

High Magnetic Field Limit of the Kinetic Equation for a Lorentzian Gas of Particles with Spin

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(Z. Naturforsch. **29 a**, 1699–1704 [1974]; received October 9, 1974)

The kinetic equation for a Lorentzian gas of particles with spin is investigated for a high external magnetic field. By time averaging over many precession periods the original kinetic equation decomposes into a set of separate equations. Each of them connects only elements of the distribution matrix with the same difference of magnetic quantum numbers. In particular, for the diagonal elements an equation of the Wang Chang-Uhlenbeck-de Boer type is obtained. The pertaining cross sections depend also on the field direction \mathbf{h} . The eigenvalues of the dynamical operator are shown to have a positive real part. As an application, the \mathbf{h} -dependent cross sections for spin-1/2-particles and the heat conduction in the high field limit are treated.

Introduction

The kinetic equation for a Lorentzian gas of particles with spin has been derived in 1957¹ and was then used to describe multiple scattering and diffusion of polarized particles^{2,3}. In the last decade the kinetic theory of transport and orientation phenomena in pure gases^{4,5} and mixtures⁶ of rotating molecules in an external homogeneous magnetic field has emerged from that and was applied to many experiments⁷. In the present paper the kinetic equation is investigated in the limiting case of high magnetic field when the precession frequency of the magnetic moments appreciably exceeds the molecular collision frequency. This question has briefly been treated earlier⁸. Here, a more detailed discussion is given.

For simplicity a spatially homogeneous Lorentzian gas of particles with spin is considered. According to the original kinetic equation the time derivative of any element of the distribution matrix is a functional of all its elements. In a high magnetic field a particle undergoes many precessions between two collisions. By time-averaging over many precession periods the original kinetic equation decomposes into a set of separate equations, viz. the time derivative of any element of the distribution matrix with quantum numbers M, M' becomes a functional only of the elements with the same difference $M - M'$. As a special case the diagonal elements, $M - M' = 0$, obey a closed Wang Chang-Uhlenbeck-de Boer (WUB-) equation⁹. The ensuing cross sections

depend also on the direction \mathbf{h} of the magnetic field. In the equations for the non-diagonal elements, $M - M' \neq 0$, which might be termed "collateral WUB-equations", still the original scattering amplitudes appear.

The eigenvalues of the dynamical operator (sum of precession and collision term) have a positive real part which guarantees the approach of the system to thermal equilibrium. This is also true for the eigenvalues of the high-field collision term. The corresponding eigensolutions are, in general, non-Hermitian.

Finally the theory is applied to spin-1/2-particles where the scattering amplitude is very simple. An expression for the \mathbf{h} -dependent WUB-cross sections is given. The corresponding WUB-equation is used to treat the heat conduction in a high magnetic field.

1. Kinetic Equation for High Magnetic Field

The kinetic equation for a spatially homogeneous Lorentzian gas of neutral particles with mass m and spin $\hbar s$ in a homogeneous magnetic field $\mathbf{H} = H \mathbf{h}$ is¹

$$\partial f / \partial t - i \omega_H [\mathbf{h} \cdot \mathbf{s}, f]_- + \omega(f) = 0. \quad (1)$$

Here, $f = f(\mathbf{c}, \mathbf{s}, t)$ respectively $f' = f(\mathbf{c}', \mathbf{s}, t)$ is the Hermitian $(2s+1) \times (2s+1)$ distribution matrix, $\omega_H = \mu H / \hbar s$ denotes the precession frequency of the magnetic moment μ and $\omega(f)$ abbreviates the collision (super-) operator

$$\omega(f) = -n c \left[\int a f' a^\dagger d^2 e' - \frac{\hbar}{i m c} (a(0)f - f a(0)^\dagger) \right]. \quad (2)$$

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Here, n is the number density of the fixed isotropic spinless scatterers, $\mathbf{c} = c \mathbf{e}$ and $\mathbf{c}' = c \mathbf{e}'$ are molecular velocities involved in an energetically elastic collision. The binary scattering amplitude and its adjoint (in spin space)

$$a = a(E, \mathbf{e}, \mathbf{e}', \mathbf{s}), \quad a^\dagger = a(E, \mathbf{e}, \mathbf{e}', \mathbf{s})^\dagger \quad (3)$$

are meant on the energy shell $E = m c^2/2$. They depend, apart from the unit vectors \mathbf{e}, \mathbf{e}' of the asymptotic velocities after and before collision, on the spin operator of the scattered particle. The integration goes over all solid angle elements $d^2\mathbf{e}'$ of

direction \mathbf{e}' before a gain-collision. The loss-collisions depend on the scattering amplitude

$$a(0) = a(E, \mathbf{e}, \mathbf{e}, \mathbf{s}) \quad (4)$$

and its adjoint in forward direction \mathbf{e} ; h/mc is the de Broglie wavelength.

