

Melting of the Electron Glass

A. A. Pastor and V. Dobrosavljević

Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306

(Received 19 March 1999)

A model of spinless interacting electrons in the presence of disorder is examined using an extended dynamical mean-field formulation. When the interaction strength is large compared to the Fermi energy, a low temperature glassy phase is identified, which in our formulation corresponds to a replica symmetry breaking instability. The glassy phase is characterized by a pseudogap in the single-particle density of states, reminiscent of the Coulomb gap of Efros and Shklovskii. Because of ergodicity breaking, the “zero-field-cooled” compressibility of this electron glass vanishes at $T = 0$, consistent with absence of screening. When the Fermi energy exceeds a critical value, the glassy phase is suppressed, and normal metallic behavior is recovered.

PACS numbers: 75.20.Hr, 71.55.Jv

Understanding the basic physical processes determining whether a material is a conductor or an insulator continues to be a central theme of condensed matter physics. In recent years, much progress has been achieved in understanding weakly disordered metals [1], but the physics of the metal-insulator transition (MIT) in the presence of disorder remains largely an open problem.

The interplay of the electron-electron interactions and disorder is particularly evident deep on the insulating side of the MIT. Here, both experimental [2,3] and theoretical studies [4] have demonstrated that this can lead to the formation of a soft “Coulomb gap,” a phenomenon that is believed to be related to the glassy behavior of the electrons. Such glassy freezing has long been suspected [5] to be of importance, but very recent work [6] has suggested that it may even dominate the MIT behavior in certain low carrier density systems. The classic work of Efros and Shklovskii [4] has clarified some basic aspects of this behavior, but a number of key questions remain: (1) What is the precise relation of this glassy behavior and the emergence of the Coulomb gap? (2) What should be the order parameter for the glass phase? (3) How should the glassy freezing affect the compressibility and the screening of the electron gas? (4) How do the quantum fluctuations (electron tunneling) melt this glass and influence the approach to the MIT?

In this Letter, we examine a simple model for which all these questions can be rigorously answered in the limit of large coordination. Within our model, the universal form of the Coulomb gap proves to be a direct consequence of glassy freezing. The glass phase is identified through the emergence of an extensive number of metastable states, which in our formulation is manifested as a replica symmetry breaking instability. As a consequence of this

ergodicity breaking, the zero-field-cooled compressibility is found to vanish at $T = 0$, suggesting the absence of screening in disordered insulators. Finally, we show that quantum fluctuations can melt this glass even at $T = 0$, but that the relevant energy scale is set by the electronic mobility, and is therefore a nontrivial function of disorder.

In order to concentrate on the physics of the electron glass, we focus on a simple lattice model of spinless interacting electrons in the presence of randomness, as given by the Hamiltonian

$$H = \sum_{ij} (-t_{ij} + \varepsilon_i \delta_{ij}) c_i^\dagger c_j + \sum_{ij} V_{ij} n_i n_j. \quad (1)$$

Here, $n_i = c_i^\dagger c_i$ are the occupation number operators, t_{ij} are the corresponding hopping elements, V_{ij} describes the intersite electronic repulsion, and ε_i are the random site energies. Motivated by the long range nature of the Coulomb interaction, we wish to examine the situation where a given electron interacts with a large number z_v of other electrons. The analysis is simplest if the interaction $V_{ij} = V$ is taken to be uniform within a volume containing z_v neighbors, as opposed to the more realistic Coulomb interactions. Nevertheless, most of the *qualitative* features of the Coulomb glass are still captured if we consider $z_v \gg 1$, as follows.

