Quantum Spin Liquids and the Metal-Insulator Transition in Doped Semiconductors

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We describe a new possible route to the metal-insulator transition in doped semiconductors such as Si:P or Si:B. We explore the possibility that the loss of metallic transport occurs through Mott localization of electrons into a quantum spin liquid state with diffusive charge neutral "spinon" excitations. Such a quantum spin liquid state can appear as an intermediate phase between the metal and the Anderson-Mott insulator. An immediate testable consequence is the presence of metallic thermal conductivity at low temperature in the electrical insulator near the metal-insulator transition. Further, we show that though the transition is second order, the zero temperature residual electrical conductivity will jump as the transition is approached from the metallic side. However, the electrical conductivity will have a nonmonotonic temperature dependence that may complicate the extrapolation to zero temperature. Signatures in other experiments and some comparisons with existing data are made.

Phenomena near the metal-insulator transition (MIT) in doped semiconductors such as Si:P or Si:B have been studied extensively for more than three decades [1–4]. Nevertheless, several aspects of the physics, for instance the detailed critical behavior [4–6], remain mysterious. In this Letter, we explore and develop the consequences of a new possible route to the MIT where a quantum spin liquid insulator appears as an intermediate phase between the metal and the Anderson-Mott insulator. In recent years, such a quantum spin liquid Mott insulator has been observed to intervene between the Fermi liquid metal and conventional magnetically ordered Mott insulators in a few different clean materials [7–9]. Here, we study the strongly disordered situation appropriate to doped semiconductors and describe a variety of experimental consequences.

When P is doped into Si, the extra electron of P forms a hydrogenlike state with an effective Bohr radius of about $a \approx 20$ Å [1,10]. A simple picture of the doped semiconductor is as a collection of randomly placed "hydrogen" atoms. The system may then be described as a half-filled Hubbard model on a random lattice supplemented by the inclusion of the long-range Coulomb interaction V_{ij} between the electrons,

$$H = -\sum_{ij;\alpha} t_{ij}(c_{i\alpha}^{\dagger} c_{j\alpha} + \text{H.c.}) + U\sum_{i} n_{i\uparrow} n_{i\downarrow} + \sum_{i \neq j} V_{ij} n_i n_j. \quad (1)$$

At low concentrations, the $t_{ij} \approx t_0 e^{-r_{ij}/a}$ are small, the on-site U dominates and a Mott insulator of local moments results. The local moments are coupled antiferromagnetically and due to their random placement, preferentially form singlets with their closest available neighbor. The resulting random-singlet phase has an extremely broad distribution of singlet-binding energies, giving rise to a diverging density of states for low-energy spin excitations, contributing a divergent coefficient of heat capacity, $\gamma = C/T$ and spin-susceptibility, χ [11].

As the concentration of dopants, n, is increased, eventually the typical t_{ij} dominates over the U and a diffusive metal is obtained. A continuous phase transition between metal and insulator occurs at some critical intermediate concentration, n_c, where $t_{ij} \approx U$ [10]. Because of the random placement of dopants, a fraction of the local moments are very weakly coupled to the conducting electrons and survive unscreened into the metallic phase. The diffusive metal appears to be well described by a "two-fluid" model where the conducting electrons exist essentially decoupled from a random fraction of weakly coupled local-moments [1,12]. As in the insulating phase, these local moments continue to dominate the low-temperature thermodynamic and magnetic properties of the metallic phase but do not appear to strongly modify its transport properties.

It is natural to ask: What is the fate of the conducting fluid across the metal-insulator transition? The conventional answer, implicitly adopted by most existing work [2,3], is that all electron degrees of freedom are localized by disorder [13], which is perturbatively enhanced by interactions. In this scenario, shown in Fig. 1(a), decreasing $n < n_c$ gives a localized Anderson-Mott insulator with nonzero average density of states. As n is further decreased, the system crosses over continuously towards a correlation driven Mott-insulator of local moments.

