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研究成果

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黎明・勃興期にあった電子計算機を活用する物理学（計算物理学）の研究を、物性物理学の分野で主導して推進するとともに、国内外でコミュニティの確立に貢献した。物性物理学分野唯一のスーパーコンピュータの物性研究所への導入を推進し、共同利用システムを確立し、その後の我が国の物性物理学における大規模計算を用いた研究の発展の基礎づくりに貢献した。

種々の量子モンテカルロ法、変分波動関数法等の効率的計算手法を開発し、その後大きな発展を遂げている量子多体現象の理解に物理、化学の分野で貢献した。開発・改良した手法の中には連続空間量子モンテカルロ法、量子転送モンテカルロ法、量子分子動力学法、経路積分繰り込み群法、階層的第一原理強相関電子状態計算法、多変数変分モンテカルロ法、テンソルネットワークやニューラルネットワークを組み合わせた変分モンテカルロ法等が含まれる。

強相関物質の電子構造の第一原理的かつ定量的で高精度な解明を可能にする数値計算手法を開発し、定量的標準手法として確立した。さらに手法を高温超伝導体などの多くの現実物質に適用してその精度の高さを検証するとともに、超伝導機構などの未知の物理の解明を行なった。

より具体的には「フェルミレベル付近の疎構造と大局密構造が作る階層性」が強相関電子系の電子構造が持つ必然的な特性であることに着目、積極利用し、繰り込み群的な手法で第一原理的に強相関電子系を解明する汎用性の高い手法（階層的第一原理強相関電子状態計算法、Multi-scale ab initio scheme for Correlated Electrons（MACE)、以下 MACE と略称）を、21 世紀初頭に提案した。手法開発も進め、MACE を構成する種々の有効模型導出手法の開発、さまざまな低エネルギーソルバーの開発も世界に先駆けて行った。また遷移金属化合物、有機導体などの多数の現実の強相関物質群に応用し精度を実証した。密度汎関数法を超えるこの方法は様々な物質への応用に大きく広がり、今世界的潮流となっている。

低エネルギーソルバーとして世界的に追究されている方法に、(変分）モンテカルロ法、密度行列繰り込み群、テンソルネットワーク、経路積分繰り込み群などの高精度変分関数手法、動的平均場法及びその拡張、機械学習法等がある。これまで、以下の例のように多くの方法でこれらの手法の進歩と応用による強相関多体現象の解明に本質的貢献をした。

[1] 経路積分に基づく連続空間での高次補正を含む量子モンテカルロ法を開発、長距離クーロン相互作用する２次元電子ガスで電子濃度と温度の平面で、ウィグナー結晶が量子融解する相図を近似なしに求め、15 年後に高い定量精度で実験的に立証された。この量子モンテカルロ法は量子化学研究者により量子化学分野へも応用が広げられ、活発に利用されている。

[2] 格子フェルミオン模型のための補助場法を用いた量子モンテカルロ法を開発整備した。さらに変分モンテカルロ法開発およびこれとテンソルネットワーク法、機械学習（ニューラルネットワーク法）との融合による高精度化も実現し、これを適用して銅酸化物超伝導体において、モット転移（強相関物質の金属絶縁体転移）の様相を解明した。また第一原理的に超伝導を含む実験相図を再現し、スピン・電荷の相分離・不均一化や長周期構造と超伝導との間の激しい競合の普遍性を解明した。加えて、強相関効果が生む創発的な「隠れた複合フェルミオン」を発見し、これにより牽引される高温超伝導などの新概念をもとに、超伝導機構の解明を行なった。鉄系超伝導体の第一原理有効ハミルトニアンも初めて導いて解き、強相関効果の本質的重要性を立証し、実験相図を再現するとともに計算科学手法で超伝導発現機構を特定した。

[3] 量子転送行列モンテカルロ法，経路積分繰り込み群法を開発した。前者は最近量子純粋状態

法として他研究者が継承発展させた。後者を用いて、遍歴的な三角格子等フラストレートした反強磁性体等での量子スピン液体状態を予言し、その後有機導体(分子性結晶)の実験でスピン液体が発見された。またその後に発展させた高精度の変分モンテカルロ法を用いてギャップレスな量子スピン液体の様相をより詳細に解明した。

[4] 量子ダイナミクスや有限温度、電子格子相互作用、界面系を扱える手法拡張を行ない、例えば超伝導の空間不均一との競合を克服するために、レーザー照射による非平衡状態が不均一を抑制して超伝導を増幅する機構を提案し、不均一を界面で克服し高温超伝導を実現するアイデアなど、強相関非平衡･非周期系研究を先導している。

[5] スピン軌道相互作用の生むトポロジカル相と電子相関の絡み合いを追究し、イリジウム酸化物の可動制御性のあるトポロジカルな金属磁壁界面を提唱し、その後実験立証された。

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