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First principles computation of dynamical structure factor in real and momentum space in cuprates YUNG JUI WANG, B. BARBIELLINI, HSIN LIN, TANMOY DAS, SUSMITA BASAK, Northeastern Univ. (NU), P. E. MIJNARENDS, Delft Univ. of Tech. and NU, S. KAPRZYK, NU and AGH (Poland), R. S. MARKIEWICZ, A. BANSIL, NU — We present a method for efficient, accurate first-principles calculations of the dynamical structure factor $S(\mathbf{q}, \omega)$ in periodic systems, using products of real space Green functions and fast Fourier transforms (FFT). We further invert $S(\mathbf{q}, \omega)$ via Fourier transformation [1] to reconstruct the propagator of electron density $X(\mathbf{x}, t)$ in real space and time domain, thereby visualising spatially the dynamics of an electron doped cuprate system in real time. The present method is useful for many-body perturbation theories of excitations based on Density Function Theory (DFT) and modeling of various highly resolved spectroscopies going beyond the standard LDA [2-5]. Some illustrative examples will be presented. Work supported by the US DOE.

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