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Dynamical structure factor computations in extended momentum space in electron doped 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, Northeastern Univ. (NU) — We report first principles computations of the dynamical structure factor $S(q,\omega)$ in the electron doped cuprates $Nd_{2-x}Ce_xCuO_2$ as a function of energy ω and momentum q extended over several Brillouin zones. We show the efficacy of obtaining $S(q,\omega)$ through the use of simple products of real space Green functions and fast Fourier transform (FFT). We also calculate the susceptibility $\chi(q,\omega)$ efficiently by recalling that $S(q,\omega)$ is proportional to the imaginary part of the susceptibility $\chi(q,\omega)$. The present work is useful in going beyond the standard LDA-based modeling of various highly resolved spectroscopies.[1-4] We will provide some illustrative examples.
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