Critical behavior of disordered degenerate semiconductors. II. Spectrum and transport properties in mean-field theory

Eduardo Fradkin
Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801
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The critical behavior of disordered degenerate semiconductors is studied within a mean-field theory valid when the number of degeneracy points is large. I show that above two dimensions there is a semimetal-metal transition at a critical impurity concentration. The mean free path and the one-particle density of states exhibit scaling behavior with universal exponents. The transition is smeared at nonzero temperature. An equation of state, relating temperature, disorder, and bare conductivity, is presented. In two dimensions, the semimetallic phase is unstable. I show that a localization transition follows except in two dimensions where all states are localized. The bare conductivity appears to be a universal number in two dimensions. Applications to zero-gap semiconductors and other systems are discussed.

I. INTRODUCTION

This is the second of a series of two papers devoted to the study of the critical properties of degenerate semiconductors.[1] In the previous paper, hereafter indicated by I, I introduced models that describe the physics of the electronic states of degenerate semiconductors near their N_c degeneracy points. In this paper I discuss their spectral and transport properties in detail, in particular near the semimetal-metal transition. I show the following:

(i) Above two dimensions, a semimetal-metal transition takes place and it is followed by a localization transition.

(ii) Two is the lower critical dimension of this transition.

(iii) The density of states (DOS) and the elastic mean free path display a critical behavior with universal exponents.

(iv) The transition is smeared at finite temperature. I show that temperature has an effect analogous to that of a magnetic field in a ferromagnet. I present an "equation of state" relating disorder, temperature, and bare conductivity. I find an anomalous temperature dependence in the specific heat at the transition of the form T^{α} with $\alpha=\frac{3}{2}$ at $N_c=\infty$.

(v) The localization transition is of the standard (noninteracting) type. The system is investigated by an approximate solution valid when the number of degenerate points (N_c) is large. The localization transition is studied by deriving the associated nonlinear σ model (Refs. 2 and 3) and its relation to the semimetal-metal transition is discussed.

(vi) In two dimensions the semimetallic phase is unstable. The bare (Boltzmann) conductivity appears to be universal. The mean free path and localization length are shown to be related and a wide separation of length scales is possible for N_c large.

The paper is organized as follows. In Sec. II the large-N_c limit is studied. The transition is studied in both two and three dimensions. The localization transition is considered in the framework of the nonlinear σ model. Section III is devoted to applications and conclusions.

II. SEMIMETAL-METAL AND LOCALIZATION TRANSITIONS: THE LARGE DEGENERACY LIMIT

In paper I (Ref. 1) I showed that the problems of calculating the averaged Green's functions of dirty degenerate semiconductors (at the Fermi energy) reduces to the study of a field theory of self-interacting Dirac fields $\psi_{\alpha ars}(x)$ with Lagrangian

$$\mathscr{L}=\bar{\psi}\nabla\!\!\!/\,\psi+\epsilon\bar{\psi}\Lambda\psi-gN_c\bar{\psi}^{a}_{rs}\psi^{a}_{r's'}\bar{\psi}^{a'}_{r's'}\psi^{a'}_{rs}\ , \tag{2.1}$$

where $\bar{\psi}\psi\equiv\bar{\psi}_{\alpha ars}\psi_{\alpha ars}$ and repeated indices are summed. The fields ψ and $\bar{\psi}$ are Grassmann (anticommuting) variables and the indices $\alpha=1,2$ (for the conduction and valence bands), $a=1,\ldots,N_c$ are the degeneracy points, $r=1,\ldots,n$ (the replica indices, $n\to 0$), and $s=\pm 1$ (for advanced and retarded). The matrix Λ is

$$\Lambda^{\alpha\alpha'}_{aa',rr',ss'}=\delta_{\alpha\alpha'}\delta_{aa'}\delta_{rr'}\delta_{ss'}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}_{ss'}\ . \tag{2.2}$$

At finite temperature T ($k_B=1$), ϵ is replaced by πT. In Eq. (2.1), g is the width of the probability distribution of random fields, i.e., a measure of the impurity concentration. I first show that the path integral

$$\mathscr{Z}=\int\mathscr{D}\bar{\psi}\mathscr{D}\psi\exp\left[-\int d^dx\,\mathscr{L}\right] \tag{2.3}$$

can be solved in the large-degeneracy limit ($N_c\to\infty$), where the average Green's functions can be calculated explicitly. In the following I shall show that this approximation is only qualitatively correct.

