MM 26: Electronic properties III

Time: Wednesday 16:45–18:15 Location: H6

MM 26.1 Wed 16:45 H6

Density matrix functional theory versus density functional theory: application to the Hubbard model — •Ryan Requist and Oleg Pankratov — Lst. für Theoretische Festkörperphysik, Universität Erlangen-Nürnberg

While the Hohenberg-Kohn theorem was long ago extended to prove a one-to-one correspondence between the first order reduced density matrix (RDM) and a nonlocal external potential [1], only recently have approximate RDM functionals been applied to systems such as atoms, small molecules, and the homogeneous electron gas. We study a two site Hubbard model which is exactly solvable; therefore, it provides a context for an explicit comparison of the density functional (DFT) and RDM functional approaches. In the RDM formalism, the Kohn-Sham (KS) system generally has fractionally occupied states, and all of these are degenerate, which is quite different from the common KS-DFT approach. The iteration of the self-consistent RDM equations leads to a nonlinear discrete map. Due to the degeneracy of the KS spectrum of the ground state RDM, an analogue of the Jahn-Teller theorem implies that the ground state is an unstable fixed point of the iteration map. The RDM energy functional constructed here may be useful for studying strongly correlated systems.
[1] T. L. Gilbert, Phys. Rev. B **12**, 2111 (1975).

MM 26.2 Wed 17:00 H6

topolgical defects in the crystalline state of the non-uniform density one component plasma — •adil mughal and mike moore — department of physics and astronomy, university of manchester, manchester, m13 9pl, u.k.

We study the ground state properties of classical Coulomb charges moving on a plane but confined either by a circular hard wall boundary or by a harmonic potential. The charge density in the continuum limit is determined analytically and is non-uniform. Because of the non-uniform density there are both disclinations and dislocations present and their distribution across the system is calculated and shown to be in agreement with numerical studies of systems of N charges, where values of N up to 5000 have been studied. A consequence of these defects is that although the charges locally form into a triangular lattice structure, the lattice lines acquire a marked curvature. A study is made of conformal crystals to illuminate the origin of this curvature. The scaling of various terms which contribute to the overall energy of the system of charges viz, the continuum electrostatic energy, correlation energy, surface energy (and so on) as a function of the number of particles N is determined. "Magic number" clusters are those at special values of N whose energies take them below the energy estimated from the scaling forms and are identified with charge arrangements of high symmetry.

MM 26.3 Wed 17:15 H6

Ionicity of $Fe_{1-x}Co_xSi$ single crystals from far-infrared spectroscopic ellipsometry — •Dirk Menzel[1], Pavlo Popovich[2], Alexander Boris[2], Matthias Neef[3], Klaus Doll[2,3], and Joachim Schoenes[1] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany — [3]Institut für Mathematische Physik, TU Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany

The nonmagnetic narrow-gap semiconductor FeSi transforms into a ferromagnetic metal by doping between 5 at.% and 80 at.% Co. High-quality tri-arc Czochralski grown $Fe_{1-x}Co_xSi$ single crystals were investigated by spectroscopic ellipsometry in the far-infrared spectral range between 100 and 700 cm^{-1}. Four infrared active T-modes are observed at 206, 330, 351, and 459 cm^{-1} for FeSi. The best fit of the dielectric function is achieved with a sum of Fano oscillators reflecting a coupling of the optical phonons with electronic excitations. Interestingly, at Co concentrations $x > 0.05$ the phonons remain visible although they should be screened by free carriers as expected in a metal. This is even more surprising since the Szigeti effective charge is lower than $0.1e$ for all the investigated Co concentrations whereas the Born effective charge is $3.0e$. For pure FeSi the indirect optical band gap is 33 meV which decreases with increasing x and closes at 5 at.% Co.

MM 26.4 Wed 17:30 H6

Optic phonon anomaly as a precursor to polaron formation in a layered CMR manganite — •Dmitry Reznik[1], Frank Weber[1,2], Nadir Aliouane[3], Dimitri Argyriou[3], Marcus Braden[4], and Winfried Reichardt[1] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany — [2]Physikalisches Institut, Universität Karlsruhe (TH), D-76128 Karlsruhe, Germany — [3]Hahn-Meitner Institut, Glienicker Straße 100, D-14109 Berlin, Germany — [4]II. Physikalisches Institut, Universität zu Köln, D-50937 Köln, Germany

We found evidence of a precursor effect to polaron formation in the bond stretching phonons in the bilayer CMR manganite $La_{2-2x}Sr_{1+2x}Mn_2O_7$ at 10K. Neutron scattering measurements of these phonons in the XX0 direction show that both the transverse and longitudinal branches broaden abruptly from X=0.15, where they are resolution limited, to X=0.25 where FWHM=13meV. They then narrow again on approach to the zone boundary (X=0.5). The shell model predicts a downward dispersion following the cosine function for the transverse branch and upward dispersion for the longitudinal branch, which is exactly what is observed in undoped cuprates. But in $La_{2-2x}Sr_{1+2x}Mn_2O_7$ both branches show a steep downward dispersion above x=0.15. The anomalous dispersion and broadening can be understood as a precursor effect to the CMR transition. This behavior is very unusual, because such precursor effects have previously been associated with phase transitions where charge order appears on cooling, not on heating as in CMR manganites.

MM 26.5 Wed 17:45 H6

Theory of tunneling spectroscopy in UPd_2Al_3 — •David Parker[1] and Peter Thalmeier[2] — [1]MPIPKS, Nothnitzer Str. 38, Dresden 01187 — [2]MPI CPFS, Nothnitzer Str. 40, Dresden 01187

There is still significant debate about the symmetry of the order parameter in the heavy-fermion superconductor UPd_2Al_3, with proposals for $\cos(k_3)$,$\cos(2k_3)$, $\sin(k_3)$, and $e^{i\phi}\sin(k_3)$. Here we analyze the tunneling spectroscopy of this compound and demonstrate that the experimental results by Jourdan et al (Nature **398**, 47 (1999)) are inconsistent with the last two order parameters, which are expected to show zero-bias conductance peaks. We propose a definitive tunneling experiment to distinguish between the first two order parameters.

MM 26.6 Wed 18:00 H6

High-resolution ARUPS on single crystalline FeSi[100] — •M. Klein[1], D. Zur[2], D. Menzel[2], J. Schoenes[2], M. Neef[3], K. Doll[3], G. Zwicknagl[3], and F. Reinert[1] — [1]Universität Würzburg, Experimentelle Physik II, Am Hubland, 97074 Würzburg — [2]Technische Universität Braunschweig, Institut für Physik der Kondensierten Materie, Mendelssohnstraße 3, 38106 Braunschweig — [3]Technische Universität Braunschweig, Institut für Mathematische Physik, Mendelssohnstraße 3, 38106 Braunschweig

The transition metal compound FeSi shows unique magnetic and transport properties which have been subject to many theoretical proposals but have never been explained completely. To reveal the electronic band structure we have prepared high quality single crystals with a [100] surface and investigated them with high-resolution ARUPS ($\Delta E \sim 3$ meV). Close to the Fermi level we see a narrow band with a small dispersion and a strong temperature dependence. We discuss our results in comparison with band structure calculations and with theoretical models involving narrow bands near the edges of the small gap.