Controlling the Fermions in Models of Disordered Conduction

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Format of This Talk

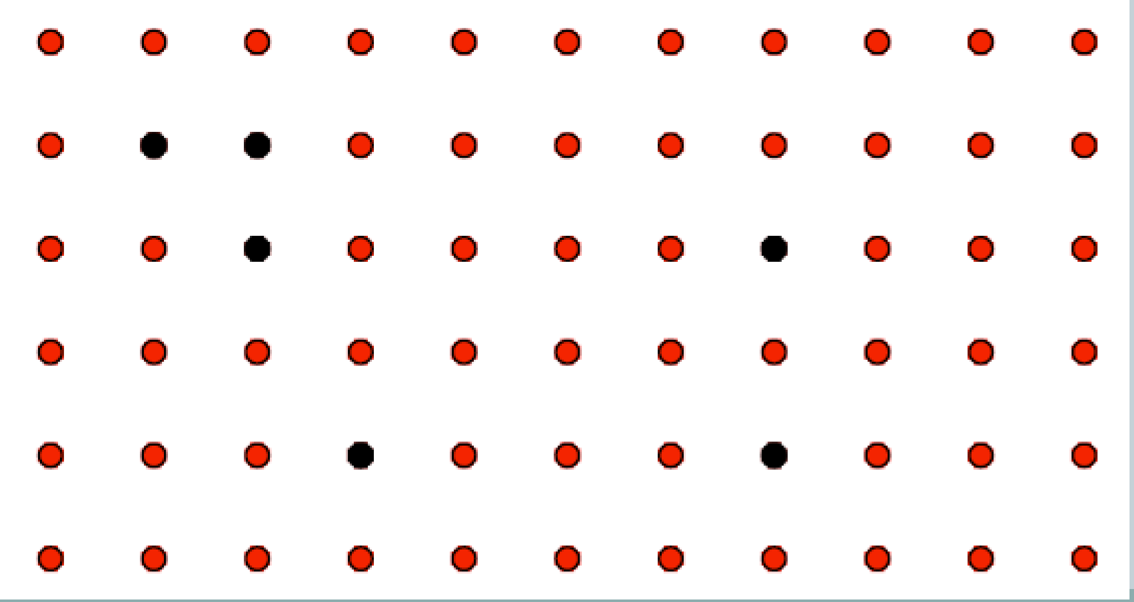
- Conduction in Disordered Materials:
  - Physical Problem, Mathematical Model
- Green's Functions, Path Integral Formulation
- Physical Degrees of Freedom, Fermions
- New Choice of Variables, Summary of Advantages
    - More precise mathematical treatment, with full perturbative control.
    - More powerful algorithms for numerical simulations.
    - A better, non-perturbative, picture of the strong disorder regime.

- Questions, ***PLEASE!***

  - ***15 Slides***

What is a Disordered Material?

- If you examine it closely (at small scales) you find a complicated structure.
- Looks random, complicated, complex, lots of detail.
- Not a repeating structure; not a crystal.



Green's Functions

- Advanced and Retarded Green's Functions:

  $G_A(E) = (E - w - H)^{-1}$, $G_R = (E + w - H)^{-1}$

- Averaged single Green's function $\langle G_{A,R}(E) \rangle_V$ gives $\rho(E)$, density of states, random scattering. Not sensitive to the Anderson localization transition.
- Average of two Green's functions $\langle G_A(E) G_R(E+\omega) \rangle_V$ gives the conductance via Landauer's formula. It is sensitive to Anderson localization: in the localized phase it dies off exponentially with distance.
- No electronic interactions; simply the Schrodinger equation with a random Hamiltonian; study the Green's functions. $H\psi = E\psi$
- The KEY here is ***quenched*** randomness– have to average.

Path Integral/Statistical Mechanics Approach

- Calculating a single Green's Function:
  - First calculate a single partition function: $Z(E, J^f, J^b) = \langle \frac{\det(E - H - J^f)}{\det(E - H - J^b)} \rangle_V$
  - J is an infinitesimal source. The first derivative produces the averaged Green's Function: $G(E, x_1, x_2) = \frac{dZ}{dJ^b(x_1, x_2)}|_{J=0}$
  - Rewrite Z as a path integral:

$$Z(E, J^f, J^b) \propto \langle \int d\psi dS \;\; e^{\mathcal{L}} \;\rangle_V$$

$$\mathcal{L} = i\psi(E - H - J^f)\overline{\psi} + iS(E - H - J^b)S^*$$

  - Averaging over the random potential produces interactions:

$$\psi^4, \;\; S^4, \;\; \psi^2 S^2$$

Supersymmetry

- Exact symmetry between numerator and denominator:

$$Z(E, J^f, J^b) = \langle \frac{\det(E - H - J^f)}{\det(E - H - J^b)} \rangle_V$$