The first step is to introduce a set of collective Hermitian (c-number) $Q^{rr'}(x)$ fields to decouple the quartic term of the Lagrangian. This is done using the standard Gaussian integral

$$\int \mathscr{D}Q_{rr'}(x)\exp\left[-\int d^dx[\tfrac{1}{2}\mathrm{tr}Q^2(x) + \lambda Q_{rr'}(x)\bar{\psi}^a_{r'}(x)\psi^a_r(x)]\right] = \mathscr{N}\exp\left[+\frac{\lambda^2}{2}\int \bar{\psi}^a_r(x)\psi^a_{r'}(x)\bar{\psi}^{a'}_{r'}(x)\psi^{a'}_r(x)d^dx\right], \quad (2.4)$$

where $\lambda^2=2gN_c$ and $\mathscr{N}$ is a numerical normalization constant. In Eq. (2.4) I have abolished the s label to simplify notation. We can now regard the replica index r as taking the values $r=1,\ldots,2n$ with Λ trivially redefined. Thus the Lagrangian (2.3) reads

$$\mathscr{L}=\bar{\psi}\nabla\!\!\!/\,\psi+\epsilon\bar{\psi}\Lambda\psi+\tfrac{1}{2}\,\mathrm{tr}Q^2+\lambda Q_{rr'}\bar{\psi}^a_{r'}\psi^a_r\,. \quad (2.5)$$

By integrating out the Dirac fields I find the effective action for the Q variables

$$S_{\rm eff}[Q]=\tfrac{1}{2}\int d^dx\,\mathrm{tr}Q^2(x) - N_c\mathrm{tr}\ln(\nabla\!\!\!/+\epsilon\Lambda+\lambda Q)\,. \quad (2.6)$$

I now define rescaled fields $\tilde{Q}_{rr'}(x)=\lambda Q_{rr'}(x)$ and a coupling constant $g_0=N_c^2 g$. The resulting path integral is

$$\mathscr{Z}=\int \mathscr{D}\tilde{Q}e^{-N_cS_{\rm eff}[Q]}, \quad (2.7a)$$

with the effective action

$$S_{\rm eff}[\tilde{Q}]=\frac{1}{4g_0}\int d^dx\, tr\tilde{Q}^2(x)-\mathrm{tr}\ln(\nabla\!\!\!/+\epsilon\Lambda+\tilde{Q})\,. \quad (2.7b)$$

Thus if the number of degeneracy points N_c is large, the path integral will be dominated by configurations of the $\tilde{Q}$ field close to the solutions to the coherent-potential-approximation- (CPA) looking saddle-point equations.[4] They are[5]

$$\frac{1}{2g_0}\langle\tilde{Q}_{rr'}(x)\rangle=\sum_a S^{aa}_{rr'}(x,x)\,. \quad (2.8)$$

In Eq. (2.8) I have used the propagator

$$S^{aa}_{rr'}(x,x')=\left\langle ar\left|\frac{1}{\nabla\!\!\!/+\epsilon\Lambda+\langle\tilde{Q}\rangle}\right|a'r'\right\rangle. \quad (2.9)$$

A. Solution of the saddle-point equation (SPE)

I now look for a translationally invariant solution of the SPE. This solution is not unique. This nonuniqueness is related to the existence of diffusive modes.[2,4] I further assume a solution $\langle\tilde{Q}_{rr'}\rangle$ proportional to Λ

$$\langle\tilde{Q}_{rr'}\rangle=q\Lambda\,. \quad (2.10)$$

Therefore I obtain

$$q\Lambda=2g_0\int_p\frac{1}{ip\!\!\!/+(\epsilon+q)\Lambda}, \quad (2.11)$$

which yields

$$q=4g_0\int_p\frac{q+\epsilon}{p^2+(q+\epsilon)^2}\,. \quad (2.12)$$

To simplify matters I define $\mu=q+\epsilon$.

