

Development of Dynamical DMRG Method using Regulated Polynomial Expansion and its Application to One-Dimensional Correlated Electron Systems

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We have developed a finite temperature dynamical DMRG procedure concentrated on low-temperatures [1] and an effective computational method to calculate a correction vector of the dynamical DMRG [2]. Our finite temperature dynamical DMRG method employs the target state given by the Boltzmann distribution. The target state is calculated by the recursive formula of the regulated polynomial expansion [1, 3]. The correction vector is also calculated by the regulated polynomial expansion. In this method, the δ -functions in the spectrum functions are broaden by a Gaussian. We apply our methods to one-dimensional correlated electron systems. In a spin-1/2 zigzag XY chain, we find that the spin chirality correlation is enhanced by the temperature effect in the dimer phase [4]. Employing a Hubbard-Holstein model, we reproduce the optical conductivity of the Sr_2CuO_3 in the spin excited and the charge-transfer energy region simultaneously as shown in Fig. 1 [2].

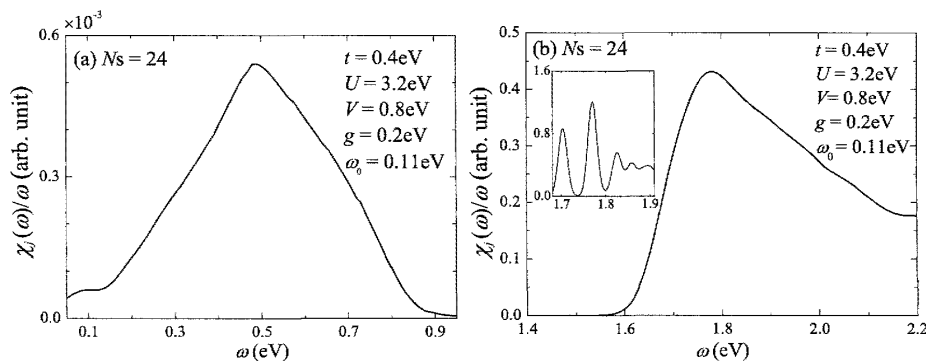


Figure 1: The calculated optical conductivity corresponding to the Sr_2CuO_3 .

References

- [1] S. Sota and T. Tohyama, Phys. Rev. B **78**, 113101 (2008).
- [2] S. Sota and T. Tohyama, arXiv:1007.5166
- [3] S. Sota and M. Itoh, J. Phys. Soc. Jpn. **76**, 054004 (2007).
- [4] T. Sugimoto, S. Sota, T. Tohyama, Phys. Rev. B **82**, 035437 (2010).