- Supersymmetry: There is always an exact symmetry between fermions and bosons ψ, S. Many exact identities, similar to Ward identities, result from SUSY. Extremely symmetric theory.
- Physical meaning: the disorder is ***quenched***; independent of the electrons; built into the substrate.
- Our new variables express the supersymmetry in a new way that is mathematically easier.

Average of two Green's Functions $\langle G_A(E) G_R(E+\omega)\rangle_V$

$$\mathcal{L} = i\psi_1(E_1 - H - J_1^f)\overline{\psi}_1 + i\psi_2(E_2 - H - J_2^f)\overline{\psi}_2 + iS_1(E_1 - H - J_1^b)S_1^* - iS_2(E_2 - H - J_2^b)S_2^*$$

- Continuous symmetry: when $\omega = E_1 - E_2 = 0$ the Lagrangian is completely symmetric under linear mixings of S_1, S_2, and also of ψ_1, ψ_2. This continuous symmetry is the source of the long distance physics (spontaneous symmetry breaking).
- Exact supersymmetry between ψ, S.
- These symmetries imply that ψ, S are not the natural variables for describing the long distance physics of conduction.

The Natural Variables (Spins) for this Theory

- Pairs of variables (matrices) are what matter:

$$Q^b \propto \begin{bmatrix} S_1 S_1^* & S_1 S_2^* \\ S_2 S_1^* & S_2 S_2^* \end{bmatrix}, \quad (Q^f)^{-1} \propto \begin{bmatrix} \psi_1 \bar{\psi}_1 & \psi_1 \bar{\psi}_2 \\ \psi_2 \bar{\psi}_1 & \psi_2 \bar{\psi}_2 \end{bmatrix}, \quad Q^g \propto \begin{bmatrix} \psi_1 S_1^* & \psi_1 S_2^* \\ \psi_2 S_1^* & \psi_2 S_2^* \end{bmatrix}$$

- Physical meaning: Q is spatially constant in conducting phase, fluctuates in the insulating phase.
- Physical meaning of bosons Q^f and Q^b :

$$\langle Q^b \rangle_{11} \propto \langle (Q^f)^{-1} \rangle_{11} \propto G(E_1), \quad \langle Q^b \rangle_{22} \propto \langle (Q^f)^{-1} \rangle_{22} \propto G(E_2),$$

- Physical meaning of fermions Q^g :
  - Responsible for preserving supersymmetry; contain the physics of quenched disorder.
- Our new formulation treats Q^g differently than before.

Changing to matrix variables: The standard SUSY approach

- Group everything into a single matrix:

$$Q \propto \begin{bmatrix} Q^f & Q^g \\ (Q^g)^\dagger & Q^b \end{bmatrix}$$

- Q contains both ordinary entries, and Grassmann entries; it is a *graded* matrix, with complicated mathematics.
- Mathematically exact change of variables obtains a new integral written in terms of the Q matrix.

- Grassmann variables Q^g occur to all powers. Integrating them produces a sum, with a number of terms which grows factorially with the volume. This makes further progress difficult, esp. at strong disorder. Little known about the ground state at large disorder.

New matrix variables

- Focus on avoiding cubic and higher powers of Q^g fermions, so that they can be integrated to produce a determinant.
- Treat Q^f , Q^b , Q^g separately.
- Overall effect is similar to integrating out the Grassmann variables in the SUSY theory's Q matrix.
- Isolates the theory into a Q^f sector, a Q^b sector, and a Q^g determinant which couples the two.

Advantages of the new variables

- The model can be simulated numerically: Many powerful algorithms for simulating fermion determinants can be copied from lattice QCD.
  - Sigma model computations at the phase transition and in the localized phase.
  - Extremal statistics associated with rare disorder configurations.
  - Large volumes with large scattering lengths.
  - Large N = number of electronic orbitals per site.
- Previous field theories of disordered conduction were inaccessible to numerical techniques because of the fermions, which occurred at all powers. Therefore previous numerical works treated individual realizations of disorder, and treated all length scales in the same way.

