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Phonon contribution to RIXS spectra calculated with a cumulant expansion for the quasiparticle Green's function KEITH GILMORE, ANDREY GEONDZHIAN, European Synchrotron Radiation Facility, JOSH KAS, Physics Department, University of Washington — Much of the effort in many-body techniques for going beyond standard density functional theory seeks to improve the accuracy of quasiparticle energies, particularly for large or complex systems. A quantity that is sometimes overlooked is the quasiparticle spectral function. Accurately calculating satellite features due to boson excitations is essential for providing a meaningful interpretation of many experimental results, particularly for X-ray spectroscopies. Resonant inelastic x-ray scattering (RIXS) is a relatively new experimental probe of the coupling of electronic states to various excitations in a material such as plasmons, magnons and phonons. The localized nature of the core hole in X-ray spectroscopies allows one to use linked-cluster formulations, as in the seminal work of Nozieres [1], that express the electron Green's function as a cumulant expansion rather than via a Dyson equation. Kas et al. have recently used this approach for electron-plasmon coupling in X-ray photoemission [2] and X-ray absorption [3]. We perform analogous work for the case of coupling to phonons, with a particular focus on RIXS. RIXS is increasingly used to study electron-phonon coupling in unconventional superconductors and it is essential to improve our interpretation of these spectra. TiO2, for which high energy resolution RIXS data was recently reported, serves as our test case. [1] Nozieres and Dominicis, Phys Rev 178, 1097 (1969). [2] Kas et al., Phys Rev B 91, 121112R (2015). [3] Kas et al., Phys Rev B 94, 035156 (2016).

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