The integral in Eq. (2.12) diverges in two dimensions. We have to cut it off at a momentum exchange scale $K\sim 1/a_0$ (where a_0 is of the order of the lattice spacing). I use the smooth cutoff

$$\mu-\epsilon=4g_0\mu\left[\int_p\frac{1}{p^2+\mu^2}-\int_p\frac{1}{p^2+K^2}\right]. \quad (2.13)$$

The result can be put in the form of an equation of state[6]

$$\frac{\mu-\epsilon}{g_0}=\frac{\mu}{g_0^c}\left[1-\left[\frac{\mu}{K}\right]^{d-2}\right], \quad (2.14)$$

where the *critical coupling* g_0^c equals

$$g_0^c=\frac{(d-2)(4\pi)^{d/2}}{8\Gamma[(2-d/2)]}K^{-(d-2)}\,. \quad (2.15)$$

If ϵ is set to zero, Eq. (2.14) has the solution ($\mu=q$), for $d>2$

$$\mu=0,\quad g_0<g_0^c \quad (2.16a)$$

$$\mu=K\left[\frac{g_0-g_0^c}{g_0}\right]^{1/(d-2)},\quad g_0>g_0^c\,. \quad (2.16b)$$

This solution means that the average one-particle Green's function[1] $G(x,y)$ decays exponentially at distances larger than the mean free path l

$$l=K^{-1}\left[\frac{g_0-g_0^c}{g_0}\right]^{-\nu}\quad (d>2) \quad (2.17)$$

with $\nu=1/(d-2)$. In two dimensions Eq. (2.14) becomes

$$\mu=Ke^{-\pi/2g_0}\quad (d=2) \quad (2.18)$$

for all $g_0>0$. Hence the mean free path is finite. This agrees with the results of Fisher and Fradkin.[7] The density of states (DOS) is

$$N(0)=\frac{N_c\mu}{2g_0\pi}\,. \quad (2.19)$$

Thus, below g_0^c the DOS vanishes and above g_0^c it increases with a critical exponent s

$$N(0)=A(g_0-g_0^c)^s,\quad g_0>g_0^c\quad (d>2) \quad (2.20)$$

and $s=1/(d-2)$, for $d>2$. In two dimensions $N(0)$ is always nonzero and equals

$$N(0)=\frac{KN_c}{2g_0\pi}e^{-\pi/2g_0}\,. \quad (2.21)$$

These results should be contrasted with analogous calculations in dirty metals.[8] In dirty metals the CPA equation (2.8) yields a finite mean free path of the order of atomic distances. The equation has essentially the same behavior in all dimensions because the DOS is nearly constant close enough to the Fermi energy. In dirty degenerate semimetals the extra phase space associated with the pointlike Fermi "surface" enhance fluctuations and is the cause of this critical behavior.

The strong dependence on the cutoff of the equation of state (2.14) suggests the use of the renormalization group

(RG). I define a dimensionless renormalized coupling constant t by

$$g_0 = tK^{-(d-2)}Z_1(t) , \tag{2.22a}$$

where the scale parameter K is arbitrary. Likewise

$$\epsilon = \epsilon_R Z(t) , \tag{2.22b}$$

$$\mu = \mu_R . \tag{2.22c}$$

Equation (2.22c) is valid only *at* $N_c = \infty$. There are corrections of order of $1/N_c$. The renormalization constants $Z_1(t)$ and $Z(t)$ can be calculated using the condition that Eq. (2.12) be finite.[9] Substituting I obtain

$$Z_1 = Z \tag{2.23a}$$

and

$$\frac{1}{Z_1} = 1 - \frac{8t}{(4\pi)^{d/2}} \frac{\Gamma[2-(d/2)]}{d-2} , \tag{2.23b}$$

which yields a renormalized equation of state

$$1 - \frac{\epsilon_R}{\mu_R} = \frac{t}{t_c}\left[1 - \left[\frac{\mu}{K}\right]^{d-2}\right] , \tag{2.24}$$

where $t_c = g_0^c K^{d-2}$. The arbitrariness of K generates the RG flow through the β function, $\beta(t)$

$$\beta(t) = -K\frac{\partial t}{\partial K} . \tag{2.25}$$

Explicit calculation yields

$$\beta(t) = -(d-2)t + \frac{(d-2)}{t_c}t^2 . \tag{2.26}$$

The β function has two fixed points ($d>2$): $t^* = 0$ (stable) and $t^* = t_c$ (unstable), which controls the semimetal-metal transition. The eigenvalue is equal to $d-2$ which agrees with the explicitly calculated exponents.