In this Letter, we point out a new and conceptually distinct scenario for the metal-insulator transition in doped semiconductors. In this scenario, the charged conducting fluid is localized into a gapless quantum spin liquid, but the electron thermal transport remains
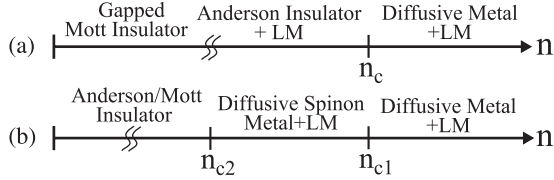
FIG. 1. Two scenarios for the MIT in doped semiconductors. (a) Conventional picture electron localization transition to Anderson-Mott insulator, which crosses over continuously to a pure Mott insulator (indicated by wiggly lines). (b) In the newly proposed scenario, the transition is to a spin liquid with gapless fermionic spinon excitations, here the electrical MIT at n_{c1} occurs separately from the spin and thermal transitions at n_{c2}. "+LM" indicates the fraction of randomly decoupled local spin-moments that inevitably accompany all phases.

diffusive into the weakly insulating regime. There is growing theoretical and experimental evidence that such gapless spin liquids occur in clean Mott insulators, where strong charge fluctuations and frustration prevent magnetic ordering [7–9]. This experience makes it natural to ask whether or not one should expect a spin-liquid phase to form in (uncompensated) doped semiconductors near the MIT, where charge fluctuations are strong, the system is at half-filling, and magnetic order is prevented by the random lattice structure, the competition between antiferromagnetic direct-exchange and random-sign RKKY exchange, and by quantum fluctuations.

The possibility of a spin-liquid phase in doped semiconductors due to multiparticle ring-exchange effects was previously suggested but not explored in [14]. Also, fractionalization of the random singlet phase of local moments was suggested [15] as a possible mechanism for unconventional superconductivity in B doped diamond.

Nature of the possible spin-liquid phase(s).—The proposed spin-liquid phase is most conveniently described by formally dividing the electron into a bosonic U(1) rotor $e^{i\theta}$ that carries the electron charge, and a fermionic spinon f_α that carries the electron spin: $c_i = e^{i\theta_i} f_{i\alpha}$ [16,17]. This description allows extraneous unphysical states that must be removed by constraining $n_{b,i} - \sum_\alpha f_{i\alpha}^\dagger f_{i\alpha} = 1$ on each site, i. Here, n_{bi} is the number operator conjugate to θ_i. The above decomposition has a U(1) gauge redundancy associated with $\theta_i \rightarrow \theta_i + \Lambda_i$ and $f_i \rightarrow e^{-i\Lambda_i} f_i$, which manifests itself in the low-energy effective theory as an emergent U(1) gauge field, $\mathbf{a}(\mathbf{r}, t)$ [18]. A similar slave-particle description was previously developed for the weakly disordered two-dimensional (2D) case for the triangular lattice organics [19].

Decoupling the hopping term $-t_{ij} c_{i,s}^\dagger c_{j,s} = -t_{ij} e^{i(\theta_i - \theta_j)} f_{i,s}^\dagger f_{j,s}$ in a mean-field approximation and including gauge fluctuations gives the effective action, $S_{\text{eff}} = \int d\tau (L_b + L_f)$, with

$$L_b = \sum_i \frac{1}{2}(\partial_\tau \theta_i + a_i^0)(U\delta_{ij} + V_{ij})^{-1}(\partial_\tau \theta_j + a_j^0)$$
$$- t_{ij} \sum_{ij} \chi_{ij}^f e^{i(\theta_i - \theta_j + a_{ij})} L_f$$
$$= \sum_{ij} f_i^\dagger [(\partial_\tau - a_i^0 - \mu)\delta_{ij} - t_{ij}\chi_{ij}^b e^{-ia_{ij}}]f_{j,s,} \quad (2)$$

where $\chi_{ij}^f = \langle f_{i,s}^\dagger f_{j,s} \rangle$ and $\chi_{ij}^b = \langle e^{i(\theta_i - \theta_j)} \rangle$ are determined self-consistently. Note that, due to the random placement of sites, in general $\sum_s \langle f_{i,s}^\dagger f_{i,s} \rangle$ will be spatially varying. Consequently, even at the mean-field level, the bosons will experience a random chemical potential; this changes the universality class of the Bose-Mott transition compared to the clean case (where $\langle n_b \rangle = 1$ for every site on both sides of the Mott transition).

The metallic Fermi-liquid state corresponds to a superfluid-ordered phase of the bosonic rotors with $\langle e^{i[\theta(\mathbf{x}) + \int^{\mathbf{x}} \mathbf{a}(\mathbf{y}) \cdot d\mathbf{y}]} \rangle \neq 0$, coexisting with a diffusive Fermi liquid of spinons. In this phase, the emergent gauge field is gapped by the condensate of charged rotors through the Anderson-Higgs mechanism, and the rotors and spinons are "glued" together into ordinary electrons.