To obtain the relevant dynamical mean-field (DMF) equations [7], we focus on a given lattice site, and formally integrate out [7] all the other degrees of freedom. For large coordination, the corresponding local effective action simplifies, since it suffices to consider contributions up to the second order in the hopping elements t and the interaction amplitudes V [8]. We concentrate on a Bethe lattice at half filling, where the equations are simple, and we find

$$S_{\text{eff}}(i) = \sum_a \int_0^\beta \int_0^\beta d\tau d\tau' \{ c_i^{\dagger a}(\tau) [\delta(\tau - \tau') \partial_\tau + \varepsilon_i + t^2 G(\tau, \tau')] c_i^a(\tau') + \frac{1}{2} V^2 \delta n_i^a(\tau) \chi(\tau, \tau') \delta n_i^a(\tau') \} \\ + \frac{1}{2} V^2 \sum_{a \neq b} \int_0^\beta \int_0^\beta d\tau d\tau' \delta n_i^a(\tau) q_{ab} \delta n_i^b(\tau'). \quad (2)$$

We have used standard functional integration over replicated Grassmann fields [9], where $a = 1, \dots, n$ ($n \rightarrow 0$) are the replica indices [10]. Here, the operators $\delta n_i^a(\tau) = [c_i^{\dagger a}(\tau)c_i^a(\tau) - 1/2]$ represent the *density fluctuations* from half filling. The order parameters $G(\tau - \tau')$, $\chi(\tau - \tau')$, and q_{ab} satisfy the following set of self-consistency conditions:

$$G(\tau - \tau') = \int d\varepsilon_i P(\varepsilon_i) \langle c_i^{\dagger a}(\tau) c_i^a(\tau') \rangle_{\text{eff}}, \quad (3)$$

$$\chi(\tau - \tau') = \int d\varepsilon_i P(\varepsilon_i) \langle \delta n_i^{\dagger a}(\tau) \delta n_i^a(\tau') \rangle_{\text{eff}}, \quad (4)$$

$$q_{ab} = \int d\varepsilon_i P(\varepsilon_i) \langle \delta n_i^{\dagger a}(\tau) \delta n_i^b(\tau') \rangle_{\text{eff}}. \quad (5)$$

In these equations, the averages are taken with respect to the effective action of Eq. (2), and $P(\varepsilon_i)$ is the probability distribution of random site energies. Physically, the quantity $G(\tau - \tau')$ represents the single-particle electronic spectrum of the environment, as seen by an electron on site i . The second quantity $\chi(\tau - \tau')$ is the averaged dynamic compressibility. This *mode-coupling* term reflects the retarded response of the density fluctuations of the environment. Finally, the quantity q_{ab} ($a \neq b$) is the familiar Edwards-Anderson order parameter [11]. Its nonzero value indicates that the time averaged electronic density is spatially nonuniform.

We should emphasize that in the presence of randomness, the electronic density will remain *nonuniform* at any temperature. As a result, the Edwards-Anderson order parameter $q = \langle \delta n \rangle^2 \neq 0$ everywhere, and thus cannot be used to identify the glass transition. However, in the classical ($t = 0$) limit, a simple transformation $S_i = 2\delta n_i$, $J = V/4$, and $h_i = \varepsilon_i/2$ reduces our problem to the familiar random-field Ising model. Here, recent work [12] has suggested that a glassy phase can be identified at low temperatures by carrying out an appropriate replica symmetry breaking (RSB) stability analysis.

To carry such a RSB analysis in our approach, note that our self-consistency conditions Eqs. (2)–(5) can be derived from an equivalent *infinite-range* model given by Eq. (1), but having *random* hopping elements t_{ij} and *random* intersite interactions V_{ij} [13], with zero mean and variance t^2/N , and V^2/N , respectively (N is the number of lattice sites). This model is similar to familiar spin-glass models, and the RSB analysis can be carried out using standard methods [11]. The resulting stability criterion takes the form

$$1 = V^2 \int d\varepsilon_i P(\varepsilon_i) [\chi_{\text{loc}}(\varepsilon_i)]^2. \quad (6)$$