The corrections of order $1/N_c$ and higher are expected to modify systematically these exponents. This I do not do here. Still fluctuations make an even more significant contribution to transport properties.

B. Fluctuations, conductivity, and localization

The analysis of the role of fluctuations *above* the transition is completely analogous to localization theory.[2,3,7,10] Below g_c the system is a semimetal and the conductivity is zero. Above g_c the bare (or microscopic) conductivity does not vanish. However, in order to determine whether the states near the Fermi surface are localized or not it is necessary to construct the corresponding nonlinear σ model[2] and, in particular, to determine its bare coupling constant. By expanding around the solution of the SPE I find

$$S(\tilde{Q}) = \frac{1}{4g_0}\int d^dx\, \mathrm{tr}\langle Q\rangle^2 - \mathrm{tr}\ln[\nabla + \epsilon\Lambda + \langle Q\rangle] + \frac{1}{4g_0}\int d^dx\, \mathrm{tr}Q^2 + \tfrac{1}{2}\int d^dx \int d^dy\, \mathrm{tr}[S(x,y)Q(y)S(y,x)Q(x)] + O(Q^3) \tag{2.27}$$

with

$$\tilde{Q}_{rr'}(x) = \langle \tilde{Q}_{rr'}\rangle + Q_{rr'}(x) . \tag{2.28}$$

Hence, at $N=\infty$, the correlation function of diffusive modes[2,4]

$$K^{+-}(p) = \langle Q^{+-}(\mathbf{p})Q^{-+}(\mathbf{p})\rangle \tag{2.29}$$

has the small-momentum-transfer limit form

$$K^{+-}(p) = \frac{4\pi g_0^2}{N_c^2}\frac{N(0)}{Dp^2+\epsilon} , \tag{2.30}$$

where the bare diffusion constant D equals

$$D = \frac{1}{12}\frac{(d-2)g_0}{g_0^c K^{d-2}}\mu^{d-3} . \tag{2.31}$$

The bare (or microscopic) conductivity can be calculated using the Einstein relation

$$\sigma = \frac{e^2}{\hbar}N(0)D , \tag{2.32}$$

which yields

$$\sigma = \frac{e^2}{\hbar}\frac{N_c}{3\pi}\frac{\Gamma[2-(d/2)]}{(4\pi)^{d/2}}\mu^{d-2} . \tag{2.33}$$

In three dimensions this is

$$\sigma_{3d} = \frac{e^2}{\hbar}\frac{N_c}{24\pi^2}\mu , \tag{2.34}$$

while in two dimensions I get

$$\sigma_{2d} = \frac{e^2}{\hbar}\frac{N_c}{12\pi^2} . \tag{2.35}$$

This is a rather remarkable result. In two dimensions the microscopic (or Boltzmann) conductivity appears to be a universal number independent of the width of the distribution. Of course fluctuations (i.e., higher orders in the $1/N_c$ expansion) may still modify this essentially semiclassical result.

The local density of states fluctuates over distances of the order of $1/\mu$, the mean free path. These fluctuations are described by the correlation function $\langle \tilde{Q}^{++}(x)\tilde{Q}^{++}(y)\rangle$. In a metal such correlations are always short-ranged because the mean free path remains small. In dirty degenerate semiconductors DOS correlations become long ranged at the semimetal-metal transition. Once the mean free path has become finite (and the DOS nonzero) localization effects set in. Such fluctuations take place on length scales longer than the mean free path l. We know from localization theory that a system with underlying unitary symmetries has a localization transition in the universality class of the unitary nonlinear σ model.[11] This model describes the physics of fluctuating diffusive modes. Following Hikami,[10] I write a compact[12] nonlinear σ model with degrees of freedom $U(x)$ defined on the symmetric space $U(2n)/U(n)\times U(n)$ in the replica $n\to 0$ limit. The Hamiltonian is ($\epsilon=0$)

$$H=\frac{1}{16u}\int d^dx\,\mathrm{tr}[\nabla U(x)\cdot\nabla U(x)^{-1}]\ . \tag{2.36}$$

