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論文目次

論 文 内 容 要 旨

The 4f electrons of rare-earth ions have the localized nature even in crystals, and their magnetic moments give rise to various phenomena. A single magnetic moment in a metal is screened by polarized conduction electrons to form the singlet ground state. On the other hand, the polarization of the conduction electrons propagates and leads to an effective exchange interaction between two moments. The former is referred to as the Kondo effect, and the latter as the RKKY interaction. Although both phenomena are consequences of hybridization between 4f and conduction electrons, they compete with each other and may lead to the heavy-fermion states at low temperatures.

If we neglect the charge fluctuation of the 4f electrons, a starting point for theoretical studies is the Kondo lattice or the Coqblin-Schrieffer (CS) lattice model. These models correspond to localized and strong-correlation limits of the periodic Anderson model. It is important to clarify properties of these fundamental models in creating a better understanding of the heavy-fermion systems.

Two contrasting approaches may be used to deal with lattice models theoretically: one is to solve the model on a finite cluster by a method such as exact diagonalization, the other involves the solution of an effective impurity system within the framework of dynamical mean-field theory (DMFT). The former approach is more suitable for low-dimensional systems, while the latter becomes exact in infinite-dimensional systems. As for the one dimension, the Kondo lattice model has been extensively investigated and its basic properties have already been revealed. However, there are few numerical studies of higher dimensions. The purpose of this thesis is to elucidate properties of the infinite-dimensional Kondo lattice model quantitatively. To this end, (i) we derive a formula of the spatial correlations between local spins within the DMFT, and (ii)

develop a new impurity solver which give numerically exact solutions.

In the Kondo and CS lattice model, the Green function cannot be defined for the 4f electrons, since the 4f-charge degree of freedom has been eliminated. A many-body effect of the exchange scattering can be taken account of in the impurity t-matrix instead. We rewrite the DMFT equations in terms of the t-matrix to be applicable to the localized limit.

For a description of the instabilities of the paramagnetic ground state, two-particle correlation function is required. In order to address the spatial correlations of local moments, we extend the t-matrix, defined from the single-particle Green function, to the two-particle Green function. The "two-particle t-matrix" is then shown to give the susceptibility of local moments, and make it possible to deal with the spin correlations by means of the ordinary technique in the periodic Anderson model. We consequently derive spatial correlations in the Kondo and CS lattice model based on the DMFT.

To solve the self-consistent equations of the DMFT accurately, we develop an impurity solver based on the continuous-time quantum Monte Carlo method (CT-QMC) for the CS model. The Monte Carlo simulations does not encounter a sign problem for antiferromagnetic interactions, and accurately reproduces the Kondo effect. Our algorithm can deal with an arbitrary number N of local degrees of freedom, becomes more efficient for larger values of N, and is hence suitable for models with orbital degeneracy.

With use of the new impurity solver, we first examine the Fermi liquid relations of the single impurity model. We point out that the Korringa-Shiba relation, which connects the imaginary part of the dynamical susceptibility with the static ones, needs correction for a finite value of the exchange interaction. On the other hand, the Friedel sum rule, which involves the single-particle excitation with the occupation number, is confirmed to be satisfied with high accuracy.

With the CT-QMC and the DMFT, we employ the Kondo lattice model with a tight-binding band of the infinite-dimensional hyper-cubic lattice. The half-filled Fermi surface exhibits a perfect nesting property, so that instabilities are expected to arise. We evaluate the correlation function of the local spins, and the charge and spin susceptibilities of conduction electrons. Transition temperatures are calculated from divergences of the susceptibilities, and then we obtain a ground-state phase diagram for arbitrary fillings.

In the weak-coupling regime around the half filling, we find an antiferromagnetic ordering due to the nesting. The ordering is suppressed by the Kondo effect as the coupling increases. The critical value agrees with the estimation by the comparison between the Kondo temperature and the RKKY interaction. Namely, the Doniach's picture is confirmed to be valid at the half filling. In the low-carrier-density regime, on the other hand, we find a divergence of the ferromagnetic susceptibility. This ordering is expected from the polarization function of conduction electrons. However, unlike the antiferromagnetic phase, the ferromagnetic phase exists beyond the critical coupling estimated by comparison between the Kondo temperature and the RKKY interaction. This follows from the fact that all the local spins cannot be screened by a fewer number of conduction electrons in the low-carrier-density regime.

In addition to the magnetic orderings of the local spins, we find a divergence of the conduction-electron charge susceptibility, i.e., a charge-density wave (CDW) ordering, at the quarter filling. This transition is accounted for by the strong-coupling picture, where each conduction electron strongly couples the Kondo singlet. Therefore, it is a novel mechanism of the CDW transition, in which the Kondo effect plays an essential role.

論文審査の結果の要旨

本論文は、局在電子と遍歴電子が共存する系の基礎的模型である近藤格子模型の熱力学的、動的性質を理論的に調べたものである。

重い電子系に代表される遍歴電子と局在電子が共存する系では、電子の波動性と粒子性という量子力学の根幹を成す電子の二重性を反映した多彩な現象が現れるが、このような系の基礎的モデルの中で、局在電子の電荷の自由度を消去した強相関の極限に相当するモデルが近藤格子模型である。

この系の性質は強相関であることの難しさから、これまで１次元の場合を除いて未解明であったが、このような強相関の困難を克服し、この系の熱力学的、動的性質を理解することが本論文の目的となっている。

本論文では、まずこの強相関であるために生じる、電荷の自由度が消去された局在電子を取り扱うために、２体の散乱行列を導入し、動的平均場理論に基づいて空間相関を求める表式を導出した。さらに、2006年にWernerらによって考案された精度の高い連続時間モンテカルロ法を用いて近藤模型の散乱行列を統計誤差の範囲で厳密に求め、これまで明確に認識されてこなかった近藤模型の帯磁率の実部と虚部の関係を与えるコリンハ斯波の関係式への有限バンド幅の場合の補正の存在と、未解明であった無限次元の近藤格子模型の基底状態の相図、動的相関関数を明らかにした。

この無限次元における研究成果は、これまでの１次元の研究と相補的なものであり、現実の３次元系を理解するための重要な足掛かりを与えた。このような成果は自立して研究活動を行うに必要な高度の研究能力と学識を有することを示しており、大槻純也提出の博士論文は、博士（理学）の学位論文として合格と認められる。