What is the Model for Ferromagnetism in Itinerant Fermions?

Itinerant ferromagnetism in a Fermi gas with contact interaction: Magnetic properties in a dilute Hubbard model
Authors: C-C. Chang, S. Zhang and D.M. Ceperley,
arXiv.org: 1009.1409v1

Itinerant ferromagnetism of a repulsive atomic Fermi gas: a quantum Monte Carlo study
Authors: S. Pilati, G. Bertaina, S. Giorgini, and M. Troyer,
arXiv.org 1004.1169v1

Recommended and a Commentary by Chandra Varma,
University of California, Riverside.

The study of correlations in itinerant fermions may be said to have begun with Wigner in connection with the problem of ferromagnetism in metals. Wigner argued that there may be no ferromagnetism in a free-electron gas with Coulomb interactions at any density, unlike in the Hartree-Fock calculation of Bloch, which shows ferromagnetic polarization in free-electrons for densities lower than $r_s > 5.45$. The Hartree-Fock calculation favors ferromagnetism because of the "spin-hole" in the pair correlation function $g_{\sigma,\sigma'}(r)$: the parallel spins avoid each other at small distances due to the Pauli principle, thus avoiding the exchange energy $1/r_s$, at the cost of increased kinetic energy, which is only $1/r_s^2$. Wigner pointed out that due to Coulomb interactions, the anti-parallel spins also avoid each other almost equally well and presented an approximate calculation for his conclusion. The calculation of what came to be called the correlation energy: the exact energy minus the energy in the Hartree-Fock approximation, is analytically impossible except in the small r_s limit. Various approximate numerical schemes have been devised. One of the best are variational Monte-Carlo calculations, for example by Ceperely and Alder [1], who found the paramagnetic state to state to be stable at least for $r_s \gtrsim 75$. Extreme precision is required in such calculations; the difference in energy between the paramagnetic and the ferromagnetic state at $r_s = 50$ is 6^{-5} Rydberg.

So, what then is the physical basis for ferromagnetism at large temperatures in a wide variety of metals? Well reasoned arguments supported by a variety of empirical data by Mott, van Vleck and Herring[2] suggest that a lattice of atoms with orbital degeneracy and associated Hund's rule is essential. But there is room for much theoretical work here which has been ignored for very long. Especially interesting is the fact that the spin-splitting of the bands in ferromagnetic metals is often more than an order of magnitude larger than the transition temperature. This appears to be occurring also for itinerant anti-ferromagnetism in the pnictides which have received more attention due to their superconductivity. The physics of superconductivity cannot however be usefully thought about without addressing the questions about their magnetism and the magnetic fluctuations above the transition temperature which lead to the above large ratio.

The question of the model for ferromagnetism has also arisen in quite a different context. In recent experiments in cold fermionic atoms without confining periodic potentials, Jo et al.[3] found evidence for significant ferromagnetic correlations for $k_F a \gtrsim 1$, where a is the (repulsive) scattering length of the neutral atoms (the experiments give evidence of ferromagetic correlations that extend over distances of 3 to 4 inter-atomic distances), exciting a flurry of theoretical activity. The physics of ferromagnetism in such a problem is quite different from that of a problem with Coulomb interactions. Herring[2] summarized earlier variational and perturbative calculations for hard spheres and concluded that there may in fact be ferromagnetism in such a model for $k_F a \gtrsim 1.7$.

Very recently variational quantum Monte-carlo calculations have been done both for the single band Hubbard model (first paper above) on a cubic lattice with varying ratio of U/t and for hard sphere fermions characterized by a scattering length a and varying density, with results which appear to be quite different. In order to avoid the dreaded sign problems, some approximations have been made in both cases. But to the best of my limited knowledge on this matter, the results do not depend in any serious way on these approximations.

For the Hubbard model, an academic result due to Nagaoka is well known: a single hole polarizes the system ferromagnetically for $U = \infty$. The work of Reference (4) below implies that the range of Nagaoka's result extends at least to a density of holes proportional to $LogN/N$ in two dimensions and $N^{1/3}/N$ in two dimensions, where N is the number of sites. The first paper cited above does the calculations far away from this limit. Results are presented for densities between 0.0625 and 0.25 per site and U/t varying from 0 to 32. No ferromagnetism is found. The pair-correlations functions $g_{\sigma,\sigma'}(r)$ are calculated and they show that Wigner's idea mentioned above for particles interacting with Coulomb interactions works for the Hubbard model as well. The paramagnetic state energy is lower than the ferromagnetic energy at all U/t examined with no sign that the results will change at higher U/t. I do not know why these calculations were not done also for hole densities near half-filling.

In the second paper above, hard sphere fermions are treated and it is found that a partially polarized ferromagnetism is stable for $k_F a \gtrsim 0.8$ and full polarization for $k_F a \gtrsim 0.95$. While these results are in rough accord with Herring's surmise, the complete lack of correspondence with the Hubbard model is surprising. In the Hubbard model with large U, the maximum scattering length is bounded by a given by the lattice spacing or $k_F a = 1.03 n^{1/3}$. That may explain why for the densities investigated for the Hubbard model, no ferromagnetism was found.

I do not know why the Hubbard model calculations were not done also for hole densities near half-filling, i.e $n \approx 1$. It would also be very useful to understand aspects of ferromagnetism in real metals to have calculations with orbital degeneracy and local exchange or Hund's rule couplings beside the local repulsion parameter U.

I wish to thank Steve Kivelson for introducing me to the paper by Barbieri, Riera and Young.

1. D. M. Ceperley and B. J. Alder, Phys. Rev. Lett. 45, 566 (1980)

2. C. Herring, "Exchange Interaction among Itinerant electrons" *Magnetism, vol. IV* Edited by G.T. Radoa and H. Suhl, Academic Press, New York (1966).

3. G.-B. Jo et al., Science 325, 1521 (2009).

4. A. Barbieri, J. A. Riera, and A. P. Young, Phys. Rev. B 41, 11697 (1990).