X-ray photoemission and absorption in strongly correlated electron systems

A.M. Shvaika[a] and J.K. Freericks[b]

[a] *Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, 1 Svientsitskii Street, 79011 Lviv, Ukraine*

[b] *Department of Physics, Georgetown University, Washington, DC 20057, USA*

We solve for the X-ray photoemission (XPS) and absorption (XAS) spectrum in correlated materials by employing dynamical mean-field theory. We focus our attention on the infinite-dimensional limit of the spinless Falicov-Kimball model, where the problem can be solved exactly, and the system can be tuned to go through a Mott-Hubbard-like metal-insulator transition. The core-hole propagator, which determines XPS, is expressed in terms of a continuous fermionic Toeplitz determinant defined only on the upper real-time branch of the Keldysh contour which produces an efficient algorithm to obtain the density of states of the X-ray edge problem for any temperature and any interaction strength. The two particle XAS is derived as a functional derivative of the core-hole propagator with respect to the dynamical mean field and is also expressed in terms of a continuous fermionic determinant. We find that both XPS and XAS contain two groups of peaks. One of them contains a sharp edge peak at finite temperature which transforms in the power law singularity or δ-peak at zero temperature on different sides of the metal-insulating transition point.