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Noncompact σ Models and the Existence of a Mobility Edge in Disordered Electronic Systems near Two Dimensions

A. Houghton, A. Jevicki, and R. D. Kenway
Department of Physics, Brown University, Providence, Rhode Island 02912

and

A. M. M. Pruisken
Institute für Theoretische Physik, Universität Heidelberg, D-6900 Heidelberg, Germany

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The properties of an electron in a disordered solid are discussed with use of a matrix nonlinear σ model first introduced by Wegner and Schäfer. The model is defined on the noncompact space $O(M,M)/[O(M)\times O(M)]$ where M is the number of replicas. This noncompact symmetry represents the essential physics of the problem. It is found that all states are localized in two dimensions; above two dimensions for weak disorder there are mobility edges, but these merge above a critical amount of disorder and all states become localized.

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The electronic properties of a disordered solid may be described by the Hamiltonian[1,2]

$$H=\frac{1}{\sqrt{n}}\sum_{\substack{\vec{r},\alpha\\ \vec{r}',\alpha'}}|\vec{r},\alpha\rangle f_{\vec{r},\alpha;\vec{r}',\alpha'}\langle\vec{r}',\alpha'| ; \tag{1}$$

at each site $\vec{r}$ of a regular lattice, spacing a, there are n orbitals α. On-site energies and inter-site hopping are randomly distributed. Here we will take $\underline{f}$ to be a real symmetric matrix. In a series of interesting papers it was first conjectured[3] and then proved[4] that the properties of the system described by Eq. (1) may be discussed in terms of a field theory with action[5]

$$A=\tfrac{1}{2}K\int d^dx\,\mathrm{Tr}[\partial_\mu V(x)][\partial_\mu V(x)],\qquad \underline{V}^2=\pm\lambda_0^2\underline{1}, \tag{2}$$

where (Refs. 2 and 4) $K=nR^2a^{-d}/4d$ and $\lambda_0=(1-E^2/E_0^2)^{1/2}$. This action arises on averaging a product of single-particle Green's functions $G(\vec{r},\vec{r}',z_p)$, $p=1,2$ over the distribution of the matrices $\underline{f}$.[4] It is defined on a set of real symmetric matrices, $\underline{V}^2=\lambda_0^2\underline{1}$, if the two energies lie on the same side of the real axis. However, in the case of most interest, the conductivity, the energies, z_p, lie on opposite sides of the real axis and a model of complex symmetric matrices, $\underline{V}^2=-\lambda_0^2\underline{1}$ results. This difference reflects the distinct symmetries of the two cases. In the first case, the system is invariant under orthogonal transformations and the matrices $\underline{V}$ are elements of the compact space $O(2M)/[O(M)\times O(M)]$ where M is the number of replicas in the spaces $p=1$ and 2. For the conductivity, the symmetry is hyperbolic and the fields belong to the noncompact space $O(M,M)/[O(M)\times O(M)]$.

In Ref. 4 it was argued that at the level of perturbation theory the two models are equivalent and therefore the critical properties in the hyperbolic case, namely the behavior of the electronic system near a mobility edge, could be described by the generalized compact nonlinear σ models

$$A=(1/2t_0)\int d^dx\,\mathrm{Tr}[\partial_\mu g^{-1}(x)][\partial_\mu g(x)],\qquad \underline{g}^2=\underline{1},\quad g\in O(2M)/[O(M)\times O(M)], \tag{3}$$

discussed previously by Brézin, Hikami, and Zinn-Justin.[6] In this Letter we will point out the important difference between the compact and noncompact models in a $2+\epsilon$ expansion. As we shall see, it is precisely this difference which represents the essential physics of the mobility-edge problem.

First, we note that the action Eq. (2) for $\underline{V}^2=-\lambda_0^2\underline{1}$ can be written in terms of real matrices $\underline{g}$ as

$$A=-(1/2t_0)\int d^dx\,\mathrm{Tr}[\partial_\mu g^{-1}(x)][\partial_\mu g(x)],\qquad \underline{g}^2=\underline{1},\quad g\in O(M,M)/[O(M)\times O(M)], \tag{4}$$

where $t_0 = 1/K\lambda_0^2$; $\underset{\sim}{g}$ can be parametrized, for real φ, as

$$\underset{\sim}{g} = \underline{U}\begin{pmatrix} \cosh\varphi & -\sinh\varphi \\ \sinh\varphi & -\cosh\varphi \end{pmatrix}\underline{U}^T, \tag{5}$$

where $\underline{U}$ is a $2M\times 2M$ matrix with $M\times M$ orthogonal blocks on the diagonal and zeros elsewhere. If one takes $\underline{U}$ constant, it is easy to check that $A=(M/t_0)\int d^dx(\partial_\mu\varphi)(\partial_\mu\varphi)$ which is positive definite. Hence, the partition function $\mathrm{Tr}e^{-A}$ is well defined. We will discuss these noncompact σ models in detail and show how the questions of localization and a mobility edge are described naturally in this context.