Equation (2) also naturally describes a deconfined state in which the rotors form a Bose glass/Mott insulator, while the spinons remain diffusive. This results in an exotic charge insulator with finite density of states for gapless spin 1/2 excitations. We suggest that this spin-liquid phase may occur near the MIT for doped semiconductors. In this scenario, shown in Fig. 1(b), the magnetic properties of the system change only gradually across the MIT at n_{c1} and are qualitatively identical in both the metal and insulator. In particular, we expect that one would still find a decoupled fraction of local moments. As these local moments dominate the low-temperature thermodynamics and magnetic properties, the clearest signature of the spin liquid is metallic thermal conductivity, $\kappa \sim T$ at low T [8]. While there has been extensive experimental analysis of the conductivity of doped semiconductors near the MIT, very little is known about thermal transport.

In the slave-rotor language, the formation of local moments comes from rare strong fluctuations in disorder that locally bind the rotor and fermion back into a correlation-localized electron. We assume that the principal effect of correlated disorder among the rotor, spinon, and gauge-field sectors is to produce such local moments, and that the physics of the remaining nonlocal moment bulk can be well described by treating disorder separately in each sector.

In the spin-liquid phase, the emergent gauge field is deconfined, and in clean systems its fluctuations lead to singular self-energies for the spinons resulting in non-Fermi liquid behavior (2D) [20–27] or marginal Fermi-liquid behavior (3D) [28–30]. For the strongly disordered doped semiconductors, the inelastic scattering rate for the spinons from gauge fluctuations scales as $\tau_g^{-1} \sim T$ and is

dominated by the elastic impurity scattering for low T (see Supplemental Material [31]). Consequently, the low-energy properties of the disordered spinon Fermi liquid will be largely unaltered by the emergent gauge field. Furthermore, the gauge field propagation is strongly damped by the diffusive spinons, leading to an $\omega \sim q^2$ scaling of gauge excitations. This scaling implies that the gauge-field contribution to thermodynamic quantities is subdominant compared to the spinon contribution. For example, the gauge-field specific heat scales as $C_a \sim T^{3/2} \ll C_{\text{spinon}} \sim T$.

In two dimensions, a deconfined phase for the gauge field requires the presence of extended, gapless fermionic excitations to suppress instanton configurations [32,33]. In three dimensions, however, a compact U(1) gauge field may remain deconfined even without extended, gapless matter [32]. Therefore, in addition to the gapless, thermally conducting spinon Fermi-surface state described above, it is also possible to form an insulating state where the charge degrees of freedom are Mott localized and the spinons are Anderson-localized by disorder. Such a spinon Anderson insulator is distinguished (in principle) from the conventional Anderson-Mott insulator by the presence of a gapless emergent U(1) gauge field (though experimentally detecting the emergent gauge field would be challenging).

Generalized phase diagram.—The MIT achieved by changing n, though experimentally relevant, is conceptually complicated since disorder and interactions are simultaneously affected. It is conceptually simpler to consider a generalized phase diagram, where disorder strength W and interaction strength U can be separately adjusted, as in Fig. 2. Here, we restrict our attention to three dimensions, half-filling, and non-nested Fermi surfaces (which are not inherently unstable to magnetic ordering). Furthermore, we remain agnostic about the particular realization of disorder, with the expectation that such details will not alter the qualitative discussion that follows.

We begin by considering various limiting cases. The $(U = 0, W \neq 0)$ limit is completely understood [13]: here, a diffusive Fermi liquid occurs up until a critical disorder strength beyond which all states near the Fermi-energy become localized leading to an Anderson insulator (AI). Each of these phases is known to be stable to infinitesimal interactions, and therefore extends at least to small U. The limit of $(U \neq 0, W \to \infty)$ is also straightforward. Here the Anderson localized insulator at weak interactions crosses over continuously to the Mott insulator of local moments at strong interactions. At $T = 0$, the local moments are magnetically ordered in either a random-singlet or spin-glass phase.

Finally, the line $(U \neq 0, W = 0)$ is also reasonably well understood [17], albeit with slightly less confidence. The clean Fermi liquid survives up until some critical interaction strength, beyond which it becomes a weak Mott-insulator with a spinon Fermi surface. For large U, the emergent gauge field undergoes a confinement transition

and antiferromagnetic order develops. Here again, each of the clean interacting phases is stable to infinitesimally small amounts of disorder and extends to finite W. The only distinction being that, for any $(U \neq 0, W \neq 0)$, disorder creates a nonzero density of decoupled local moments (indicated in Fig. 2 by "+LM").