If the eigenstates of $s_z = \mathbf{s} \cdot \mathbf{h}$

$$s_z |M\rangle = M |M\rangle \quad (5)$$

are introduced as a special basis of representation, Eq. (1) with (2) takes the detailed form

$$\begin{aligned} \partial f_{MM'}/\partial t - i \omega_H (M - M') f_{MM'} = n c \left\{ \sum_{M''} \int \sum_{M'''} a_{MM''} f_{M''M'''} a_{M'M'''}^* d^2\mathbf{e}' \right. \\ \left. - \frac{h}{i m c} \sum_{M''} [a(0)_{MM''} f_{M''M'} - f_{MM''} a(0)_{M'M''}^*] \right\}. \end{aligned} \quad (6)$$

This will be our starting point in discussing the high field limit.

“High magnetic fields” is understood in such a way that the precession time $\tau_H = 2\pi/\omega_H$ is much smaller than the time τ_{free} between two collisions, but still larger than the duration τ_{coll} of a collision

$$\tau_{\text{coll}} \ll \tau_H \ll \tau_{\text{free}}.$$

The condition $\tau_{\text{coll}} \ll \tau_H$ implies that the scattering amplitude will be fairly independent of the magnetic field which has already tacitly been assumed in Equation (2). The condition $\tau_H \ll \tau_{\text{free}}$ means that a particle undergoes many precessions between two successive collisions. To get rid of the corresponding rapid time variation of the distribution matrix we put

$$f_{MM'}(t) = \bar{f}_{MM'}(t) \exp\{i \omega_H (M - M') t\}, \quad (7)$$

where $\bar{f}_{MM'}(t)$ is now a function varying slowly with time due to the collisions only. The rapid oscillations are contained in the exponential factor (“interaction picture”). If Eq. (7) is inserted into Eq. (6), if the result is “tranquilized” by multiplication with $\exp\{-i \omega_H (M - M') t\}$, and averaging over many precession times $N \tau_H$, and if finally

$$\frac{1}{N \tau_H} \int_t^{t+N \tau_H} \exp\{i \omega_H (M - M') t'\} dt' \approx \delta_{MM'}$$

is observed, one obtains

$$\partial \bar{f}_{MM'}/\partial t \approx n c \left\{ \sum_{M''} \int a_{MM''} \bar{f}_{M'', M'' + M' - M} a_{M', M'' + M' - M}^* d^2\mathbf{e}' - (h/i m c) [a(0)_{MM} - a(0)_{M'M}^*] \bar{f}_{MM'} \right\}. \quad (8)$$

This is already the desired kinetic equation in the high field limit. It is important to realize that the elements $a_{MM'}$ of the scattering matrix depend not only on $E, \mathbf{e}, \mathbf{e}'$ but also on the direction \mathbf{h} of the magnetic field which had been taken as the axis of quantization. To cope with the boundaries of the M'' -summation it is sufficient to stipulate that any matrix element of a or f vanishes if the modulus of at least one of its indices exceeds the spin value s .

2. Diagonal and Nondiagonal Parts of the High Field Kinetic Equation

The kinetic Eq. (8) decomposes into separate sets, one set for each “parallel of the diagonal”, i. e. for elements with fixed difference $M - M'$. In order to make this even more explicit, let us introduce new subscripts by putting

$$M = \mu + m, \quad M' = -\mu + m$$

so that

$$M - M' = 2\mu, \quad \text{with } \pm 2\mu = 0, 1, 2, \dots,$$

is constant within a particular set. The elements of the distribution matrix \bar{f} are renamed according to

$$\bar{f}_{MM'} = F_{\mu m}$$

and for the summation index M'' we write

$$M'' = \mu + m'.$$

Then Eq. (8) goes over into

$$\partial F_{\mu m} / \partial t = n c \left\{ \sum_{m'} \int a_{\mu+m, \mu+m'} F'_{\mu m'} a_{-\mu+m, -\mu+m'}^* d^2 e' - (h/i m c) [a(0)_{\mu+m, \mu+m} - a(0)_{-\mu+m, -\mu+m}^*] F_{\mu m} \right\}. \quad (9)$$

This shows that only F 's with the same index μ are connected.