Here, $\chi_{\text{loc}}(\varepsilon_i)$ is the *unaveraged* local compressibility that can be expressed as

$$\chi_{\text{loc}}(\varepsilon_i) = \frac{\partial}{\partial \varepsilon_i} \frac{1}{\beta} \int_0^\beta d\tau \langle \delta n(\tau) \rangle_{S_{\text{eff}}(i)}. \quad (7)$$

We continue by concentrating on the classical ($t = 0$) limit, where $\chi(\tau, \tau') = 1/4$, and the problem can

easily be solved in closed form. We first focus on the replica symmetric (RS) solution, which is valid at high temperatures, and set $q_{ab} = q$ for all replica pairs, giving

$$q = \frac{1}{4} \int_{-\infty}^{+\infty} \frac{dx}{\sqrt{\pi}} e^{-x^2/2} \tanh^2 \left[\frac{1}{2} x \beta W_{\text{eff}}(q) \right], \quad (8)$$

where we have introduced an effective disorder strength $W_{\text{eff}} = \sqrt{W^2 + V^2 q}$, and have considered a Gaussian distribution of random site energies of variance W^2 . Even for weak disorder, $q \neq 0$ at any temperature, but it becomes appreciable only for $T \leq V/4$. These frozen-in density fluctuations introduce an added component to the random potential seen by the electron. In this way W_{eff} can become appreciable at low temperatures even if the “bare” disorder W is weak; this represents an interaction-driven mechanism for resistivity enhancement.

Next, we examine the stability of this RS solution. From Eq. (6) we find an expression for the instability line, which takes the form

$$1 = \frac{(\beta V)^2}{16} \int_{-\infty}^{+\infty} \frac{dx}{\sqrt{\pi}} e^{-x^2/2} \cosh^{-4} \left[\frac{1}{2} x \beta W_{\text{eff}}(q) \right], \quad (9)$$

where $q(T, W)$ is given by Eq. (8). The resulting expression for the glass transition temperature simplifies for $W \gg V$, where using the fact that $q \leq 1/4$ we find $T_G \approx (1/6\sqrt{2\pi})(V^2/W)$. This reduction of T_G at large W reflects the *reduction* of frustration in the strong disorder limit, where the electrons simply populate the lowest potential wells. Still, in contrast to the well known “AT line” [11], T_G decreases slowly with disorder, suggesting that the glassy behavior of electrons may be observable at finite temperatures, in agreement with some recent experiments [14].

To understand this behavior, we investigate the structure of the low-temperature glass phase. Consider the single-particle density of states at $T = 0$, which in the classical limit can be expressed as

$$\bar{\rho}(\varepsilon, t = 0) = \frac{1}{N} \sum_i \delta(\varepsilon - \varepsilon_i^R), \quad (10)$$

where $\varepsilon_i^R \equiv \varepsilon_i + \sum V_{ij} n_j$ are the renormalized site energies. In the thermodynamic limit, this quantity is nothing but the probability distribution $P_R(\varepsilon_i^R)$. It is analogous to the “local field distribution” in the spin-glass models, and can be easily shown to reduce to a simple Gaussian distribution in the RS theory, establishing the *absence* of any gap for $T > T_G$. Obtaining explicit results from a replica calculation in the glass phase is more difficult, but useful insight can be achieved by using standard simulation methods [15,16] on our equivalent infinite-range model; some typical results are shown in Fig. 1.

We find that as a result of glassy freezing, a pseudogap emerges in the single-particle density of states, reminiscent of the Coulomb gap of Efros and Shklovskii (ES) [4]. The low energy form of this gap appears *universal*,

$$\rho(\varepsilon) \approx C |\varepsilon|^\alpha / V^2; \quad C = \alpha = 1, \quad (11)$$

