Whither Correlated Electron Theory?

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This is the text of the 'Theory' opening talk at the 2001 Strongly Correlated Electron Systems conference. It contains opinions about some of the outstanding scientific challenges facing the theory side of the correlated electrons field.

I. INTRODUCTION

The intellectual excitement of the 'Strongly Correlated Electrons' field comes from the amazing variety of behaviors exhibited by actual materials; behaviors which apparently cannot be understood within the well established framework of electronic condensed matter physics, and which suggest the existence of as yet undiscovered classes of collective behavior. I think the organizers of the 2001 Strongly Correlated Electron Systems (SCES) conference have done a wonderful job of selecting talks which exhibit the diverse and fascinating behavior of correlated systems. In this, the 'Conference Introduction: Theory' talk, I will present my own opinions of the intellectual challenges and opportunities presented to the theoretical side of our field. I am sure that this audience will disagree with many aspects of what I have to say, and I look forward to hearing why.

I would like to begin by explaining what I mean by 'the well established framework of electronic condensed matter physics', and then to go on by building up a series of ways in which that framework has recently been challenged or extended. I shall be concerned mainly with the excitations which govern transport and other response functions and will not discuss energy calculations at all. The conventional picture is based on Landau’s fermi liquid theory, which shows how in many circumstances the low energy physics of interacting electrons in solids can be reduced to the physics of basically free electrons, moving in self consistent fields generated by other electrons. The self consistent fields may lead to a condensation into a paired state (either of particle-hole pairs, giving rise to a magnetic or charge density wave state, or of particle-particle pairs, giving rise to a superconducting state). The leading corrections to this picture involve electron-electron, electron-phonon, or electron-collective mode scattering and may be treated basically perturbatively, for the usual phase space reasons. In more formal language, these calculational techniques and understandings are associated with the existence of an infrared stable (or marginally unstable) fixed point (the fermi liquid fixed point discussed by Shankar).

This set of ideas (coupled with the tremendously successful complex of ideas and techniques associated with density functional band theory) describes many materials quite well; our field is concerned with those where it fails. One clear example is the quasi one dimensional materials. It is by now theoretically well established that strictly one dimensional electron systems are described by a Luttinger liquid, rather than a fermi liquid fixed point. The properties of Luttinger liquids are well understood, and while there are serious and important questions related to the degree to which any actual material with a strong unidirectional anisotropy is well described by a Luttinger model, I will not discuss these questions here. Another very well studied set of phenomena concerns the electron gas in a very high magnetic field. In a certain sense this involves the artificial creation (by suppression of kinetic energy) of a non-fermi-liquid. To keep this article within reasonable bounds I will restrict attention to zero magnetic field.

In what follows I discuss the following topics, not all of which are entirely orthogonal:

- The approach to the fermi liquid fixed point
- New kinds of ordered phases
- Problems with the present theory of quantum criticality in metals
- The possible existence of and characterization of 'Non-fermi-liquid' phases
- Non-quasiparticle physics: the exciting new techniques for dealing with \( T > 0 \) and with the 'incoherent' part of the electron spectral function.
• The importance, demonstrated to us by the 'colossal' magnetoresistance manganites, of first order phase transitions and of regimes of strong fluctuation.

