nanoscale views

Saturday, December 02, 2006

This week in cond-mat

Two papers on the arxiv this week that give me an excuse to talk about the standard picture of metals and how bits of it can fail.

cond-mat/0611714 - Pisana *et al.*, Born-Oppenheimer breakdown in graphene
The Born-Oppenheimer approximation is one of the most commonly made in quantum mechanical treatments of atoms, molecules, and solids. It's a specific example of the *adiabatic approximation*: if the potential energy term $V(t)$ of the single-particle Schroedinger equation changes slowly enough (basically compared to \hbar divided by the energy difference between the single-particle energy levels of the system at some instant in time), then it's ok to say that the true single-particle solutions are well approximated at time t by the solutions to the *static* Schroedinger equation with $V = V(t)$. The Born-Oppenheimer approximation applies this to electrons around atoms. It assumes that the atoms move slowly compared to the electronic energy timescales, so that one can do calculations of molecular (for example) states by assuming that the ions are fixed in space. This paper reports Raman scattering measurements of the vibrational modes of graphene as a function of gate voltage (and hence electronic density). What they find is that the electronic population affects the lattices vibrational modes in a way that violates the Born-Oppenheimer approximation. I haven't read this very carefully, but this is interesting and surprising, at least to me. Given how well the basic graphene electronic structure can be approximated by a simple tight-binding calculation, a big violation here seems weird.

cond-mat/0611724 - Qazilbash *et al.*, Correlated metallic state of vanadium dioxide
The mean free path is a simple concept: it's the average distance a particle travels before scattering off of something. For a classical gas of hard spheres, the mean free path would be the inverse of (number density times cross-section). For quantum mechanical electrons in a metal, the electrons scatter off anything that breaks the periodicity of the crystal lattice - grain boundaries, defects, impurities, distortions of the lattice due to phonons. The mean free path in a metal is typically found from the conductivity, via something called the Einstein relation. Tacit here is the assumption that the electrons behave like well-defined particles that can propagate along for a while between scattering events. Indeed, a general requirement for the validity of this quasiparticle picture for electronic states in a metal is that the ratio of the mean free path to the wavelength of the electron is much greater than one. If the electron scatters many times before even traveling one wavelength, obviously the traveling wave picture of the electron is not valid. The point of this is that there is a physical lower limit to the mean free path: in a "good metal", the mean free path should never be shorter than the lattice spacing between atoms. This is called the Ioffe-Regel-Mott limit.
Now look at vanadium dioxide, which has a transition at 340 K between a high temperature metallic phase and a low temperature insulating phase. The

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phase transition is complicated, and includes a change in the unit cell shape. The authors of this paper have used optical techniques to infer the frequency-dependent conductivity in both phases. They confirm that the Ioffe-Regel-Mott limit is violated in the metallic phase at high temperatures, and they infer that the dominant scattering mechanism is due to electron-electron interactions. Basically this is one more nice piece of evidence that VO2 is a "bad metal", in which the quasiparticle way of thinking about distinct electrons isn't really valid.

posted by Doug Natelson at 1:39 PM

5 Comments:

You have to wonder if charging of the graphene couldn't cause stress in the ultrathin layer that would shift the phonon energies.

Speaking of phonons and graphene, on Friday afternoon I heard a talk by Eric Pop of Intel/Stanford about thermal conductivity of single-wall carbon nanotubes. Then this week there's a paper in _Science_ by Arun Majumdar's Berkeley group about asymmetric (rectifying transport) in nanotubes. All this got me to thinking: could there be quantized conductance of heat? The answer might be no since phonons are bosons whose phase need not be a multiple of 2*pi when making a circuit around a magnetic field line. In other words, it seems like quantized electron conductance is related to the Aharonov-Bohm effect, which bosons do not participate in. OTOH, maybe there would be another source of phonon quantized conductance? The spin-statistics theorem is not the subject I understand the best!

By Alison Chaiken, at 8:40 PM

Alison, Keith Schwab (now at Cornell) actually demonstrated quantized thermal conductance as his big postdoc project with Mike Roukes. See Nature **404**, 974 (2000).

By Doug Natelson, at 8:10 AM

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thanks for that link to schwab's work. fascinating!

By Anonymous, at 9:03 AM

I second the thanks for the link. The result that quantized thermal conductance is independent of particle statistics is particularly thought-provoking. I don't have to struggle with the spin-statistics theorem again after all.

By Alison Chaiken, at 9:28 AM

Here is a recent paper on quantized thermal conductance. Nature **444**, 187 (2006)

By Xiaosong Wu, at 11:58 PM

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