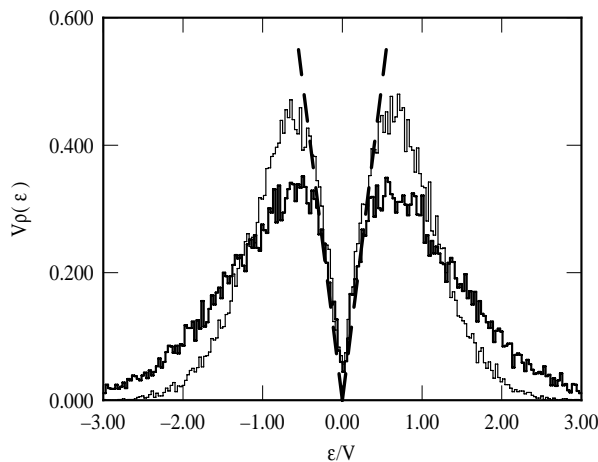


FIG. 1. Single-particle density of states in the classical ($t = 0$) limit at $T = 0$, as a function of disorder strength. Results are shown from a simulation on $N = 200$ site system, for $W/V = 0.5$ (thin line) and $W/V = 1.0$ (full line). Note that the low energy form of the gap takes a *universal* form, independent of the disorder strength W . The dashed line follows Eq. (11).

independent of the disorder strength W , again in striking analogy with the predictions of ES [17]. To establish this result, we have used stability arguments very similar to those developed for spin-glass (SG) models [16], demonstrating that the form of Eq. (11) represents an exact *upper bound* for $\rho(\varepsilon)$. For *infinite-ranged* SG models, as in our case, this bound appears to be *saturated*, leading to universal behavior. Such universality is often associated with a critical, self-organized state of the system. Recent work [16] finds strong numerical evidence of such criticality for SG models; we believe that the universal gap form in our case has the same origin. Furthermore, assuming that the universal form of Eq. (11) is obeyed immediately allows for an estimate of $T_G(W)$. Using Eq. (11) to estimate the gap size for large disorder gives $T_G \sim E_g \sim V^2/W$, in agreement with Eq. (9).

The ergodicity breaking associated with the glassy freezing has important consequences for our model. Again, using the close similarity of our classical infinite-range model to standard SG models [11], it is not difficult to see that the *zero-field-cooled* (ZFC) compressibility vanishes at $T = 0$, in contrast to the field-cooled one, which remains finite. Essentially, if the chemical potential is modified *after* the system is cooled to $T = 0$, the system immediately falls out of equilibrium and displays hysteretic behavior [16] with vanishing *typical* compressibility. If this behavior persists in finite dimensions and for realistic Coulomb interactions, it could explain the absence of screening in disordered insulators. We emphasize that our picture does not agree with the recently proposed scenario of Si and Varma [18], where the two compressibilities are not distinguished, and are *both* proposed to vanish in the $T = 0$ insulating state.

Finally, we examine the effect of quantum fluctuations on the stability of the glass phase. We generally expect

that for a sufficiently large Fermi energy $E_F \sim t_G, T_G \rightarrow 0$, but of particular interest is the disorder dependence of $t_G(W)$. In the quantum case, solving our DMF equations becomes a nontrivial many-body problem, which cannot be solved in closed form. The problem simplifies in the strong disorder limit, where the exact expression for the RSB boundary can be obtained. As in the classical case, to examine the $W \gg V$ limit, we use the fact that $q \leq 1/4$, $\chi(\tau - \tau') \leq 1/4$, so that in solving Eq. (6) we can eliminate the corresponding terms in the expression for the local effective action Eq. (2). The calculation of the local compressibilities of Eq. (7) then reduces to computing the same quantity for noninteracting electrons in the presence of disorder, and we find

$$\chi_{\text{loc}}(\varepsilon) = \frac{\beta}{4} \int_{-\infty}^{+\infty} d\omega \rho_{\varepsilon}^{\infty}(\omega) \cosh^{-2}\left(\frac{1}{2} \beta \omega\right). \quad (12)$$