First, we will illustrate the main points of the argument for the simplest examples: the original compact $O(N)/O(N-1)$ σ model whose fields are defined on a sphere[7] ($N=3$, 2, and 1 are the Heisenberg, planar, and Ising models, respectively), and the noncompact $O(N-1,1)/O(N-1)$ σ model whose fields take values on a hyperboloid. Both surfaces have constant Riemannian curvature; $+1$ for the sphere, -1 for the hyperboloid. The coupling-constant renormalization may be calculated using a method developed by Polyakov.[8,9] The action for a spin confined to an N-dimensional sphere is

$$A^S(n) = (1/2t_0)\int d^2x(\partial_\mu n_\alpha)(\partial_\mu n_\alpha),\qquad n_\alpha n_\alpha = 1, \tag{6}$$

where $\alpha = 1,2,\ldots,N$ and we will work explicitly in two dimensions. If $\tilde{n}_\alpha$ is a slowly varying background field with wavelengths greater than $\tilde{\Lambda}^{-1}$, then fluctuations on the sphere (with wavelengths between $\Lambda^{-1}=a$ and $\tilde{\Lambda}^{-1}$) relative to $\tilde{n}_\alpha$ may be parametrized as

$$n_\alpha = (1-\vec{\pi}^2)^{1/2}\tilde{n}_\alpha + \sum_{i=2}^{N}\pi_i e_{i\alpha}. \tag{7}$$

The orthonormal basis $\{e_{i\alpha},\ i=1,\ldots,N\}$ obeys $e_{1\alpha}=\tilde{n}_\alpha$, $e_{i\alpha}e_{j\alpha}=\delta_{ij}$, and $\vec{\pi}^2=\sum_{i=2}^{N}\pi_i^2$. Introducing "gauge" fields $A_{\mu ij}=e_{i\beta}\partial_\mu e_{j\beta}$, we arrive at an effective action, to one-loop order,

$$A_{\mathrm{eff}}^S = (1/2t_0)\int d^2x[(1-\vec{\pi}^2)(\partial_\mu\tilde{n}_\alpha)(\partial_\mu\tilde{n}_\alpha)+(\partial_\mu\vec{\pi})(\partial_\mu\vec{\pi})-\pi_i A_{\mu i1}A_{\mu 1j}\pi_j]. \tag{8}$$

If one isolates the divergent terms in the integration over $\vec{\pi}$ fields, one gets

$$A^S(\tilde{n}) = (1/2t)\int d^2x(\partial_\mu\tilde{n}_\alpha)(\partial_\mu\tilde{n}_\alpha), \tag{9}$$

where

$$\frac{1}{t}=\frac{1}{t_0}-\frac{N-2}{2\pi}\ln\frac{\Lambda}{\tilde{\Lambda}}. \tag{10}$$

On the other hand, the action for an N-dimensional hyperboloid is

$$A^H(n) = -(1/2t_0)\int d^2x(\partial_\mu n^\alpha)(\partial_\mu n_\alpha),\qquad n^\alpha n_\alpha = 1, \tag{11}$$

where raised indices are defined via a metric $g_{\alpha\beta}$ which has one "+1" and $N-1$ "-1" on the diagonal and zeros elsewhere. The fluctuations on the hyperboloid relative to a background field $\tilde{n}_\alpha$ are given by

$$n_\alpha = (1+\vec{\pi}^2)^{1/2}\tilde{n}_\alpha + \sum_{i=2}^{N}\pi_i e_{i\alpha}, \tag{12}$$

where the basis $\{e_{i\alpha},\ i=1,\ldots,N\}$ obeys $e_{1\alpha}=\tilde{n}_\alpha$, $e_i{}^\alpha e_{j\alpha}=g_{ij}$. The "gauge" fields in this case are $A_{\mu ij}=e_i{}^\beta\partial_\mu e_{j\beta}$ and the effective action is

$$A_{\mathrm{eff}}^H = (1/2t_0)\int d^2x[-(1+\vec{\pi}^2)(\partial_\mu\tilde{n}^\alpha)(\partial_\mu\tilde{n}_\alpha)+(\partial_\mu\vec{\pi})(\partial_\mu\vec{\pi})+\pi_i A_{\mu i1}A_{\mu 1j}\pi_j]. \tag{13}$$

We recover an action of the same form as Eq. (11), but with a coupling constant

$$\frac{1}{t}=\frac{1}{t_0}+\frac{N-2}{2\pi}\ln\frac{\Lambda}{\tilde{\Lambda}}. \tag{14}$$