Advantages of the new variables

- Full control over the Grassmann variables Q^g , since there are many powerful theorems about determinants, and well defined perturbation theory.
- Possibility of rigorous proofs about the conducting phase, which has not been accessible until now.
- Very easy algebra. The SUSY model of disorder has very complicated algebra because of the graded matrices. This has imposed a practical limit on analytical computations.

New Perspective on Strong Disorder: Analysis of the Fermions

- Divide the Q^f, Q^b phase space into many sectors divided by infinite potential walls.
  - Therefore the system has many competing ground states.
  - Localized phase is a fermionic glass.
  - By comparison, SUSY in the localized phase is unable to determine which configurations are favored or disfavored. No possibility of determining a ground state in the localized phase.
- Impose a very large energy penalty on spatially uniform configurations.
  - Uniform configurations lie close to the potential walls.
  - Every ground state exhibits large fluctuations, driven by the fermions, not by entropy.
  - Phase transition is controlled by competition between kinetics, entropy, and fermions.
    - By comparison, SUSY model has competition between Entropy vs. Kinetics, but on a graded manifold which is hard to understand.

Other Novel Aspects of this Work: More Rigor

- Lattice not Continuum
- Establish and use Locality of the Massive Modes
- Analyze Higher Orders in the expansion of the Logarithm
- Analyze Corrections to the Sigma Model.
- Consider competition between saddle points and local fluctuations in the saddle point.
- Exact integration of the spatially invariant degrees of freedom.
- Careful analysis of the large N limit when omega is of order 1/N.

Thank You!

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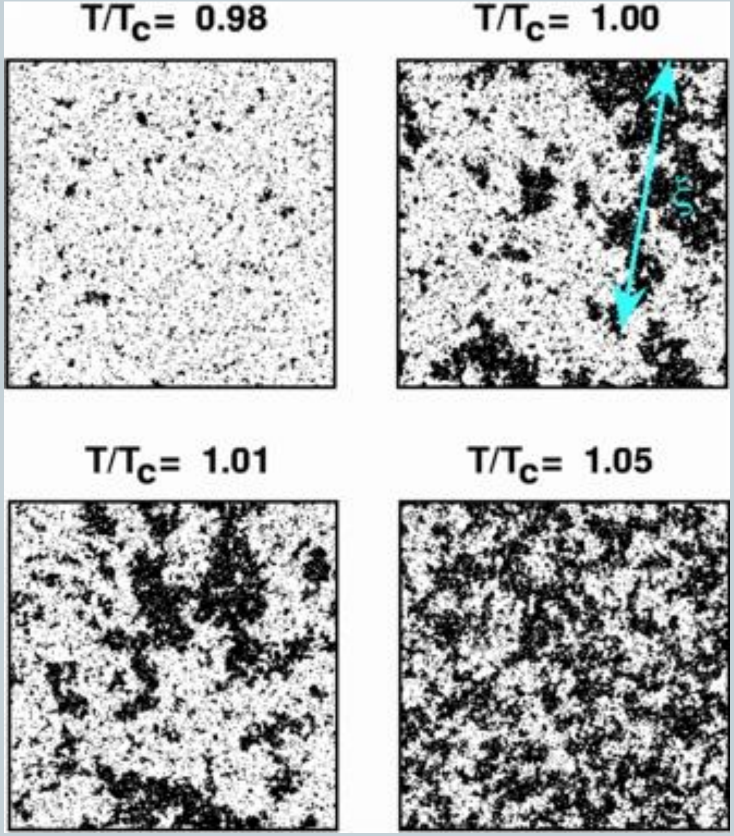
Long Distance Physics and Matrix Variables

- The exact symmetries at $\omega = E_1 - E_2 = 0$, and the corresponding long distance physics, are just rotations of Q^f and Q^b : $Q^f \rightarrow U Q^f U^\dagger$.
- Possible that system will get locked into a particular value of Q^f and Q^b , with the same value everywhere, breaking the symmetry.

