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研究課題名（和文）クーロン相互作用する電子系におけるアンダーソン転移への新規なアプローチ

研究課題名（英文）A new approach to the Anderson transition in electron systems with Coulomb interactions

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研究成果の概要（和文）：本プロジェクトでは，大規模数値シミュレーションを用いて，単純化されたモデルとドープされた半導体の金属 - 絶縁体転移のより現実的なモデルの両方で，アンダーソン転移の臨界現象の理解に貢献した。単純化したモデルにおけるアンダーソン転移の臨界指数の次元依存性を数値的に詳細に研究し、その結果が解析的予測と一致していることを示した。また、アンダーソン転移に対する磁性不純物の影響を調べ，解析的な理論的予測と一致することを確認した。また，臨界指数（したがって相転移の普遍性クラス）が電子間の長距離クーロン相互作用によって変化するという証拠も見出した。

研究成果の学術的意義や社会的意義
本プロジェクトは，ランダムポテンシャルと電子 - 電子相互作用の両方を含む問題を扱っている。この問題は，物性物理学において最も困難なものの一つである。この研究プロジェクトの学術的意義は2つあると思われる。まず、この研究はアンダーソン遷移を説明するために提案された理論的な考え方が正しいという確信を与えた。第二に、この研究はランダムポテンシャルと電子 - 電子相互作用を（近似的にではあるが）同等に扱う研究への道を示唆した。

研究成果の概要（英文）：Using extensive numerical simulations, this project has contributed to a better understanding of the critical phenomena of the Anderson transition both in simplified models, and in more realistic models of the metal-insulator transition in doped semiconductors. We studied the dimensionality dependence of the critical exponent of the Anderson transition in simplified models in detail numerically and found the results to be in reasonable agreement with analytical predictions. We also studied the effect of magnetic impurities on the Anderson transition and found the results to be consistent with analytical theoretical predictions. We also found evidence that the critical exponent (and hence the universality class of the phase transition) is changed by the long-range Coulomb interaction between electrons.

研究分野：物性理論

キーワード：disordered systems　Anderson transition　critical phenomena

１．研究開始当初の背景

In semiconductors, there is a zero temperature metal-insulator transition as a function of doping concentration. Below a certain critical concentration, the semiconductor is an insulator, i.e. the finite temperature conductivity extrapolates to zero at zero temperature. While above a certain critical concentration, the finite temperature conductivity extrapolates to a nonzero value. At the critical concentration, a quantum phase transition occurs. This transition has been the subject of experimental study over several decades. There is no theoretical consensus on the mechanism that drives the transition. One possibility is that it is a type of Anderson transition. This latter well-studied phase transition occurs for gases of non-interacting electrons in a random potential as a function of the magnitude of the potential fluctuations. In a semiconductor, the randomness comes from the random positions of the dopant atoms. In this scenario, however, it is important to understand how the Coulomb interaction, magnetic impurities etc. affect the critical behavior of the Anderson transition.

２．研究の目的

To understand how various factors such as the long-range Coulomb interaction between electrons and the presence of magnetic impurities affect the critical phenomena and critical exponents of the Anderson transition. The goal was to study this both in simplified models such as Anderson's model of localization, and also in more realistic models of the metal-insulator transition in doped semiconductors with a view to better understanding the critical phenomena observed in such systems.

３．研究の方法

We performed large-scale computer simulations using a variety of methods. We used the transfer matrix method and the kernel polynomial method extensively when simulating non-interacting electrons. When simulating interacting electrons, we used the Kohn-Sham formulation of density functional theory in the local density approximation. This allowed us to take into account the Coulomb interaction between electrons in an approximate manner. We analyzed the results of the simulations using ideas from renormalization group theory in particular the method of finite size scaling. For the Kohn-Sham wavefunctions, we also used machine learning. The basic assumption underlying our work is that the metal-insulator transition in doped semiconductors is a type of Anderson transition.

４．研究成果

Effect of Coulomb interaction on the critical exponent of the Anderson transition

We performed a simulation of the metal-insulator transition in a doped semiconductor in a model that incorporates both the random positions of the donors and the Coulomb interaction between the electrons by means of density functional theory. We found that the wave functions are multifractal, as in the usual Anderson transition. Using a multifractal analysis of the wave functions, we found that the critical exponent of the correlation length was approximately 1.3. This differs significantly from that of the usual Anderson transition in three dimensions suggesting the importance of the Coulomb interaction. In addition, the phase diagram we obtained using the multifractal analysis was used to train a neural network. This neural network is being used in ongoing work to predict the critical concentrations in models with spin degrees of freedom.

Dimensional dependence of the critical exponent of the Anderson transition

We performed high precision numerical simulations using the transfer matrix method. We analyzed the results of these simulations using the finite size scaling method. We made new estimates of the critical exponents for the 4 and 5 dimensional orthogonal universality classes, and the 3 and 4 dimensional unitary symmetry classes. We compared these with new Borel–Padé re-summations of the perturbation series for the critical exponents and the beta functions of the scaling theory of localization. After incorporating the expected asymptotic behavior at infinite dimension, we found reasonable agreement even in 3 dimensions. We also made a new estimate of the lower critical dimension for the symplectic universality class.

Effect of magnetic impurities on the critical phenomena of the Anderson transition

Using the kernel polynomial method, we studied the effect of magnetic impurities on the Anderson transition. Magnetic impurities break both time reversal symmetry and spin rotation symmetry simultaneously. Moreover, from magnetic susceptibility measurements, it is known that magnetic moments are present near the metal-insulator transition in doped silicon. We found that a small concentration of magnetic impurities enhances the critical disorder. We also found that the dependence on the exchange coupling strength was in agreement with theoretical predictions of anomalous scaling.

Parallelization of the transfer matrix method
The transfer matrix method is one of the most widely used numerical methods in the field of Anderson localization. In its usual form, however, it is not well suited to modern massively parallel supercomputing systems. We proposed a modification of the method suitable for such computers and demonstrated its effectiveness by estimating the exponent for the three-dimensional orthogonal universality class with an improved precision.

５．主な発表論文等

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〔図書〕（計 0 件）

〔産業財産権〕
○出願状況（計 0 件）

○取得状況（計 0 件）

〔その他〕
なし

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なし

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