Note the change in sign of the correction term. This is characteristic of the transition from rotational to hyperbolic symmetry. In general, integrating out the constraints in Eqs. (6) and (11), we are led to Lagrangians of the type

$$L = (1/2t_0)(\partial_\mu\pi^i)g_{ij}(\pi)(\partial_\mu\pi^j) \tag{15}$$

in terms of the $N-1$ independent fields π_i. For the general matrix models, corresponding to compact $O(N)/[O(N-p)\times O(p)]$ symmetries, studied by Brézin, Hikami, and Zinn-Justin,[6] the fields π_i are their $V_\alpha{}^i$; $i=1,\ldots,p$; $\alpha=p+1,\ldots,N$.

To discuss the renormalizability and critical properties of the general Lagrangian Eq. (15) we use a formalism developed by Honerkamp.[10] We parametrize the fluctuations relative to a vector φ_i, the solution of the classical field equations. Schematically $\pi_i=\varphi_i+\epsilon_i$ where ϵ_i is the geodesic between φ_i and π_i. Explicitly,

$$\pi^i=\varphi^i+\Gamma^i-\tfrac{1}{2}\Gamma^i_{kl}(\vec{\varphi})\Gamma^k\Gamma^l+\dots . \tag{16}$$

Here $\Gamma^i=g^{ij}\Gamma_{,j}$ where $\Gamma(\pi,\varphi)$ is one-half of the square of the distance along the geodesic and $,j$ denotes a derivative with respect to φ^j; Γ^i_{kl} are the Christoffel symbols

$$\Gamma^i_{kl}=g^{ij}[g_{jl,k}+g_{jk,l}-g_{kl,j}].$$

Substituting in the Lagrangian, expanding and keeping terms to second order in Γ^i, we find

$$L(\vec{\pi})=L(\vec{\varphi})-(1/2t_0)(\Gamma^a\partial^2\Gamma^a+\Gamma^a\{[\rho^\mu(\varphi)\rho_\mu(\varphi)]_{ab}+C_{ab}(\varphi)\}\Gamma^b+\Gamma^a\rho_{\mu,ab}\partial_\mu\Gamma^b-\partial_\mu\Gamma^a\rho_{\mu,ab}\Gamma^b)\,, \tag{18}$$

$$\rho_{\mu,ab}=e_a{}^k\Gamma_{k,il}(\partial_\mu\varphi^i)e_b{}^l+g_{kl}e_a{}^k\partial_\mu e_b{}^l\,, \tag{19}$$

$$C_{ab}=e_a{}^ke_b{}^l(\partial_\mu\varphi^i)(\partial_\mu\varphi^j)R_{kjil}. \tag{20}$$

R_{kjil} is the Riemann tensor and we have introduced fields $e_i{}^a(\varphi)$ associated with the metric, $e_a{}^ke_a{}^l=g^{kl}$, $e_a{}^ke_{kb}=\delta_{ab}$. Equations (16)–(20) are the generalizations of Eqs. (7), (8), (12), and (13) to spaces of arbitrary curvature. As before, we obtain an effective Lagrangian by integrating the partition function over the quantum fluctuations Γ^a. To one-loop order we find

$$L(\vec{\pi})=L(\vec{\varphi})-\mathrm{Tr}[C(\vec{\varphi})]I(\Lambda), \tag{21}$$

where

$$I(\Lambda)=\int_{\tilde{\Lambda}}^{\Lambda}\frac{d^2k}{(2\pi)^2}\frac{1}{k^2}. \tag{22}$$

The theory is renormalizable if $\mathrm{Tr}[C(\vec{\varphi})]$ has the same form as $L(\vec{\varphi})$. Now

$$\begin{aligned}C_{aa}(\vec{\varphi})&=g^{kl}R_{kijl}(\partial_\mu\varphi^i)(\partial_\mu\varphi^j)\\&=R_{ij}(\partial_\mu\varphi^i)(\partial_\mu\varphi^j),\end{aligned} \tag{23}$$

where R_{ij} is the Ricci tensor, and so the condition for renormalizability is that $R_{ij}=rg_{ij}$ for constant r. This is the definition of an Einstein space; r is known as the average curvature. It is positive for compact spaces and negative for noncompact spaces. Thus, the coupling-constant renormalization for Einstein space is

$$\frac{1}{t}=\frac{1}{t_0}-\frac{r}{2\pi}\ln\frac{\Lambda}{\tilde{\Lambda}}. \tag{24}$$