Long Distance Physics and the Ground State

- Disorder strength is like temperature.
  - These Pictures show the Ising model.
- Correlations = Conduction.
- Low disorder phase has a spatially uniform ground state, with constant long distance correlations.
- At critical disorder (phase transition) critical fluctuations appear at all distances.
- At higher disorder the fluctuations have a length scale which gets smaller as the temperature increases. Correlations controlled by an exponential.
- The disordered ground state has not been well understood, except in D=1 dimensions and the Bethe lattice.
    - Images from http://www.physik.unizh.ch/groups/keller/fluctuations/index.html



Final Result

$$
\begin{aligned}
\bar{Z} &= \gamma_D \int_{Q^b \geq 0} dQ^f\, dQ^b \sigma_3\, e^{\mathcal{L}}\, \det(Q^f - Q^b \sigma_3 (1-k)) \\
\mathcal{L} &= (N-2) \sum_v Tr \ln Q_v^f - N/2 \sum_{v_1 v_2} (k/(1-k))_{v_1 v_2} Tr(Q_{v_1}^f Q_{v_2}^f) \\
&+ zN \sum_v Tr(Q_v^f \hat{E}^f) - N/2 \sum_v Tr\,(Q_v^f Q_v^f) \\
&+ (N-2) \sum_v Tr \ln Q_v^b \sigma_3 + N/2 \sum_{v_1 v_2} k_{v_1 v_2} Tr(Q_{v_1}^b \sigma_3 Q_{v_2}^b \sigma_3) \\
&+ zN \sum_v Tr(Q_v^b \sigma_3 \hat{E}^b) - N/2 \sum_v Tr\,(Q_v^b \sigma_3 Q_v^b \sigma_3)
\end{aligned}
$$

New perspective on the phase transition

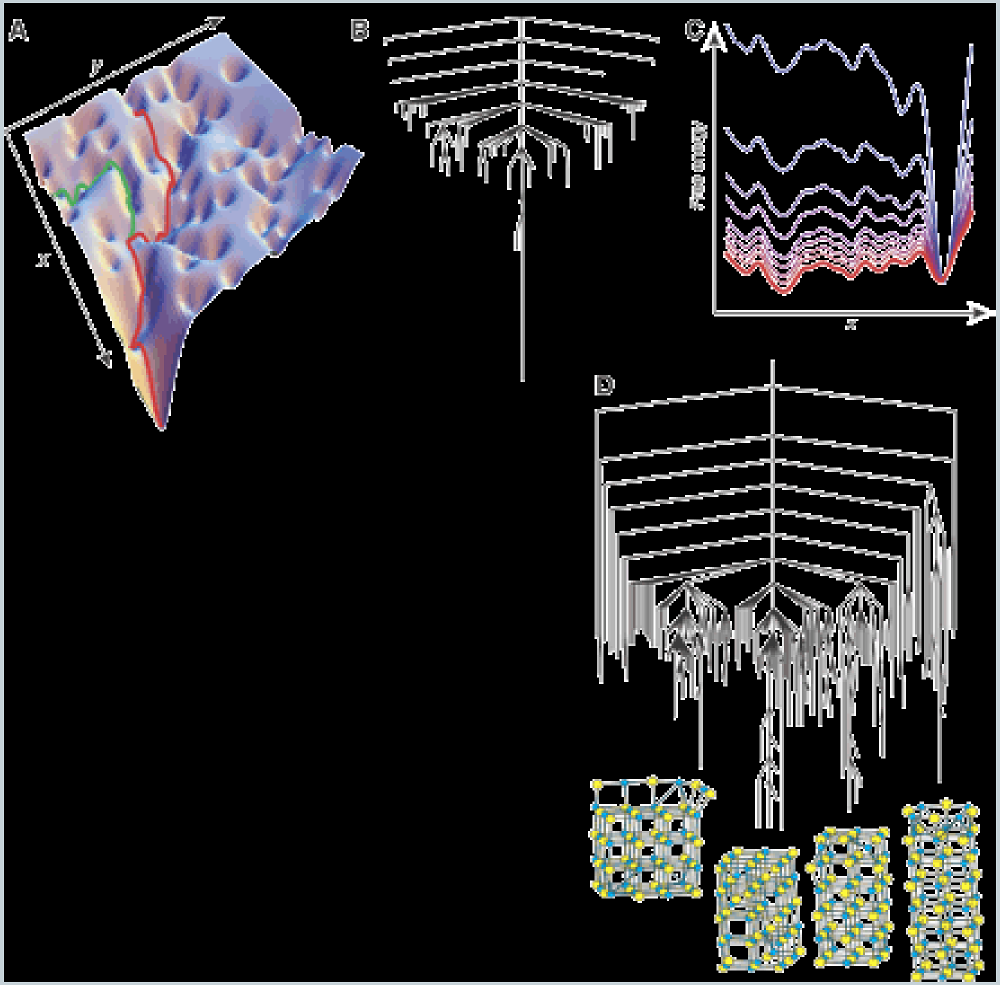
- Three competing forces acting on Q^f and Q^b :
  - Kinetic terms penalize fluctuations, and push for conduction.
  - Entropy favors fluctuations, and pushes for insulating phase.
  - Fermions (determinant) favor fluctuations and push for insulating phase. They impose a high energy cost on non-fluctuating configurations.
- New model makes all three visible.
  - Gives the physics of the Grassmann variables.
  - Much clearer picture of phase transition and localized phase. More prospects for analysis.