II. LEADING CORRECTIONS TO FERMI LIQUID THEORY: THE BELITZ-KIRKPATRICK-VOJTA $[Q]$

Fermi liquid theory is now understood as an almost infrared stable fixed point of the interacting electron problem ("almost" because fermi liquids are generically marginally unstable to superconductivity). The location of the Fermi surface, the quasiparticle fermi velocity and residue and the Landau interaction parameters are parameters characterizing the fixed point. Most workers implicitly or explicitly expected that (with one exception) corrections to physical quantities, for example the free energy or the small momentum transfer $q$ limit of the spin or charge susceptibility were analytic in the variables ($T/T_F$)$^2$, $(q/p_F)^2$, corresponding in a straightforward way to irrelevant operators of dimension 2. These ($T/T_F$)$^2$, $(q/p_F)^2$ terms constitute among other things the bare temperature dependence of parameters in theories of quantum critical phenomena. Also, the coefficient of the $(q/p_F)^2$ term in the current-current correlation function gives the Landau diamagnetism. The one exception, a $T^2 \ln T_F/T$ term ($T$ in $d = 2$) term in the specific heat coefficient $\gamma = C/T$, was understood as a special effect involving the effect of long wavelength collective modes on the specific heat only. Because it was believed to have a coefficient entirely expressible in terms of Landau parameters and the fermi velocity, it was thought of as a feature of the Fermi liquid fixed point.

Very interesting recent work of Belitz, Kirkpatrick and Vojta challenges this understanding. These authors showed, by examination of leading nontrivial terms in a perturbation series, that the leading momentum dependence of the spin susceptibility $\chi_s$ of a clean fermi liquid is

$$\chi_s(q, \omega = 0) = \chi_0 + |q| \quad (d = 2)$$

$$\chi_s(q, \omega = 0) = \chi_0 + q^2 \ln(p_F/q) \quad (d = 3)$$

In the same approximation the dependence of the charge susceptibility is simply $q^2$. This result was later confirmed and clarified by a numerical analysis of the same set of perturbative graphs. A subsequent systematic analysis of the (mathematically much simpler) possibility of a $|q|$ term ($d = 3$) or $|q|^3$ term ($d = 2$) temperature dependence clarified some aspects of the connection to fermi liquid theory and demonstrated the importance of $2p_F^2$ terms to the phenomena.

The results obtained so far have however been essentially calculational. A general understanding has apparently not been achieved, but would be desirable. For example, if the Belitz et. al. $|q|$ occurred in the current-current correlation function, it would correspond to a strongly divergent Landau diamagnetism! While the logarithmic correction expected in $d = 3$ may be difficult to unambiguously observe, a detailed experimental study of quasi-two-dimensional materials (e.g. $Sr_2RuO_4$ and especially $Sr_3Ru_2O_7$, which is near a ferromagnetic instability) would be very interesting.

III. NOVEL FORMS OF LONG RANGED ORDER

Strongly correlated materials tend to order, and the search for new forms of order is a central theme in our field. Recent attention has focussed on two possibilities: orbital order, and 'staggered flux' or 'd-density wave' order.

**Orbital order** has recently been extensively discussed in the context of the 'CMR' manganites, and, or its fluctuations, may be important in many other systems as well. The idea is that if the electrically active (and correlated) ion (e.g. the Mn in CMR compounds) sits at a site of sufficiently high symmetry (as the Mn site has cubic symmetry in the ideal perovskite structure), then several different orbital states (e.g. the $\text{Mn } d_{3z^2-r^2}$ and $d_{x^2-y^2}$ orbitals) may be degenerate, and a spontaneous breaking of the orbital symmetry may occur, in close analogy to the spontaneous breaking of spin symmetry in a magnet. Similarly, in analogy with the 'spin liquid' states extensively discussed in the context of high-$T_c$ materials (see below, also), 'orbital liquid' states have been considered. Note, though, that orbital ordering generically breaks a crystal symmetry; it thus tends to be strongly coupled to lattice distortions, which should be ncluded in any theory and which tend to make the situation less quantum mechanical. Further, orbital index (unlike spin index) tends not to be conserved by the electron hopping part of the Hamiltonian, rendering 'orbital liquid' states different from spin liquids.