Here, the *local* density of states reduces to a narrow resonance of width $\Delta = \pi t^2 P(\varepsilon_i = 0) \sim t^2/W$

$$\rho_{\varepsilon}^{\infty}(\omega) \approx \frac{1}{\pi} \frac{\Delta}{(\omega - \varepsilon)^2 + \Delta^2}, \quad (13)$$

and we get

$$t_G(T = 0, W \rightarrow \infty) = V/\pi\sqrt{2}. \quad (14)$$

In contrast to the effect of finite temperatures, we find that a *finite* value of the Fermi energy $E_F \sim t$ is needed to suppress the glass phase, even for $W \gg V$. This surprising result has, in fact, a simple physical interpretation. At $t = 0$ we have argued that the glass phase for $W \gg V$ is characterized by a small energy scale $E_g \sim V^2/W$, hence the reduction of T_G at strong disorder. In the $T = 0$ quantum case, the role of the thermal energy is replaced by an energy scale measuring the size of quantum fluctuations. However, the relevant energy scale is *not* the Fermi energy $E_F \sim t$, but instead is given by the *hybridization energy* $\Delta \sim t^2/W$ which, according to Fermi's golden rule, determines the inverse lifetime of an electron on a given site. Because of the decrease of the electronic mobility at large disorder, $\Delta(W)$ is reduced at $W \gg t$; comparing it to the $T = 0$ gap size $E_g(W)$ immediately explains Eq. (14).

Our solution, which evaluates the local compressibilities in Eq. (6) by setting $V = 0$ gives the asymptotic behavior for $W \gg V$. This approximation can be considered as a leading term in a “weak-coupling” approach, where the compressibilities are expanded in powers of the interaction, similar in spirit to the RPA of the electron gas. For our purposes of calculating the phase diagram, this strategy will provide qualitatively correct results even for weaker disorder, and the resulting phase diagram is shown in Fig. 2. Note that our glass phase persists even as $W \rightarrow 0$. However, in this regime we expect uniform charge ordering to preempt any glass formation, an effect that we have not examined, but that can easily be incorporated in our framework.

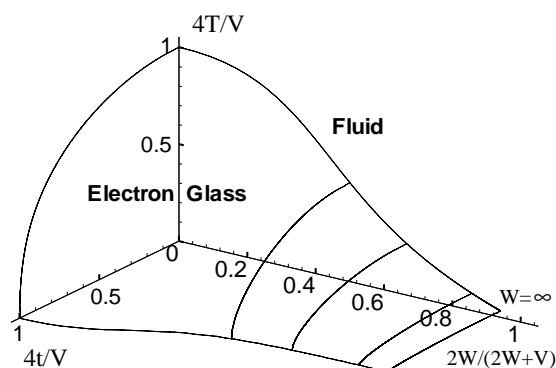


FIG. 2. Phase diagram as a function of temperature T , disorder strength W , and hopping element t . Note how the glass transition temperature T_G decreases as $1/W$ in the strong disorder limit. In contrast, the critical value of the hopping element t_G remains *finite* as $W \rightarrow \infty$.

Our results clearly demonstrate that the quantum fluctuations become a nontrivial function of disorder in this electronic context, which plays a key role in controlling the glassy phase. We emphasize that, within our theory, the relevant hybridization energy Δ remains *finite* at any $t \neq 0$, since Anderson localization [19] is absent at $z_t = \infty$. As a result, while the glass phase will persist for all $t < t_G$, the systems will become metallic for any $t \neq 0$. Similarly as finite temperatures, $\Delta \neq 0$ will introduce a cutoff for both our Coulomb gap, and the corresponding ZFC compressibility. On the other hand, Anderson has demonstrated [19] that $\Delta \rightarrow 0$ in an Anderson insulator, even in the absence of interactions. We thus expect that Anderson localization will strongly stabilize the glass phase, as well as restore the ZFC incompressibility and the existence of the Coulomb gap in the entire insulating phase. Our theory can be readily extended to incorporate the Anderson localization effects within the DMF framework, following the approaches of Ref. [20], but these interesting issues will be addressed elsewhere.