In the case of diagonal elements, $M = M'$ or $\mu = 0$, Eqs. (8) or (9) can be simplified further by aid of the optical theorem for the scattering matrix (completeness and normalization relations). This theorem connects the forward amplitude with integrals over all directions of scattering:

$$(h/i m c) [a(0) - a(0)^\dagger] = \int a a^\dagger d^2 e' = \int a'^\dagger a' d^2 e'. \quad (10)$$

Here, the abbreviation

$$a' = a(E, \mathbf{e}', \mathbf{e}, \mathbf{s}) \quad (11)$$

for the scattering from direction \mathbf{e} into direction \mathbf{e}' has been introduced. Now, in particular for the diagonal elements, one finds from (8), or (9) equivalently.

$$\partial f_{MM} / \partial t = -n c \sum_{M''} \int \sigma_{MM''} (f_{MM} - f'_{M''M''}) d^2 e' \quad (12)$$

with the cross sections

$$\sigma_{MM''} = |a_{MM''}|^2 = \sigma_{MM''}(E, \mathbf{e}, \mathbf{e}', \mathbf{h}) \quad (13)$$

relevant to a transition $M'' \rightarrow M$ between magnetic states. The bar over f_{MM} could be omitted after Equation (7). Equation (12) is an equation for the occupation numbers f_{MM} alone. So, it represents a kinetic equation of the WUB-type⁹. Again, the cross sections $\sigma_{MM''}$ depend on \mathbf{h} , our special choice of the quantization axis. More specifically it can be said that they will — as scalars — depend on all the scalars which can be constructed from the unit vectors $\mathbf{e}, \mathbf{e}', \mathbf{h}$. An example will be given in section 4.

For nondiagonal elements, $M \neq M'$ in Eq. (8) or $\mu \neq 0$ in Eq. (9), no further simplification is possible. These “collateral equations” still contain the scattering amplitudes, not just cross sections. In particular, for $M = -M' = s$ or $M = -M' = -s$,

M'' in (8) can only be s or $-s$. In version (9) this means that one has $\mu = \pm s$, hence $m = m' = 0$. Therefore, simple equations for the matrix elements $\bar{f}_{s,-s}$ and $\bar{f}_{-s,s}$ (or $F_{\pm s,0}$) alone exist.

3. Eigenstates of the Collision Operator

The collision operator (2) has the well-known property³

$$\omega(f)^\dagger = \omega(f^\dagger).$$

From this one concludes that

$$\partial(f - f^\dagger) / \partial t = i \omega_H [\mathbf{h} \cdot \mathbf{s}, f - f^\dagger] - \omega(f - f^\dagger),$$

which implies the persistence of Hermiticity: if $f - f^\dagger$ vanishes at time t , it vanishes at any time.

Let us again look at an arbitrary non-Hermitian f and define the “quadratic entropy” by

$$S = -\int \text{tr}(f^\dagger f) d^2 e$$

where “tr” means the trace in spin state. The time derivative is, after (1) and its adjoint, expressed by

$$dS/dt = \int \text{tr}[f^\dagger \omega(f) + \omega(f^\dagger) f] d^2 e.$$

The magnetic field term which is purely mechanical does not contribute. Insertion of the detailed form (2) of the collision operator and use of the optical theorem (10) under the trace yields the H-theorem^{10, 11} for the “quadratic entropy”

$$\begin{aligned} dS/dt &= n c \iint \text{tr}[(a f' - f a)(a f' - f a)^\dagger] d^2 e d^2 e' \\ &= n c \iint \text{tr}[(a f' - f^\dagger a)(a f' - f^\dagger a)^\dagger] d^2 e d^2 e' > 0. \end{aligned} \quad (14)$$

The second alternative form of the entropy production term follows also by appropriate use of the optical theorem or simply by interchanging f and f^\dagger in the first expression: as S is symmetrical in f, f^\dagger , the same must be true for the production term.

The preceding reminder on the H-theorem shall now be used in discussing eigensolutions of the

dynamical operator, viz. solutions with exponential time dependence

$$e^{-\omega t} g.$$

The g 's have to fulfill the eigenvalue equation

$$-\omega g = i \omega_H [\mathbf{h} \cdot \mathbf{s}, g]_- - \omega(g). \quad (15)$$

In general the eigensolutions g will be non-Hermitian, the eigenvalues ω will be complex. From (15) one takes

$$-\omega^* g^\dagger = i \omega_H [\mathbf{h} \cdot \mathbf{s}, g^\dagger]_- - \omega(g^\dagger),$$

which means that with g also g^\dagger is an eigensolution with ω^* as the corresponding eigenvalue. Only in passing it shall be noticed that the g 's for different

ω 's are in general not orthogonal in some sense. To obtain orthogonality one has to introduce a second set of eigensolutions, based on the collision (super-) operator $\omega^\dagger(f)$ which originates from $\omega(f)$ by interchanging the scattering amplitude a and its adjoint a^\dagger .

