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学 位 論 文 題 目 モット転移の二段階性と光電子スペクトルの経路積分理論

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The photoemission spectroscopy is the most standard method to determine the density of states (DOS) of electrons in solids. At present, the energy resolution of this photoemission spectrum (PES) overreaches a few meV, and the momentum resolution is also high enough to clarify the dispersion relation of the valence band electron. Thus, the photoemission spectroscopy can now clarify the natures of the electronic states more precisely than before. In particular, to clarify the natures of the electronic states just around the Fermi level is one of the most important issues in the solid state physics.

In connection with this high resolution photoemission spectroscopy, the nature of the electronic states around the Fermi level of the perovskite-type compounds such as CaVO_3 and SrVO_3 is the matter of great interest. According to the recent experiments, a new peak structure has been observed around the Fermi level for CaVO_3 and SrVO_3 , in addition to the well-known Hubbard-band peaks. This new peak at the Fermi level has such a double-peak structure that the intensity are suppressed just at the Fermi level but enhanced at slightly below and above this level. These experiments are performed by Osaka Univ. group and Tokyo Univ. group independently from each other. However, the resultant spectra are entirely same between these two independent groups. Thus, the origin of these new peaks, which are slightly below and above the Fermi level, has become a hot debating point.

From the theoretical point of view, the PES directly corresponds to the Lehmann spectrum of the one-body Green's function. Looking back on these past theoretical studies, the Lehmann spectra were calculated for the infinite dimensional Hubbard model by using the dynamical mean-field method. While the finite dimensional cases are also calculated by using the quantum Monte Carlo simulations, and by various other approximation methods. In particular, for one-dimensional systems, there are many studies including the exact results.

In the infinite dimensional case, as is already well-known, a significant peak clearly appears at the Fermi level, if the Coulomb repulsion is weak enough to keep a metallic state. However, it has long been believed that, the peak at the Fermi level is the artifact of the infinite dimension. On the other hand, the peaked structure around the Fermi level is absent in the finite dimension. As mentioned before, for these finite dimensional cases, there are many calculations of the Lehmann spectra. However, all studies have been restricted only in strongly correlated cases. Within the quantum Monte Carlo method for one-, two- and three-dimensional systems, up to present, there is no theoretical study that predicts the appearance of such peaks around the Fermi level.

For this reason, the purpose of the present paper is to clarify the DOS and the electronic property related with this new peak appeared around the Fermi level. In particular, we focus mainly on intermediately (or weakly) correlated regions concerning with the metal-insulator transition.

We calculate the one-body Green's functions for one-dimensional half-filled Hubbard systems with various correlation strengths and temperatures, by using the quantum Monte

Carlo method. The Lehmann's spectral functions of the one-body Green's functions are obtained by using the analytic continuation. In the region of the intermediate correlation strength and temperature, we will show some new peaks appear around the Fermi level, even in the case of one-dimensional system, just like the case of the infinite dimension. This new peak at the Fermi level splits into two peaks, as the temperature decreases or the on-site Coulomb repulsion increases. These theoretical results will be shown to agree with the recent experiments on CaVO_3 and SrVO_3 qualitatively, will also be examined in terms of a single impurity model.

論文の審査結果の要旨

固体内の伝導電子が相互に強いクーロン斥力で反撥する為に起きるモットー型の金属-絶縁体転移は高温超伝導現象の機構解明等にも関連し、現在の固体物理学における最重要課題の一つであり、様々な理論的・実験的研究が行われているが、この転移の理論は、現在、相互に異なる二種類に大別される。

一方は、仮想的無限次元格子で厳密解を得る方法であり、この理論は、金属から絶縁体へと転移が進行する過程で、幾つかの過渡的で中間的な相が発生する事を预言する。

他方は、有限（1～3）次元格子での経路積分（量子モンテ・カルロ）法によって数値解を得る方法である。この方法では実際の数値計算が困難である事が災いし、此れまでは、斥力が電子の遍歴性に比較して十分強い場合のみが計算されてきた。そして、この結果によれば、強斥力領域では、金属-絶縁体転移は、金属から絶縁体へ一段階で直接起こり、途中には何等の中間相も現れないと云う結論が得られている。従って、無限次元での中間相の存在は、正に無限次元と云う仮想性の結果であると見なされてきた。

ところが、極く最近、CaVO₃やSrVO₃等の物質で、伝導電子帯全体は金属-絶縁体転移の兆候を示しながらも、僅かフェルミ面近傍だけは金属的なまま残ると云う中間相の存在が高分解光電子分光により実験的に発見された。

この状況に鑑み、山崎才弘君は、経路積分（量子モンテ・カルロ）法が抱えている種々の数値計算上の難点を克服し、強斥力領域のみならず、中間斥力及び、弱斥力領域でも計算が可能になるように、新たに、この理論を拡張する事に成功した。そして、この新しい理論的方法による精密な計算を中間及び弱斥力領域で実行した。この結果、中間斥力及び弱斥力領域では、金属絶縁体転移は、前述の実験にあるように、一段階ではなく、金属絶縁体中間相を経由して二段階で起きる事が世界に先駆けて理論的に立証された。

以上、本論文により得られた知見は、専門的にも総合的にも極めて水準の高い研究であると認められる。従って、数物科学研究科物質構造科学専攻の博士学位論文としてふさわしい内容を持つと判断した。