The fields $U(x)$ are just the matrices $\widetilde{Q}(x)$ constrained to satisfy the SPE exactly (after rescaling them by the expectation value μ). The nonlinear σ-model coupling constant is (as $N_c\to\infty$)

$$u=\frac{3}{32}\frac{(4\pi)^{d/2}}{\Gamma[2(d/2)]}\frac{l^{d-2}}{N_c}\ , \tag{2.37}$$

where in three dimensions (3D) I get $u_{3D}=(3\pi/4N_c)l^{-1}$ and in two dimensions $u_{2D}=(3\pi/8N_c)$. Defining once again a dimensionless coupling constant $u_0=u\overline{K}^{2-d}$ where $\overline{K}<(1/l)$, one can write down the β function for the unitary nonlinear σ model known from localization theory[10,13] as

$$\beta(u_0)=-K\frac{\partial u_0}{\partial K}=-(d-2)u_0+\frac{u_0^3}{2\pi^2}\ , \tag{2.38}$$

which is accurate to two loops.

In two dimensions this implies a relation between the localization length ξ and the mean free path l

$$\xi\lesssim l\exp(\frac{64}{9}N_c^2)\ . \tag{2.39}$$

Notice that the numerical proportionality constant can be very large. A naive substitution $N_c\sim 1$ in (2.39) yields a ratio $\xi/l\sim 10^3$.

In three dimensions there is a localization transition. A very poor estimate of its location can be found using the unstable fixed point of (2.38) valid to leading order in $d-2$. Therefore,

$$u_0^*\cong[2\pi^2(d-2)]^{1/2}+O((d-2)^2)\ , \tag{2.40}$$

where the condition that ratio

$$\frac{u_0}{u_0^*}\cong\frac{3}{4N_c\sqrt{2(d-2)}}$$

be less than one implies that all states near the Fermi energy are extended if

$$N_c\gtrsim\frac{3}{4\sqrt{2(d-2)}}+O(d-2)\ .$$

Estimates of this sort are exceedingly unreliable in three dimensions. Therefore, all one can tell is that there should be a critical value N_c^* *above* which all states near the Fermi energy should be extended. This value N_c^* surely is a slowly varying function of the impurity density. It is likely that at high disorder N_c^* should eventually become less than one. There is no reliable way of computing these effects with the methods of this paper. Nevertheless it is clear that for general N_c a localization transition of the standard noninteracting type follows the semimetal-metal transition.

C. Finite-temperature behavior

It was shown in I that temperature formally plays the role of a symmetry-breaking field. At finite temperature the effective Lagrangian is still given by Eq. (2.1). However, ϵ must now be replaced by the minimum Matsubara frequency in a fermionic system, i.e., $\epsilon=\pi T$. We can now find the temperature dependence of the mean free path l and bare conductivity σ by making the appropriate replacements in Eq. (2.24).

The solution to this equation yields the mean free path as a function of the disorder t and temperature T. Thus at the semimetal-metal transition ($t=t_c$) one finds

$$l(T)=K^{-1}\left[\frac{\pi T}{K}\right]^{-1/\delta}\ , \tag{2.41}$$

where $\delta=d-1$. In the pure-system limit ($t=0$) one finds $l=1/\pi T$. In the entire semimetallic region I find $l\sim cT^{-1}$ with a coefficient c, which is a function of impurity concentration (as $T\to 0$). At the transition a crossover from $1/T$ to $1/\sqrt{T}$ behavior should be observed. Above the transition l should remain finite as $T\to 0$. The singular behavior of Eq. (2.41) is universal (i.e., it does not depend on the microscopic details of the system). The actual exponent δ equals $d-1$ only in the large degeneracy limit. There should be important corrections to this number for finite N_c. These results will be published elsewhere.

