Final Report Summary - ABINITIODGA (Ab initio Dynamical Vertex Approximation)

The calculation of materials and their properties on a (super)computer is particularly challenging if the electrons interact strongly with each other, since then their movement becomes strongly correlated. This is especially relevant for many transition metal oxides and rare earth compounds because the electrons reside in spatially confined 3d or 4f orbitals, hence the electrons repel each other strongly. In the ERC project a new methodology for calculating such strongly correlated materials has been developed: ab initio dynamical vertex approximation (AbinitioDGA). This approach represents a breakthrough: beyond state-of-the-art methods also strong non-local correlations between electrons on different lattice sites are included. This now allows us to investigate, among others, long-range correlations in the vicinity of phase transitions, spin fluctuations and high-temperature superconductivity.

Thanks to this methodological progress several physical problems could be better understood and new physical effects have been discovered. Let us restrict here to some highlights: (1) It was discovered that the dynamical structure of the vertex (in particular its screening at low frequencies) is crucial for...
superconductivity. Finding the holy grail of solid state physics, room temperature superconductors, is possible if we discover a way to avoid this low frequency screening. (2) A quantum critical point is a phase transition e.g. from a paramagnet to a ferromagnet at zero Kelvin. Here, besides spatial correlations also temporal (quantum) correlations become relevant. A new universality class for the (quantum) critical behavior has been established in the ERC project. (3) A novel Mott transistor with ideal ON-OFF switching characteristics has been proposed based on SrVO3/SrTiO3 heterostructures; here vertex corrections play an important role. (4) An efficient way to inject spin currents into semiconductors has been identified using a heterostructure with a laser-excited ferromagnet such as Nickel. This spin-injection has been confirmed experimentally and has been hitherto the bottleneck for spintronics, i.e. electronics based on the spin instead of the charge of the electrons. (5) The importance of Nickel in the earth’ core for the dynamo effect which generates the earth’ magnetic field has been identified.

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