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The Heavy Electron State

Final Report

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Abstract

Theoretical investigations of electron interactions in two families of novel materials were conducted.

1. The temperature-concentration phase diagram of doped bismuthate superconductors was described using a coarse grained anisotropic Heisenberg model. This research found a robust region of coexistence between the charge density wave (CDW) and the superconducting (SC) phases. Our results explained several key experimental findings.
2. A simplified model of electron interactions on buckminsterfullerene was studied. This model is relevant for the superconductivity and ferromagnetism in doped fullerenes. The total energy in the presence of an adjustable repulsive interaction was computed by first and second order numerical perturbation theory. This approach laid the foundation for a full scale renormalization group calculation. The relevance of this model to superconductivity and ferromagnetism in doped fullerenes was discussed.
3. Studies of the electron-vibron interactions in buckminsterfullerene. We solved the model numerically and semiclassically. Molecular Aharonov-Bohm effects were found which determine the vibrational spectra, zero point fluctuations, and electrons' pair binding energies.

1 Report

1.1 Multicritical Phase Diagram and Random Field Effects In Superconducting Bismuthates

(With Amnon Aharony, Tel Aviv University). The temperature-concentration phase diagram of doped bismuthate superconductors, was described using a coarse grained anisotropic Heisenberg model. In contrast to previous treatments, we find a robust region of coexistence between the charge density wave (CDW) and the superconducting (SC) phases. Random fields break the CDW phase into metastable domains, which may explain various recent experiments. A partial Meissner effect without bulk superconductivity is predicted at low doping concentrations and at low temperatures.

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1.2 Buckminsterfullerene: Interacting Electrons on a Spherical Molecule

(With Ganpathy Murthy, Boston University). We studied a simplified model of buckminsterfullerene, where the π electrons move freely on the surface of a sphere. The total energy in the presence of an adjustable repulsive interaction is computed by first and second order perturbation theory. Second order results yield an effective attraction (pair binding) between electrons which are added above a closed angular momentum shell. For different regimes of interaction parameters, we find an $L=0$ singlet and an $L=1$ triplet ground state. Pair binding occurs at larger couplings for longer range interactions. We estimate the third order corrections, and define the region where the second order predictions are expected to hold. The relevance of this model to superconductivity and ferromagnetism in doped fullerenes is discussed.

1.3 Electron-Vibron Interactions and Berry Phases in Charged Buckminsterfullerene

(With N. Manini and E. Tosatti)

A simple model for electron-vibron interactions on charged buckminsterfullerene C_{60}^{n-} , $n = 1, \dots, 5$, was solved both at weak and strong couplings. We consider a single H_g vibrational multiplet interacting with t_{1u} electrons. At strong coupling the semiclassical dynamical Jahn-Teller theory is valid. The Jahn-Teller distortions are unimodal for $n=1,2,4,5$ electrons, and bimodal for 3 electrons. The distortions are quantized as rigid body pseudo-rotators which are subject to geometrical Berry phases. These impose ground state degeneracies and dramatically change zero point energies. Exact diagonalization shows that the semiclassical level degeneracies and ordering survive well into the weak coupling regime. At weak coupling, we discover an enhancement factor of $5/2$ for the pair binding energies over their classical values. This has potentially important implications for superconductivity in fullerenes, and demonstrates the shortcoming of Migdal-Eliashberg theory for molecular crystals.

The ground state energy shifts and excitation spectra of charged buckminsterfullerene C_{60}^{n-} , $n = 1, \dots, 5$ were calculated. The electron-vibron Hamiltonian was extended to include all A_g and H_g modes with

experimentally determined frequencies and theoretically estimated coupling constants. Complex splitting patterns of H_g vibrational levels were found. Our results are relevant to EPR measurements of spin splittings in C_{60}^{2-} and C_{60}^{3-} in solution. Spectroscopic gas-phase experiments will be of interest for further testing of this theory. As found in Part I, degeneracies in the electron and vibron Hamiltonians give rise to a dynamical Jahn Teller effect, and to a considerable enhancement of the electronic pairing interaction. This helps to overcome repulsive Coulomb interactions and has important implications for superconductivity in K_3C_{60} and the insulating state in K_4C_{60} .

2 Publications

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