**Staggered flux or d-density wave** ordering falls into the familiar class of particle-hole pair condensation, but the order parameter involves intersite correlations in a crucial way and in particular leads to the formation of lattice scale circulating current patterns. The idea was introduced in the context of high temperature superconductivity by Affleck and Marston. In their theory the circulating currents were a consequence of a particular kind of spin correlations produced (in the approximation used in Ref 8) by the competition between magnetic ordering and carrier motion. More recently, Chakravarty et al have reintroduced the concept (still in the context of high-$T_c$) and argued that one
should treat the circulating currents as fundamental, and Chandra and co-workers have proposed that something of this kind is the mysterious hidden order parameter of \( URu_2Si_2 \)

### IV. QUANTUM CRITICALITY IN METALS

An obvious place to seek for the breakdown of conventional concepts is in the vicinity of a second order \( T = 0 \) phase transition (quantum critical point), where the diverging correlation length suggests the existence of a long ranged, unscreened interaction which would invalidate the usual justification for fermi liquid theory. The theory of quantum criticality in metals was founded by Hertz and studied in more detail by the authors and many others. The basic starting point is an action \( S \) for an order parameter \( \phi \), obtained by formally integrating out the electron excitations and of the form

\[
S = S_{dyn} + \int d^dxd\tau \left[ \xi^2_0 (\nabla \phi)^2 + r\phi^2 + u\phi^4 + \ldots \right]
\]

where \( S_{dyn} \) expresses the dynamics of the order parameter. In metals, the crucial point is that the excitations are overdamped, \( S_{dyn} \sim i|\omega|/\Gamma_q \) with \( \Gamma_q \) a damping coefficient) leading to a dynamical exponent \( z \geq 4 \). The effective dimensionality is \( d_{eff} = d + z \) and for \( d \geq 2 \) \( d_{eff} \geq 4 \) so one expects the transition to be at or above its upper critical dimension and described by a Gaussian model with a dangerously irrelevant operator. The theory is then very well controlled and leads to a number of predictions which agree roughly with experiment in some cases, but in many cases disagree strongly. The reason for the disagreement is presently unclear. In some cases it may be associated with quasi-two-dimensional spin fluctuations, but I am uncomfortable with this explanation because one would expect a crossover to three dimensional behavior to occur within the experimental range. The detailed crossover behavior has however not been carefully studied theoretically or experimentally, so it is possible that the numbers are such that my concern is unwarranted.

Two other more theoretically interesting possibilities have been raised. One is that the presence of gapless electron excitations can change the form of \( S \). Chubukov and co-workers have demonstrated that in a model of two dimensional metallic antiferromagnetism the coefficient \( u \) in fact is not a constant but has a nontrivial \( \omega \), \( q \) dependence, leading to somewhat different behavior for response functions etc. In general one ought uncomfortable with integrating out gapless excitations, so it seems that this issue deserves examination in other contexts as well.

A more radical proposal was made by Schroeder, Coleman and co-workers in the context of analysing data on the \( Ceu_{x-y}Au_x \) system, which undergoes a paramagnet-antiferromagnet transition at approximately \( x = 0.1 \) with critical properties (most notably the linear scaling of the Neel temperature with control parameter and a logarithmically divergent specific heat coefficient) strikingly inconsistent with the standard analysis. These authors argued on the basis of scaling analyses of the \( \omega \), \( q \) dependence of neutron scattering measurements of the susceptibility at a range of high momenta, along with the temperature and field dependence of the uniform susceptibility, that at the critical point \( S_{dyn} \sim (i\omega)^\alpha \) with \( \alpha \approx 0.75 < 1 \). In other words, at criticality, the very low frequency spin dynamics are anomalous everywhere in the zone, not just in the vicinity of the ordering wavevector. These authors speculated that this was a signature of a new kind of critical point, at which the Korringa temperature or renormalized fermi energy vanished at precisely the point at which magnetism began. Si and collaborators have found a model of fermions coupled to two-dimensional bosons, which in the dynamical mean field approximation appears to yield the sort of behavior suggested by Coleman et. al. Further experimental and theoretical study of these extremely interesting models and phenomena would be very desirable. One issue which deserves clarification is the behavior of the specific heat coefficient. Naively, a divergence of the local spin susceptibility implies a similar divergence of the specific heat coefficient. The connection is not completely rigorous, but from the Kubo formula one has

