Abstract for GR-TR Conference on Statistical Mechanics and Dynamical Systems

Talk Invited Invited Talk

Dilute magnetic semiconductors: combined density functional theory and quantum Monte Carlo approach

Nejat Bulut*

Department of Physics, Izmir Institute of Technology Gulbahce, Urla 35430, Izmir, Turkey

* Electronic Address: nejatbulut@iyte.edu.tr

We use the Haldane-Anderson model to discuss the substitution of transition-metal impurities into semiconductors. We study this model with the Hirsch-Fye Quantum Monte Carlo (QMC) technique in the dilute limit. The QMC results show that the occupation of the impurity bound state plays an important role in determining the nature and the range of the magnetic correlations between the impurities [1] in agreement with the Hartree-Fock predictions [2]. In order to make direct comparisons with the experimental data, we combine the Density Functional Theory (DFT) with the QMC technique. In particular, we first use the density-functional theory to calculate the host band structure and the impurity-host hybridization matrix elements, which are input parameters for the Haldane-Anderson model, and then perform the QMC simulations with these realistic model parameters [3]. For the case of (Ga,Mn)As, the DFT+QMC approach leads to an impurity bound state located 100meV above the top of the valence band in agreement with the experimental value of 110meV. In addition, we observe an anisotropic distribution for the local density of states at the impurity-bound state energy, which is consistent with the STM data. Hence, we think that the DFT+QMC approach is a useful tool for performing realistic calculations for the various compounds of dilute magnetic semiconductors.

References

[1] N. Bulut, K. Tanikawa, S. Takahashi, and S. Maekawa, Physical Review B 76, 045220 (2007).

[2] M. Ichimura, K. Tanikawa, S. Takahashi, G. Baskaran, and S. Maekawa, Foundations of Quantum Mechanics in the Light of New Technology (ISOM-Tokyo 2005), eds. S. Ishioka and K. Fujikawa, World Scientific, Singapore, pp. 183186, 2006.

[3] Jun-ichiro Ohe, Yoshihiro Tomoda, Nejat Bulut, Ryotaro Arita, Kazuma Nakamura, and Sadamichi Maekawa, Journal of the Physical Society of Japan 78, 083703 (2009).