To conclude, we have presented a simple theoretical framework where several aspects of glassy freezing of electrons can be investigated in detail. We find that glassy freezing strongly enhances the effective disorder seen by the electrons, providing a new driving force for electron localization. In addition, the ergodicity breaking in the glassy state leads to the universality of the Coulomb gap, as well as the incompressible behavior in disordered insulators.

We thank E. Abrahams, A. Georges, M. Horbach, T. R. Kirkpatrick, D. Popović, A. E. Ruckenstein, Q. Si, G.

Zarand, and G. Zimanyi for useful discussions. This work has been supported in part by the NSF Grant No. DMR-9974311, the NHMFL/FSU, and the Alfred P. Sloan Foundation.

- [1] P. A. Lee *et al.*, Rev. Mod. Phys. **57**, 287 (1985).
- [2] J. G. Massey *et al.*, Phys. Rev. Lett. **77**, 3399 (1996).
- [3] Mark Lee *et al.*, e-print cond-mat/9902169.
- [4] A. L. Efros *et al.*, J. Phys. C **8**, L49 (1975).
- [5] D. Belitz *et al.*, Phys. Rev. B **52**, 13 922 (1995).
- [6] S. Chakravarty *et al.*, e-print cond-mat/9805383.
- [7] A. Georges *et al.*, Rev. Mod. Phys. **68**, 13 (1996).
- [8] Standard DMF equations [7] are formally exact in the large coordination limit, after rescaling $t \rightarrow t/\sqrt{z_t}$; $z_t \rightarrow \infty$. To examine uniform ordering, the intersite interaction has to be rescaled as $V \rightarrow V/z_v$; $z_v \rightarrow \infty$, where only the Hartree contribution (linear in V) survives. In this paper, we focus on disordered systems, and ignore any uniform ordering. The emergence of *glassy* freezing can be examined by keeping terms of up to the order V^2 , which is formally exact after rescaling $V \rightarrow V/\sqrt{z_v}$; $z_v \rightarrow \infty$. Similar “extended” DMF formulations have been proposed for clean systems in Q. Si *et al.*, Phys. Rev. Lett. **77**, 3391 (1996); J. Llewellyn-Smith *et al.*, e-print cond-mat/9903083; R. Chitra *et al.*, e-print cond-mat/9903180.
- [9] V. Dobrosavljević *et al.*, Phys. Rev. B **50**, 1430 (1994).
- [10] For mean-field glassy models [11], such as ours, there exists considerable evidence that most results obtained using replicas can also be derived using alternative approaches.
- [11] M. Mezard *et al.*, *Spin Glass Theory and Beyond* (World Scientific, Singapore, 1987).
- [12] M. Mezard *et al.*, Europhys. Lett. **18**, 653 (1992).
- [13] Related ideas have been proposed in F. Gebhard, *The Mott Metal-Insulator Transition*, Springer Tracts in Modern Physics, Vol. 137 (Springer, New York, 1997).
- [14] G. Martinez-Arizala *et al.*, Phys. Rev. B **57**, R670 (1998).
- [15] R. G. Palmer *et al.*, J. Phys. F **9**, 1451 (1979).
- [16] F. Pazmandi *et al.*, e-print cond-mat/9902156.
- [17] The result $\alpha = 1$ that we find is specific to our model. In early work, Efros and Shklovskii [4] have suggested that the precise value of this exponent should depend on both the (power-law) form of the interaction and the dimensionality, but should display universality by being insensitive to the disorder strength—in agreement with our findings.
- [18] Q. Si *et al.*, Phys. Rev. Lett. **81**, 4951 (1998).
- [19] P. W. Anderson, Phys. Rev. **109**, 1498 (1958).
- [20] V. Dobrosavljević *et al.*, Phys. Rev. Lett. **78**, 3943 (1997).