\[
\sum_q \chi''_q(\omega) = \sum_n \langle <0|m_{loc}|n> \rangle \delta(\omega - E_n)
\]

where \( D(\varepsilon) \) is the density of states (of exact eigenstates) and \( m_{loc} \) is the matrix element by which a local magnetic field couples to these eigenstates. The proposed behavior of \( \chi \) would imply that either \( D(\varepsilon)/\varepsilon \) or \( m_{loc}(\varepsilon) \) diverges as \( \varepsilon \to 0 \). As it seems unlikely that a local matrix element would diverge, one is tempted to ascribe the divergence to \( D(\varepsilon)/\varepsilon \), which would imply a stronger than logarithmic divergence of the specific heat, in contrast to observation on \( CeCtu_{x-y}Au_x \). Interestingly, Trovarelli et. al. have observed that in \( YbRh_2Si_2 \) that an apparent logarithmic divergence in the specific heat coefficient , occurring for temperatures in the range of 1-5\( K \) is changed at very low \( T \) to a stronger divergence.
V. NON FERMI LIQUID PHASES

A long-standing goal of our field is the discovery of metallic phase with no (obvious) long ranged order and with low temperature properties inconsistent with the predictions of Fermi Liquid theory. Recent detailed high-precision experimental studies have produced an intriguing finding. In a number of heavy fermion and transition metal compounds exhibiting a pressure-tuned magnetic critical point, on the paramagnetic side the low temperature resistivity does not take the $T^2$ form expected from fermi liquid theory, but instead exhibit a lower exponent, even down to the lowest temperatures. It is possible that this is a crossover phenomenon, but one should be able to estimate the crossover scale from the behavior of the Neel temperature on the low pressure side of the transition, and the temperatures attained are far below this. If these results hold up, they present a fundamental challenge to our understanding of metal physics.

On the theory side, note that the conventional dichotomy in the 'Kondo lattice' model describing heavy fermion materials is that one either dissolves the local moments into the conduction electrons, forming a heavy fermi liquid, or one magnetically orders them. Kikoin and co-workers have argued that a third alternative is possible, namely to form a 'spin liquid' state from the local moments, leaving the conduction electrons to form a small fermi surface. My understanding is that experiments so far do not support this possibility, but it is a very interesting theoretical suggestion which seems very much worth further investigation. Senthil, Fisher and co-workers have argued that the theoretical search for new physics should focus on 'fractionalized' phases in which at least some of the excitations exhibit novel quantum numbers (e.g. charge 0 and spin 1/2) and (following work by Wen in the quantum hall context) have shown that this implies the presence of a topological order revealed most clearly by the ground state degeneracy in a multiply connected sample. Luillier and co-workers have presented very suggestive numerical evidence that spin liquid phases (which, if possessing spin-Peierls order, do so on such a long length scale as to leave a reasonable regime of spin liquid behavior) actually occur in certain two dimensional frustrated Heisenberg spin models, and Sondhi and Moessner have convincingly demonstrated the existence of a spin liquid in the (perhaps less directly physical) tirangular-lattice quantum dimer model.

VI. BEYOND PARTICLES

Much attention has focussed on properties controlled either by ground state symmetries or by the excitation of a small number of quanta ('particles') in part because the theoretical treatment is simplest and the different between phases perhaps least unambiguous. In the fermi liquid context one focusses on properties controlled by the quasiparticle pole of the Green function (or by the long-wavelength collective modes); in the non-fermi-liquid context one searches for new phases, and new particles (e.g. 'semions' or 'spinons'). However, many situations arise in which a description in terms of a small number of (reasonably well-defined) particles is not appropriate, and I would like to draw your attention to recent very interesting progress in this area.

Conventionally, one thinks of superconductivity as arising from the pairing of two reasonably well-defined particles (although Eliashberg theory allows one to go a bit beyond this assumption). Chubukov and co-workers studied superconductivity near a two dimensional antiferromagnetic critical point where the electron Green function is very broad and has no coherent part at all, and were able to formulate a theory of 'incoherent pairing'. I think this work is important in a broader context, as an example of physics without (quasi)particles, and could be relevant to the long-standing mystery of $UBe_{13}$ where superconductivity apparently emerges from an extremely highly resistive and strongly scattered state.

