.1 and 0.6 eV energy loss for TiSe$_2$, after having subtracted a linear background and the elastic line. Our RIXS spectra were also corrected for self-absorption effects, following the method used in Ref. 13. The elastic line has also been removed.

IV. RESULTS

We show in Fig. 1 a resonant feature below the Fe $L_3$ threshold of Fe$_{1.087}$Te. The subthreshold peak energy locks to a constant value of 0.9 eV while the RIXS line shape preserves its shape. Interestingly, the momentum transfer of this peak is $q = 0.51$ Å, and the energy transfer of about 0.9 eV corresponds to the recoil energy of an electron or a hole $q^2/(2m^*)$ with an effective mass $m^* \sim 1$. This feature is also consistent with excitations associated with bands crossing the Fermi level around the $\Gamma$ point forming small hole pockets and around the $M$ point giving small electron pockets. Similar Fermi surfaces are also found in the LaO$_{1-x}$Fe$_2$As iron pnictide compounds$^{34,35}$. The calculated $f_1$ as a function of incident energy is shown in the top frame of Fig. 2 together with $f_1$ data from total electron yield experiments in pure iron$^{36}$. The agreement between the two curves is quite impressive. Therefore, the behavior of $f_1$ is very similar in Fe$_{1.087}$Te and in pure iron. This result confirms that the x-ray absorption for materials related to iron pnictides is qualitatively similar to Fe metal$^{37}$ but also very different from Fe ions in the Li$_x$FePO$_4$ compound for the Li-battery cathode$^{38}$, where multiplet calculations must be included. In the bottom frame of Fig. 2 the inelastic peak height is plotted against incident energy together with the theoretical enhancement $\eta$. We have used the value $r_s = 1.60$ a.u., which is consistent with the plasmon energy losses associated with the Fe 1s core level. The corresponding plasma energy of the Fe 3d shell is 23.3 eV. The overall agreement between the experimental data and $\eta$ is good below the threshold energy of 705 eV, and it remains reasonable after this threshold despite the fact that the present theory does not include the resonant x-ray emission described by KH. The enhancement

![FIG. 1. (Color online) Focus on the RIXS subthreshold feature of Fe$_{1.087}$Te. We concentrate on the 0.9 eV energy loss; however, we consider the area below 0.1 and 4.0 eV to estimate the enhancement of the peak. This spectrum has been corrected for self-absorption effects, following the method used in Ref. 13. The elastic line has also been removed.](image)

![FIG. 2. (Color online) Fe $L_3$ edge of Fe$_{1.087}$Te: In the top frame the solid curve represents the model for $f_1$ as a function of the incident energy. The dashed curve represents $f_1$ data from total electron yield experiments in pure iron. The label "solid" emphasizes that the parameter $f_1$ for the solid is different from the one calculated for free atoms. In the bottom frame the black circles and the solid curve are inelastic peak height and the model with $f_1$ from FDMNES respectively, plotted against incident energy.](image)
The factor $\eta$ is very large, and it approaches a value as large as 87.

In the case of TiSe$_2$, the choice of the parameter $r_s = 3.0$ yields a screening length $\lambda = \sqrt{1.56r_s} = 2.16 \text{ a.u.}$ within the Thomas Fermi model, which is consistent with the measured plasma frequency. This larger $r_s$ value gives a much smaller enhancement $\eta$ compared to the FeTe case, which reaches a factor of 14 at most. The FDMNES calculation of $f_1$ yields amplitudes of about $-77$ around an energy of 458 eV. In the present case, well defined particle-hole features given by $S(q, \omega)$ dominate the fluorescent contributions in agreement with the findings by Monney et al. The $L_2$ and $L_3$ edges of Ti almost overlap. Therefore, one must perform a calculation for both edges at the same time in order to have an accurate description of the amplitude $f_1$. The TDDFT must also be applied in order to describe many-electron effects which modify the ratio of the $L_2$ and $L_3$ contributions. However, as shown in the bottom of Fig. 3, the agreement with the experiment is still not perfect, despite the models ability to capture the main amplitude in the RIXS signal.