These considerations greatly constrain the structure of the generalized phase diagram. Each of the phases at the boundary are known to extend to finite values of W and U. Given the understanding of the boundaries of the phase diagram, the main issue here is not whether a strongly disordered fermionic spin liquid could exist, but rather which particular path through the generic W and U phase diagram is appropriate to tuning n in doped semiconductors. Figure 2 depicts an extension of the well-understood outer boundary of the phase diagram to the interior. While one can conceive of many intermediate insulating phases at intermediate U and W, in the slave-rotor language, the only other natural candidate is the deconfined spinon Anderson insulator described above.

Thermal conductivity.— In the spin-liquid scenario, the electrical MIT and thermal MIT occur separately: whereas electrical conductivity vanishes in the insulating phase, thermal conductivity remains metallic, scaling as $\kappa_{\text{sp}} \sim T$ at low temperatures. Since the ever-present concentration of local moments dominates the low-temperature thermodynamical properties of the system (but contributes only weakly to transport), linear-T metallic conductivity is the clearest experimental signature of the spin liquid.

While $\kappa_{\text{sp}} \sim T$ at the lowest temperatures there will be Altshuler-Aronov–type corrections to κ from interactions and disorder: $\kappa_{\text{AA}} \sim T^{3/2}$ [34–36]. Also, one expects a large contribution, κ_{ph} from phonons: $\kappa_{\text{ph}} \sim T^3$ [37]. Therefore, to observe the metallic spinon contribution, it may be necessary to work at very low temperature and carefully subtract subdominant contributions.

Quantum critical (QC) scaling.— Despite extensive experimental and theoretical effort, the quantum-critical (QC) behavior of electrical conductivity remains contentious and poorly understood. The existence of a spin-liquid
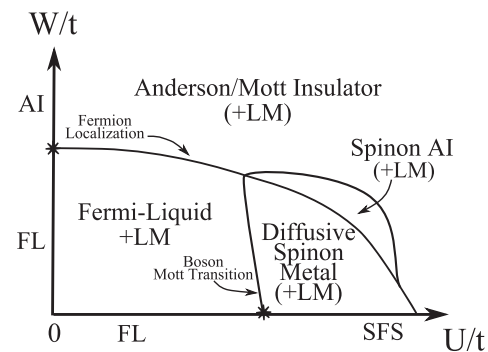

FIG. 2.   Schematic generalized phase diagram as a function of disorder strength W and interaction strength U measured with respect to the typical hopping t. SFS indicates a spinon Fermi surface.

phase would have important implications for how QC scaling should be extracted and interpreted. For $T = 0$ and $n > n_c$, the system is a Fermi liquid obeying the Wiedemann-Franz law: $\kappa/LT = \sigma$ (where the Lorenz number L is a constant). Since σ vanishes at the transition while κ/LT remains nonzero, there must be a discontinuous jump in the $T = 0$ electrical conductivity at the MIT. In the slave-rotor description, this jump arises from the Ioffe and Larkin rule [38] that the electrical resistivity ρ equals the sum $\rho = \rho_b + \rho_f$ of the resistivities of the bosonic rotors ρ_b and spinons ρ_f respectively. Crossing the MIT at $T = 0$, the bosons transition from a superfluid with $\rho_b = 0$ to an insulator with $\rho_b = \infty$. In contrast, the fermionic contribution, ρ_f evolves smoothly through the transition, implying a nonuniversal jump in the zero-temperature conductivity. Though superficially similar to Mott's early proposal [39], this jump in conductivity is unrelated to the idea of a "minimum metallic conductivity."

Evidence against a discontinuous jump in conductivity in Si:P comes mainly from pressure tuning studies [5] that show conductivity dropping sharply but apparently continuously to zero at the MIT. However, determining whether one is truly accessing the asymptotic behavior near the QC point is very challenging, and the proper interpretation of the conductivity scaling remains controversial and poorly understood [6]. For example, the pressure-tuned experiments extract a conductivity scaling exponent $\nu = 1/2$ that is incompatible with general exponent inequalities for a metal-insulator transition [40], but could be explained as a thermally rounded version of the true $T = 0$ conductivity jump. In the spin-liquid scenario, as we will argue below, issues with extrapolating to $T \to 0$ and $n \to n_c$ are further exacerbated.

Near the quantum critical point (i.e. $T \approx 0$, and $\delta n = n - n_c \ll n_c$), $\rho_b(T, \delta)$ obeys the quantum critical (QC) scaling for the disordered Bose-Hubbard model Mott transition as shown in Fig. 3(a). In the high-temperature critical regime where T is the dominant perturbation away from criticality, $\rho_b(T) \sim T^{-1/z}$. At lower temperatures $T < T^* \sim (\delta n)^{z/\nu}$, where δn is the dominant perturbation from criticality $\rho_b(T)$ crosses over from the $T^{-1/z}$ to 0 as superfluidity develops. Here z is the dynamical exponent for the disordered Bose-Mott transition with Coulomb interactions [41].