A characteristic feature of a strongly incoherent state is a lack of strong momentum dependence (put differently, the crucial aspect of a particle is its energy-momentum dispersion relation, which is absent or weak in a strongly incoherent state). This feature allowed Chubukov et. al. to make progress by reducing the problem to a self-consistent set of integral equations involving only frequency. The consequence of negligible momentum dependence (in this case of the electron self energy) has been exploited to a much greater extent in the 'dynamical mean field' or 'd = ∞' approach to correlated electron problems, introduced by Mueller-Hartmann, pursued by many workers, and brought into its present highly successful and useful form by Kotliar and many co-workers. This line of approach has had many successes, including the elucidation of many key features of the Mott metal-insulator transition and its recent 'marriage' to LMTO band theory (enabling the more or less ab-initio calculation of key features of the phase diagram of plutonium and of the magnetic transition temperatures of Fe and Ni). Here, however, I would stress the great conceptual importance of the method. The essential idea is that if the momentum dependence of the electron self energy is negligible, then all important physical quantities may be derived from a functional of the local green function $G_{loc}$ given by
where $\varepsilon_p$ is the underlying band dispersion. The key point (due to Georges and Kotliar\cite{41}) is that because $G_{\text{loc}}$ is a function only of frequency, the functional of $G_{\text{loc}}$ may be written as a quantum impurity and explicitly constructed via (not too heavy) numerics. The important object in the theory, thus, is not a particle or field with a well defined $\omega$ vs $k$ dispersion relation. Rather, it is a \textit{function of frequency} which includes coherent and incoherent parts of propagators, and $T > 0$ and $T = 0$ behaviors on the same footing. This produces the ability to calculate many things which could not be done before, and more importantly, I believe will lead to new ways of thinking about correlated electron physics.

A further advantage of the DMFT work is that there are a number of important questions in correlated electron physics which are quantitative in nature, yet extremely interesting, and which DMFT may help us to understand. One topic of current discussion is ‘Why is the ferromagnetic transition temperature of lightly doped hexaborides so high? Why does it drop rapidly for dopings beyond a few percent?\cite{42} Another topic of long standing interest is ‘Why is the pairing scale in the hole-doped cuprates so high?’ This question has recently been joined by the question ‘Why is the pairing scale in hole-doped $C_{60}$ so high?\cite{43}

### VII. FIRST ORDER TRANSITIONS LEAD TO INTERESTING BEHAVIOR ALSO!

A commonly held belief in correlated electron physics is that first order phase transitions are not interesting, because they are not accompanied by a diverging length. I wish to argue that this point of view is perhaps overly narrow. First, it rules out of consideration the many phenomena associated with metal insulator transitions (which are typically first order with a second-order end point) and mixed valence phenomena (also typically first order). Second, as is well known, correlated electron materials generically have very low energy scales and several competing phases: critical end-points of first order transitions may occur at much lower temperatures than one would guess and as a result fluctuations may be much stronger. Indeed, it is even possible by tuning a parameter to bring the critical end point of a first order line is sufficiently close to zero temperature that the physics is controlled by a \textit{quantum critical end point}.\cite{44} Apparently, the metamagnetic transitions in many heavy fermion compounds are in this category (or may be made so by applying e.g. pressure), and a very exciting recent development is that at ambient pressure the nearly two-dimensional compound $Sr_3Ru_2O_7$ may be in this category.\cite{45} Further, the classic Imry-Wortis work\cite{46} shows that in two spatial dimensions, randomness which couples to the energy density (i.e. any randomness at all) converts first order transitions into second order ones, leading (presumably) to a host of unusual phenomena. I sometimes wonder if this phenomenon is at the root of the difficulties involved in interpreting data on high-$T_c$ materials.