To illustrate our approach, we calculate the dynamical structure factor $S(q, \omega)$ for four bands near the Fermi level, as performed previously to understand electron-hole excitation dispersions in the charge density wave phase of TiSe$_2$. These four bands are depicted in Fig. 4 (a) and correspond to a model band structure of the charge density wave in TiSe$_2$, inspired by angle-resolved photoemission spectroscopy experiments. Transitions between the lowest occupied band and the highest unoccupied band give rise to the dispersive peak at high energy losses in RIXS, while transitions between the partially occupied bands and the highest unoccupied one give rise to the dispersive peak at low energy losses. The corresponding spectral functions have been broadened using a Gaussian function to account for the experimental resolution. Figure 4 (b) shows the resulting RIXS spectra as a function of the transferred momentum of light projected on the surface plane of the sample, $q_{||}$. These spectra are given by an energy-loss- and momentum-resolved convolution of the occupied and unoccupied band structure, which approximates Eq. 1. Reference 21 shows that such a convolution compares very well with the measured $q$-dependent RIXS spectra for an incident photon energy maximizing the cross section. According to Eq. 1, the cross section can be obtained using the enhancement term $\eta$ given by Eq. 11. Figure 4 (c) shows selected calculated RIXS spectra (solid lines) obtained with the dynamical structure factor function at $q_{||} = 0$ and multiplied by the enhancement factor $\eta$ for TiSe$_2$. For comparison, we show in the same panel the corresponding experimental RIXS spectra (dotted lines) of TiSe$_2$ at different incident photon energies, (see Ref. 21 for more details). Thus, this example illustrates the present RIXS model for particle-hole excitations in metallic systems. This scheme factorizes the RIXS signal in an incident-energy dependent part describing the resonance behavior multiplied by an energy-loss and momentum dependent term for the excitation dispersion.

V. CONCLUSIONS

We propose, by using a renormalization group approach, to simplify the description of RIXS for the particle-hole excitations in metallic systems. For this
purpose, we connect $S(q, \omega)$ to an effective scattering cross section where the amplification factor $\eta$ is directly related to the atomic scattering parameter $f_1(\omega)$, which is strongly modulated across resonant absorption edges. For metallic Fe and FeTe, the TDDFT calculation of $f_1(\omega)$, works very well while for TiSe$_2$ one can expect some discrepancy between theory and experiment since these calculations usually can reproduce rather well the absorption cross section (related to $f_1$) for metals, but not the absorption in ionic or correlated systems. Nevertheless, we find that the model is still able to capture the overall amplitude of the RIXS signal in TiSe$_2$. The reason for the discrepancies between model and experiment above the absorption thresholds is explained by the fact that the present model does not include the momentum independent resonant emission described by KH. An important question is what can we learn from the present approach? The band structure calculations for TiSe$_2$ shown by Monney et al. already reproduced many interesting features of the RIXS spectral shape, including the dispersion embedded in $S(q, \omega)$. However, the missing part of this previous work was the amplitude of the RIXS process involving both energy and momentum conservation, which can now be brought in by our present model. Thus, the most interesting aspect of the present model is a method to extract $S(q, \omega)$ in metallic systems in future $q$-dependent RIXS experiments.

ACKNOWLEDGMENTS

We thank Sebastian Macke for sending us $f_1$ data for iron. B.B. is supported by the US Department of Energy (USDOE) Contract No. DE-FG0207ER46352. C.M. and T.S. acknowledge support from the Swiss National Science Foundation (SNSF) and its National Centre of Competence in Research MaNEP. C.M. acknowledges support by the Swiss National Science Foundation (under Grant No. PA00P2_142054) and from the Alexander von Humboldt Foundation. We benefited from computer time from Northeastern Universitys Advanced Scientific Computation Center (ASCC) and USDOEs NERSC supercomputing center.

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