モット転移の多段階性と光電子スペクトルの経路積分理論)

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abstract

We have theoretically studied various one-, two- and three-dimensional half-filled Hubbard models from weak correlation cases to strong ones, and calculated the Lehmann's spectra of the momentum-specified one-electron Green's functions, as well as the total density of states (DOS), using the quantum Monte Carlo method. In the region of intermediate correlation strength, we have found the DOS has new characteristic peaks near the Fermi level, in addition to the well-known upper and lower Hubbard-band peaks. We show these new peaks near the Fermi level comes from quasi-coherent states, while the upper and lower Hubbard-band peaks comes from strongly incoherent ones. This multi-peaked structure, appearing only in the intermediate region, is shown to be quite insensitive to the dimensionality. Finally, we compare our results with the static single impurity model, and give a rough and intuitive explanation for the origin of this newly obtained multi-peaked structure. Our results also qualitatively agree with the recent photoemission experiments on $CaVO_3$ and $SrVO_3$ crystals.

Keywords: Mott transition, photoemission spectra, coherent and incoherent peaks, intermediate correlation, $CaVO_3$, $SrVO_3$