HL 19: Theory of electronic structure

Time: Tuesday 12:30–13:00 Location: BEY 81

HL 19.1 Tue 12:30 BEY 81

Phonons in strongly correlated materials from Hubbard-corrected density-functional-perturbation theory — Andrea Floris[1,2], Matteo Cococcioni[3], •Eberhard K. U. Gross[1,2], and Stefano de Gironcoli[4] — [1]Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — [2]ETSF, European Theoretical Spectroscopy Facility — [3]Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis MN 55455B — [4]Scuola Internazionale Superiore di Studi Avanzati (SISSA), I-34014 Trieste, Italy and INFM DEMOCRITOS National Simulation Center, I-34014 Trieste, Italy

In this contribution, the density functional perturbation theory is extended to compute the vibrational frequencies of strongly correlated systems whose ground state electronic properties are well reproduced within the DFT+U approach. The formalism, extended to both norm-conserving and Vanderbilt ultrasoft pseudo-potentials, allows to compute phonon frequencies with a computational cost that is independent from the q-vector, thus permitting the efficient exploration of the entire Brillouin zone. The main features of the implementation [1] , as the correction to the perturbed self-consistent potential and to the dynamical matrix due to the inclusion of the Hubbard U term, will be discussed along with several applications.

1. QUANTUM ESPRESSO code: http://www.quantum-espresso.org/

HL 19.2 Tue 12:45 BEY 81

Pseudospin Resonance in two Coaxial Tubes — •Benedikt Scharf[1], Jaroslav Fabian[2], and Alex Matos-Abiague[3] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Deutschland — [2]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Deutschland — [3]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Deutschland

In a 2DEG confined to two coaxial tubes the 'tube degree of freedom' can be described in terms of pseudospin-1/2 dynamics. The presence of tunneling between the two tubes leads to a collective oscillation known as pseudospin resonance. We employ perturbation theory to examine the dependence of the dispersion of this mode on a coaxial magnetic field for the case of small intertube distances. Coulomb interactions lead to a shift in the resonance frequency. The presence of the coaxial magnetic field gives rise to pronounced peaks in the shift of the resonance frequency. For large magnetic fields this shift vanishes due to the effects of Zeeman splitting.