New Perspective: Analysis of the Fermions

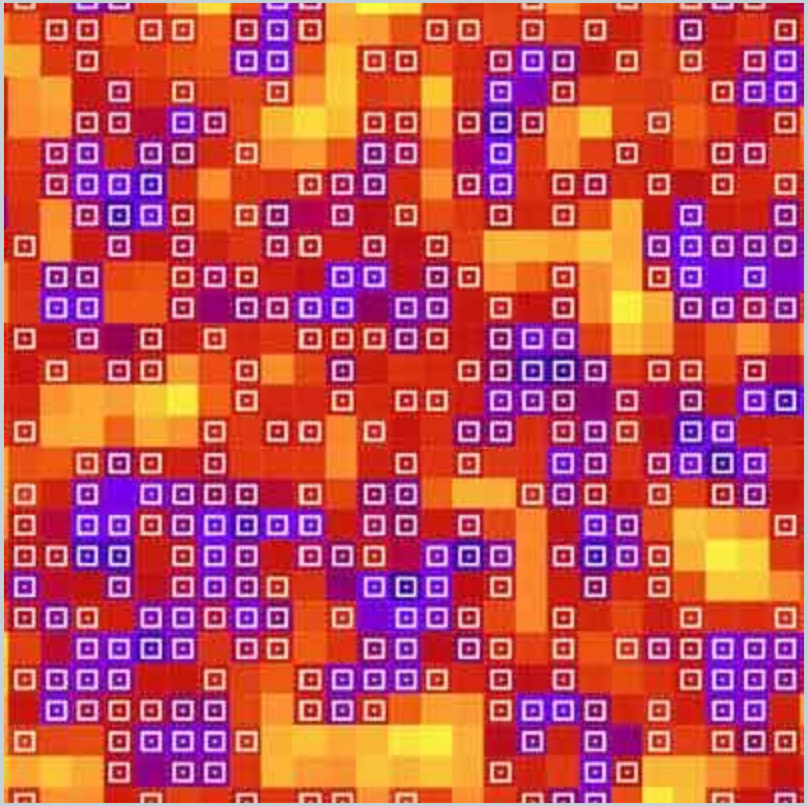
- At very small disorders the cost of fluctuations is large, and all spins are spatially uniform.
- As the disorder increases, fluctuations become possible.
- In the localized phase the fermions dominate, and force a qualitative change in the ground state.
- Because the fermions are dominant, we can learn a lot about the insulating ground state and the phase transition by focusing on the fermion determinant.

New Perspective:
Many ground states when disorder is strong

- Picture of another glassy model with many competing ground states.
- Expect that in our model all the ground states have roughly the same depth; no single one dominates.
  - *Science* Magazine > 27 July 2001 > Brooks III et al., pp. 612 - 613



New Perspective: Every single ground state has large fluctuations



- Determinant imposes a very large energy penalty for spatially uniform configurations.
- Picture of the ground state of an XY spin glass.
  - Picture from **Zero-temperature phase of the *XY* spin glass in two dimensions: Genetic embedded matching heuristic**, by Weigel and Gingras.

New Perspective: Comparison with SUSY

- SUSY in the localized phase is unable to determine which configurations are favored or disfavored.
- No possibility of determining a ground state in the localized phase.
- Gives more mystery to the physics within the conducting phase which leads up to the phase transition.
  - Entropy vs. Kinetics, but on a graded manifold which is hard to understand.

What is exciting about this new perspective?

- Previously path integral formulations of disordered conduction were limited to the conducting phase.
  - Attempts to use the renormalization group and scaling theory to evolve from conductor to insulator.
- A new and much more detailed picture of all disorders, based on exact, non-perturbative results.
- This is the first work showing that discusses fermionic dominance, glassiness, etc.
- Promising for high-efficiency numerical calculations.
    - Better ideas about how to handle fermions and small (ballistic) length scales.

Thank You!

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