These ideas are very nicely exemplified by the results obtained in the last 5 years on the ‘colossal’ magnetoresistance manganites. These materials display an amazing sensitivity of properties to external perturbations (and sample form and quality!), of which the highly-touted ‘colossal’ magnetoresistance is but one example. It is now generally accepted that linear response susceptibilities are not particularly large, and that the exotic behavior is due to a multiphase coexistence\cite{47} which is itself a consequence of the presence of several competing phases (different varieties of charge ordered insulator as well as ferromagnetic metal) with first order phase boundaries between them, along with disorder, which leads to the multiphase coexistence. Two particularly striking recent results are that in the material $La_{0.7}Ca_{0.3}MnO_3$ (which has a ferromagnetic ground state and a magnetic transition at $T_c \approx 260K$) the phase transition is in fact first order\cite{48} and the high temperature phase exhibits surprisingly strong charge/orbital fluctuations extending up to quite high temperatures\cite{49}. The percolation idea was picked up by theorists, and modelled via numerical simulations of the two dimensional random field Ising model\cite{50}, with quite plausible agreement with data. One difficulty is that the calculation relied on what the general arguments\cite{51} are quite special features of two dimensional models, which would not be expected to hold in the three dimensional cases of experimental relevance. It seems likely to the present author that the relevant disorder is long-range correlated, and arises from strain fields. This belief is supported by recent work showing a martensitic character to the charge/orbital ordering transitions.\cite{52}

In any event, the example of the manganites shows that first order phase boundaries can lead to fascinatingly complex behavior. It seems likely that this idea will be fruitful in other areas of correlated electron physics as well.

### VIII. SUMMARY

In this article I have tried to present an overview of important challenges and open issues in correlated electron theory. I apologize to all those whose work I have misrepresented or not represented.
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1. D. Pines and P. Nozieres, Theory of Quantum Liquids, (Addison Wesley: Reading, MA 1995).
2. R. Shankar, Rev. Mod. Phys. 66 199 (1994).
3. F. D. M. Haldane, J. Phys. C14, 2585 (1981); Phys. Rev. Lett. 47, 1840 (1981); 48, 569(E) (1982).
4. A. J. Millis, Physical Review B48, 7183-96 (1993)
5. C Pethick and G. M. Carneiro, and C. J. Pethick Phys. Rev. B16 1933 (1977)
6. D. Belitz, T. R. Kirkpatrick and T. Vojta, Phys Rev. B55 9452 (1997).
7. D. Hirashima and K. Takahashi, J. Phys. Soc. Jpn 67 3816 (1998) and D. Hirashima and K. Kubo, J. Phys. Soc. Jpn 68 2174 (1999).
8. G. Y. Chitov and A. J. Millis, Phys. Rev. Lett. 86 5337 (2001)and Phys. Rev B in press (2001)
9. R. Perry et. al. Phys. Rev. Lett 86 2661 (2001)
10. Colossal Magnetoresistive Oxides, Y. Tokura, ed., Gordon and Breach, 1999.
11. see, e.g. F. Mila et. al. Phys. Rev. Lett. 85 1714 (2000)
12. D. Belitz, T. R. Kirkpatrick and T. Vojta, Phys Rev. B55 9452 (1997).
13. D. Hirashima and K. Takahashi, J. Phys. Soc. Jpn 67 3816 (1998) and D. Hirashima and K. Kubo, J. Phys. Soc. Jpn 68 2174 (1999).
14. G. Y. Chitov and A. J. Millis, Phys. Rev. Lett. 86 5337 (2001)and Phys. Rev B in press (2001)
15. R. Perry et. al. Phys. Rev. Lett 86 2661 (2001)
49. J. P. Hill et al. cond-mat/0105604
50. A. Moreo et al., Science 283, 2034 (1999).
51. V. Podzorov, B. G. Kim, V. Kiryukhin, M. E. Gershenson, S-W. Cheong, cond-mat/0107609 (Phys Rev B in press (2001)).