The temperature dependence of the bare conductivity can be found by substituting the temperature-dependent mean free path in Eq. (2.33). One can write this *equation of state* in the scaling form

$$1-\pi T\left[\frac{A}{\sigma}\right]^{1/(d-2)}=\frac{t}{t_c}\left[1-\left[\frac{\sigma}{AK^{d-2}}\right]^{1/\beta(d-2)}\right]\ , \tag{2.42}$$

where the exponent β equals $1/d-2$ (at $N_c=\infty$) and A

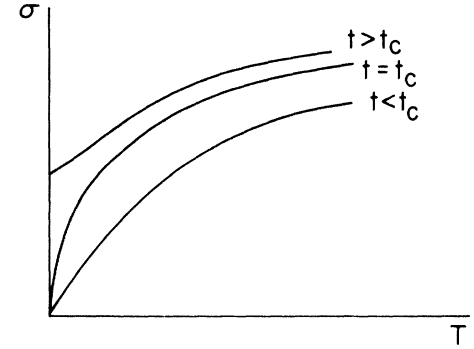

FIG. 1. Qualitative temperature dependence of the *bare conductivity* below, at, and above the semimetal-metal transition.

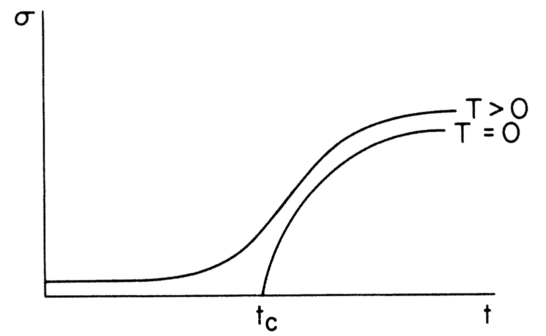

FIG. 2. Bare conductivity as a function of disorder strength t at zero and nonzero temperature. Localization effects are not included.

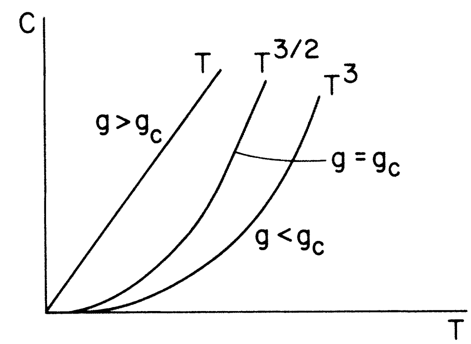

FIG. 3. Qualitative behavior of the specific heat below, at, and above the semimetal-metal transition.

is a numerical coefficient. At the semimetal-metal transition the bare conductivity behaves like

$$\sigma(t_c,T)\sim T^{(d-2)/\delta} . \tag{2.43}$$

In three dimensions (and $N_c\to\infty$) one finds $\sigma\sim\sqrt{T}$. Below the transition σ vanishes like T (in 3D), whereas above the transition it reaches the constant value given by Eq. (2.33). Again localization effects should affect these results appreciably. A qualitative picture of the temperature dependence of the bare conductivity (i.e., below the localization transition) is shown in Fig. 1. In Fig. 2 we see the bare conductivity as a function of impurity concentration at various temperatures.

Fluctuations also affect the specific-heat behavior at low temperature. Above the transition the DOS is finite and one readily finds a linear specific heat. Below the transition the system behaves roughly like free relativistic massless fermions with $N(E)\sim E^{d-1}$. At the transition one can solve the SPE at nonzero energy and one finds that the DOS behaves like

$$N(E)\sim E^{1/\delta} . \tag{2.44}$$

Thus the specific heat is, at low temperatures,

$$C\sim T^{\alpha} \tag{2.45}$$

with $\alpha=(1/\delta)+1$. In these dimensions, and for $N_c=\infty$, I find that $C\sim T^{3/2}$ (see Fig. 3).

III. CONCLUSIONS

In this paper I demonstrated that disordered degenerate semiconductors should exhibit a rich variety of critical behavior. Particularly striking are the anomalous temperature dependence of the specific heat at the critical concentration and the apparent universal character of the bare conductivity in two dimensions.

There are several experimental systems already available to study the transition in three dimensions. In Ref. 1 I noted that HgTe, SnTe, and α-Sn at high pressure, as well as alloys, could serve as typical systems. In this paper I considered only the large degeneracy limit. The actual exponents at N_c finite are expected to change smoothly with N_c. However, there is still the issue that there may be values of N_c for which the large N_c results may not apply, not even qualitatively. This can be checked by means of a $2+\epsilon$ expansion which will be published elsewhere. Preliminary results indicate that indeed for low values of N_c fluctuations do appreciably modify the results. Other effects such as spin-orbit scattering as well as the role of interactions should also be included.

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