Spectral Evolution of Finite Dimensional Holstein Model

Jiaguang Han [1,2] , Kai Ji[2] , Zhiyuan Zhu[1], and Keiichiro Nasu[2,3]

[1] *Shanghai Institute of Applied Physics,*

Chinese Academy of Sciences, Shanghai 201800, China

[2] *Solid State Theory Division, Institute of Materials Structure*

Science High Energy Accelerator Research Organization ,

1-1 Oho, Tsukuba, Ibaraki305, Japan

[3] *Department of Materials Structure Science,*

Graduate University for Advanced Studies,

1-1 Oho, Tsukuba, Ibaraki305, Japan

Abstract

we calculate the one-electron spectral function of non half-filled Holstein model in one, two and three dimensions for various correlation strengths and temperatures. In the previous work, we have reported on a new path-integral theory to calculate the photoemission spectra of Holstein model. Using quantum Monte-Carlo simulation, we presented the characteristic spectral evolution, which takes a broad Gausssian at the band bottom and a Lorentzian near Fermi level. Here, we perform a further analysis on the photoemission spectra of Holstein model in finite dimension based on a classical Monte-Carlo method. The system is simulated with the help of classic Monte Carlo technique that allows us to clarify the impact of classic e-ph interaction on the spectral evolution. Such a comparison research is helpful for ones to distinguish what is coming from the classical phonon effect and what is coming from a quantum effect. We would demonstrate that some remarkable behaviors in the evolution of photoemission spectra can be ascribed to the classical e-ph interaction. Moreover, the origin of such an evolution in the spectra of due to classical e-ph interaction is discussed within the electron localization framework. Such a evolution can be illustrated as the transmition of electronic state from a localized incoherent state to a extended coherent state. This has been identified by introducing the physical quality participation ration. These theoretical results agree with the recent ARPES experiments. Furthermore, comparing with the QMC results, we realize that the main characteristic in the evolution of spectra can ascribed to the static classical e-ph interaction.

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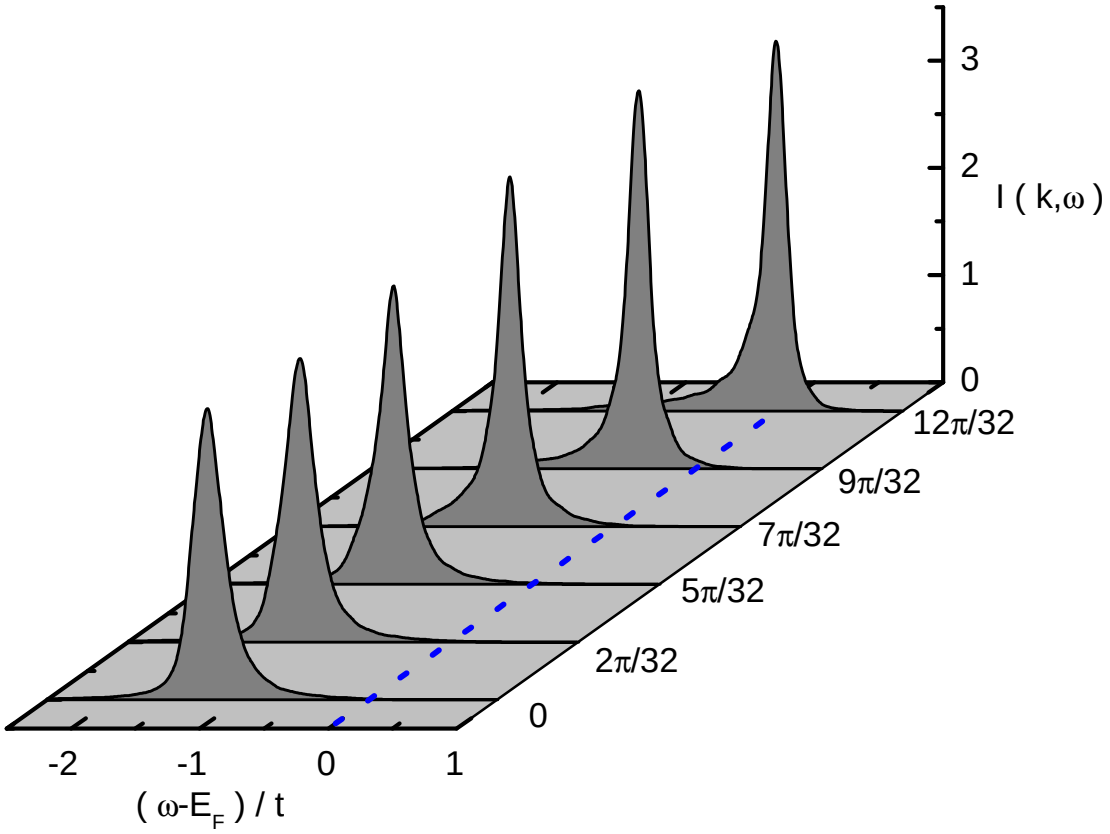

FIG. 1: The 3D profile view of 1D Holstein model with 64 sites at 37.5% filling for coulping constant g= 0.4. The dashed line indicates the Fermil level.

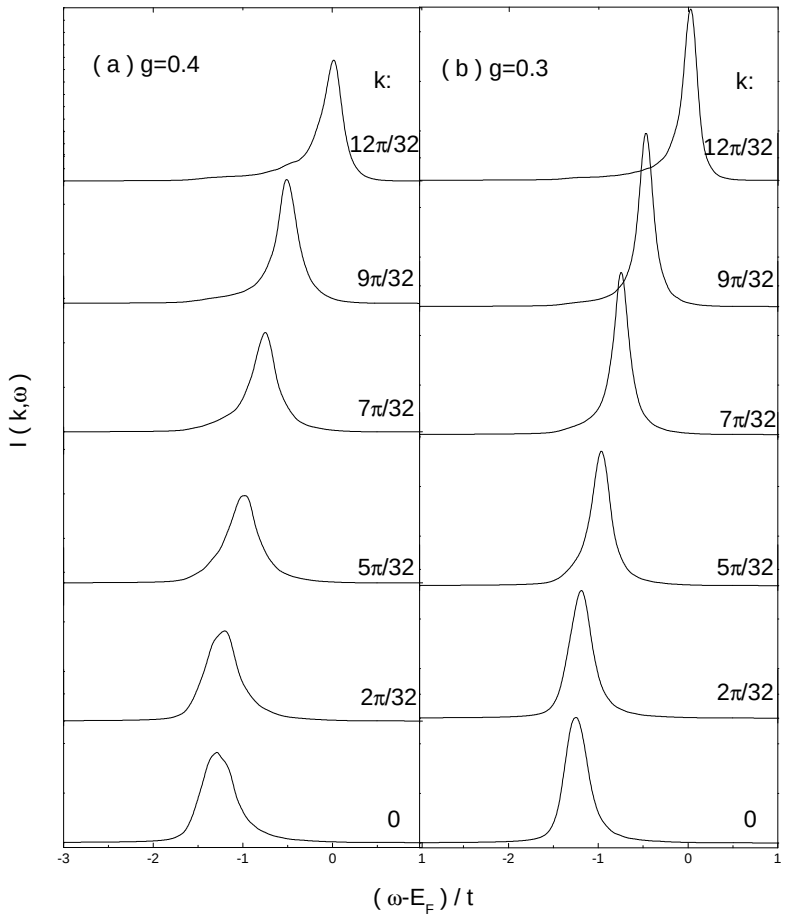

FIG. 2: Comparision results for two different coupling constants g for 1D Holstein model at 37.5% filling with fixed $\beta = 5.0$.