The spaces $O(N)/[O(p)\times O(N-p)]$ are Einstein spaces with $r=N-2$.[11] This is the result of Brézin, Hikami, and Zinn-Justin.[6] For the sphere $p=1$, we recover Eq. (10). The noncompact spaces $O(p,N-p)/[O(p)\times O(N-p)]$ are also Einstein spaces, but with $r=-(N-2)$. Our previous result Eq. (14) was for the special case of the hyperboloid, $p=1$. These results can also be obtained by a direct generalization of the method outlined in Ref. 6. The crucial difference for noncompact spaces is that the sign of the quartic interaction in the effective Lagrangian changes. This leads to the change in sign of the one-loop contribution to the β function, $\beta(t)=\partial t/\partial\ln\tilde{\Lambda}$. In $2+\epsilon$ dimensions, for the specific case $O(M,M)/[O(M)\times O(M)]$ of interest we find

$$\beta_M(t)=\epsilon t+\pi^{-1}(M-1)t^2+O(t^3) \tag{25}$$

and so there is no nontrivial fixed point for $M>1$. However, the disordered electronic system corresponds to $M=0$, so that

$$\beta_{M=0}(t)=\epsilon t-\pi^{-1}t^2+O(t^3) \tag{26}$$

and there is an infrared unstable fixed point at $t_c=\pi\epsilon$. This corresponds to a mobility edge.

The renormalized coupling t is given in terms of the physical parameters E and l ($=R/a$ is the mean range of a single hop in units of the lattice spacing) as $t^3=(c/l^2)E_0{}^2/(E_0{}^2-E^2)$, $E_0{}^2>E^2$, and c is a numerical constant. In two dimensions there is a single unstable fixed point at $t_c=0$. Therefore, for any finite amount of hopping l, flow in energy, as the length scale increases, is to the edges of the band and localized states. We conclude that all states are localized in two dimensions. Above two dimensions, two different situations can arise depending on the strength of the disorder. If the disorder is weak, so that the range l is large, specifically $l>[c/(d-2)\pi]^{1/2}$, then there are mobility edges $\pm E_c$, such that for $E^2<E_c{}^2$ flow is towards $E=0$ and extended states, whereas for $E^2>E_c{}^2$ flow is towards the edges of the band and localized states. This is illustrated in Fig. 1. However, as the disorder increases the mobility edges move in towards the center of the band and a point is reached $\{l=[c/(d-2)\pi]^{1/2}\}$ at which they merge; thereafter all states are lo-

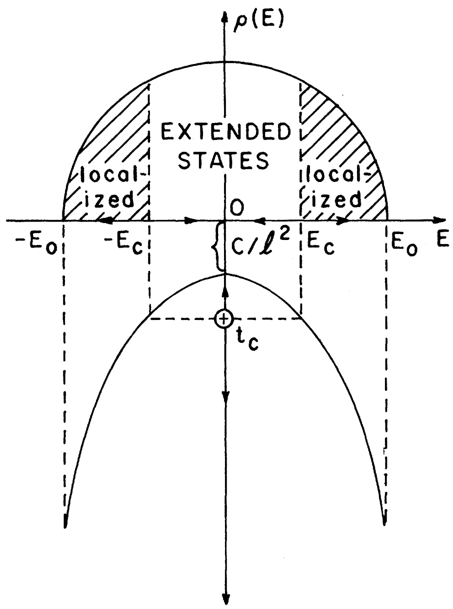

FIG. 1. Density of states $\rho(E)$ in a weakly disordered solid above two dimensions showing the existence of mobility edges at $\pm E_c$ and flow under renormalization-group transformations.

calized.

Finally, noting that t is the dimensionless resistance, we see that in Eq. (26) we have derived from first principles the β function of Abrahams *et al.*[12] ($t \propto 1/g$ of this reference). This justifies the assumption of one-parameter scaling.[13] Further we note that it is crucial for their arguments that the sign of the first correction term in the β function be negative. As we have pointed out, this follows directly from the noncompact symmetry of the model.

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Anomalous L_3/L_2 White-Line Ratios in the 3d Transition Metals

R. D. Leapman and L. A. Grunes
School of Applied and Engineering Physics and the Materials Science Center, Cornell University, Ithaca, New York 14853
(Received 7 April 1980)

The L_{23} near-edge fine structure has been investigated in electron-energy-loss spectra from thin films of 3d transition metals and an unexpected departure from the statistical L_3/L_2 "white-line" intensity ratio of 2:1 is reported. For Ti, a ratio of 0.7:1 is observed, while for Fe and Ni the ratio exceeds 3:1, indicating a systematic trend within the period. It is suggested that many-electron effects may be important.

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In this Letter we report an anomaly in the relative excitation probabilities of L_3 and L_2 inner-core levels in the 3d transition metals, which we have studied with electron-energy-loss spectroscopy (EELS). At small momentum transfer the matrix element in the cross section for inelastic