The spinon contribution to the resistance tends to a constant at zero temperature, due to the elastic scattering from disorder. At finite temperature, there will also be nonconstant contributions to ρ_f: $\rho_{AA} \sim \sqrt{T}$, [42] and $\rho_{ph} \sim T^{\sim 3-5}$, from interactions and phonons respectively. The resulting electrical resistance, $\rho = \rho_b + \rho_f$, is depicted in Fig. 3(b). for various δn near the MIT. The main feature here, is the resistance upturn due to the nearly critical fluctuating bosons, which quickly disappears below $T < T^*$ as ρ saturates to a nonuniversal constant set by ρ_f. The corresponding T dependence of $\sigma = 1/\rho$ is shown in Fig. 3(c). Notice the discontinuous jump in the very-low

temperature conductivity between $\delta n \to 0^+$ and $\delta n = 0$. As shown in Fig. 3(d), this jump will be rounded at nonzero temperature, and could escape notice [consider, for example, if the lowest achievable temperature were indicated by the vertical dotted line in Fig. 3(c)].

The spin-liquid scenario outlined here suggests a very different scheme for extracting the QC behavior of conductivity than that for a conventional localization transition. Here, one should include only data for which the resistance saturates to a nearly constant value set by the spinon contribution. In practice, there is a minimum achievable value of temperature, T_{min}. Consequently, this saturation region will disappear as the MIT is approached when $\delta n \lesssim T_{min}^{\nu/z}$. Beyond this point, extrapolations based on the curvature of σ would fail to capture the true $T \to 0$ behavior.

The spin-liquid scenario will also complicate efforts to extract the critical scaling of $\sigma(n)$ near the MIT. This difficulty is illustrated in Fig. 3(d), which shows $\sigma(T = 0, n)$. As the concentration is decreased in the metal, the conductivity curves slowly towards an eventual localization transition at n_{c2} (which may or may not occur). However, in the present scenario, the Mott transition of the rotors intervenes at $n_{c1} > n_{c2}$ before the spinons localize. In this case, extrapolations of QC scaling based on a conventional Anderson transition from the metallic side would be misleading.

Discussion.—In summary, we propose an alternative scenario to the Mott transition in doped semiconductors where the weakly insulating state is a spin liquid with fermionic excitations. While such a transition has definite consequences for the quantum critical scaling of conductivity, such quantum critical behavior is notoriously difficult to determine.

Other possible signatures of spin-liquid behavior include subgap optical conductivity [43] in the insulator from gauge fluctuations and vanishing quasiparticle residue
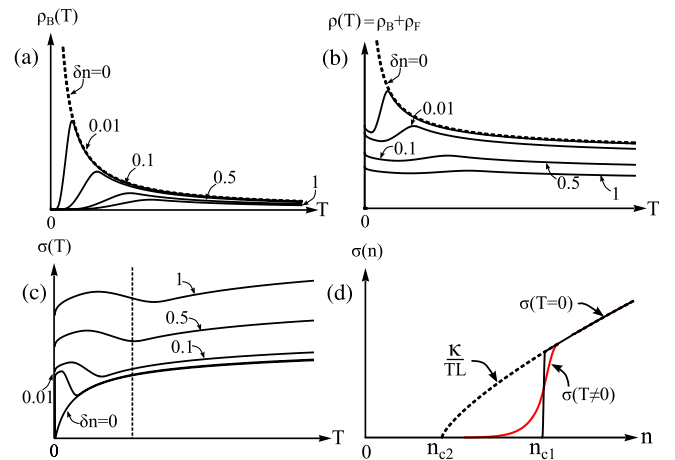

FIG. 3 (color online). Quantum critical scaling (with $z = 1$) [41] of electrical conductivity σ and linear T coefficient of thermal conductivity κ/TL (L is the Lorenz number) near the MIT as a function of concentration and temperature.

approaching the MIT (measurable by tunneling on the metallic side). However, the former coexists with subgap conductivity from exciting weakly bound local moments, and the latter behavior will also be produced by a soft Coulomb gap (which will develop at the MIT) [44]. Consequently, such probes are indirect, and would require a detailed quantitative comparison.

Therefore, we suggest that the clearest test for spin-liquid behavior in doped semiconductors would come from a careful study of thermal transport near the MIT. A spinon Fermi liquid would lead to $\kappa \sim T$ for low T, which, if observed, would strongly indicate the presence of gapless fermionic excitations.

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