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Density matrix renormalization group study of optical conductivity in the one-dimensional Mott insulator Sr_2CuO_3 SHIGETOSHI SOTA, TAKAMI TOHYAMA, Yukawa Institute for Theoretical Physics, Kyoto University — We examine the optical conductivity of Sr_2CuO_3 by using zero and finite temperature dynamical density matrix renormalization group (DMRG) methods. Employing a Hubbard- Holstein model containing Holstein-type coupling of electron to the Einstein phonons, we reproduce both the Mott-gap excitation and phonon-assisted spin excitation observed experimentally [1,2] by using the dynamical DMRG method combined with a regulated polynomial expansion [3]. We find a parameter set describing Sr_2CuO_3 . Furthermore, by using a low- temperature dynamical DMRG method which is recently developed by present authors [4], we examine the temperature effect of the Mott-gap excitation to clarify the effect of optical phonons on spectral shape at finite temperatures. We find that the presence of phonons induces the enhancement of the width of an excitonic peak in the optical conductivity. [1] M. Ono, K. Miura, A. Maeda, H. Matsuzaki, H. Kishida, Y. Taguchi, Y. Tokura, M. Yamashita, and H. Okamoto, Phys. Rev. B **70**, 085101 (2004). [2] H. Suzuura, H. Yasuhara, A. Furusaki, N. Nagaosa, Y. Tokura: Phys. Rev. Lett. **76**, 2579 (1996). [3] S. Sota and M. Itoh, J. Phys. Soc. Jpn. **76**, 054004 (2007). [4] S. Sota and T. Tohyama, Phys. Rev. B **78**, 113101 (2008).

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