The real part of an eigenvalue is positive

$$\omega + \omega^* > 0. \quad (16)$$

This follows now immediately from (14): inserting $e^{-\omega t} g$ for f yields

$$f^\dagger f = e^{-(\omega + \omega^*)t} g^\dagger g,$$

hence from (14)

$$\begin{aligned} (\omega + \omega^*) \int \text{tr}(g^\dagger g) d^2 e &= n c \iint \text{tr}[(a g' - g a)(a g' - g a)^\dagger] d^2 e d^2 e' \\ &= n c \iint \text{tr}[(a g'^\dagger - g^\dagger a)(a g'^\dagger - g^\dagger a)^\dagger] d^2 e d^2 e' > 0. \end{aligned} \quad (17)$$

The magnetic field does not show up in this relation which therefore is also valid in the high field limit. Finally a general Hermitian solution of the kinetic equation is obtained by a superposition of all eigensolutions g , with arbitrary coefficients a , of the type

$$f = \sum (a e^{-\omega t} g + a^* e^{-\omega^* t} g^\dagger).$$

The positiveness of the real part of the ω 's guaran-

tees that with increasing time the system goes to thermal equilibrium as far as the directions of the velocity and the spin are concerned.

The positiveness of $\omega + \omega^*$ for the high field limit must also follow directly from the high field equations (8) or (9). Indeed, the exponential factor split off in (7) affects only the imaginary part of the eigenvalues. The eigenvalue equation (15), in the notation used in (9), takes the form

$$\begin{aligned} -\omega_\mu G_{\mu m} &= n c \left\{ \sum_{m'} \int a_{\mu+m, \mu+m'} G'_{\mu m'} a_{-\mu+m, -\mu+m'}^* d^2 e' \right. \\ &\quad \left. - (h/i m c) [a(0)_{\mu+m, \mu+m} - a(0)_{-\mu+m, -\mu+m}^*] G_{\mu m} \right\}. \end{aligned} \quad (18)$$

The eigenvalues ω_μ and eigensolutions $G_{\mu m}$ now have an index μ from the beginning because the kinetic equation decomposes into separate sets characterized by that index. Again, with ω_μ , $G_{\mu m}$ also ω_μ^* , $G_{\mu m}^*$ is an eigensolution, the latter however corresponding to the ("adjoint") value $-\mu$, as an inspection of (18) shows. So, one can affiliate

$$G_{-\mu m} = G_{\mu m}^*, \quad \omega_{-\mu} = \omega_\mu^*.$$

These form "adjoint pairs" of eigensolutions. Now let us discuss the positiveness of $\text{Re}(\omega_\mu)$. By multiplying (18) with $G_{\mu m}^*$, by summation over m , integration over \mathbf{e} and by adding the conjugate complex, one obtains, again by use of the optical theorem (10)

$$\begin{aligned} (\omega_\mu + \omega_\mu^*) \sum_m \int |G_{\mu m}|^2 d^2 e &= n c \sum_m \sum_{m'} \iint |a_{\mu+m, \mu+m'} G'_{\mu m'} - G_{\mu m} a_{-\mu+m, -\mu+m'}|^2 d^2 e d^2 e' \\ &= n c \sum_m \sum_{m'} \iint |a_{-\mu+m, -\mu+m'} G'_{\mu m'}^* - G_{\mu m}^* a_{\mu+m, \mu+m'}|^2 d^2 e d^2 e'. \end{aligned} \quad (19)$$

Again, the second alternative form of (19) follows by appropriate alternative use of the optical theorem

or simply from the symmetry of the expression in $G_{\mu m}$ and $G_{\mu m}^* = G_{-\mu m}$. The identities (19) are

valid for any fixed value μ ; they are, so to say, the independent parts into which the over-all identities (17) decompose in the high field case. From (19) one infers once more that

$$\omega_\mu + \omega_\mu^* > 0;$$

all the eigenvalues, if discrete, signify exponential decay into equilibrium.

4. Application to Spin-1/2-Particles

In this section the simplest example, namely neutral spin-1/2-particles (e.g. neutrons), is considered. The spin structure of the scattering amplitude is very simple in this case. The spin operator

can occur only linearly. Due to rotational and parity invariance of the interaction the scattering matrix is

$$a(E, \mathbf{e}, \mathbf{e}', \mathbf{s}) = a_0(E, \mathbf{e} \cdot \mathbf{e}') + a_1(E, \mathbf{e} \cdot \mathbf{e}') \mathbf{n} \cdot \mathbf{s}, \quad (20)$$

where

$$\mathbf{n} = \mathbf{e}' \times \mathbf{e} \quad (21)$$

is the vector normal to the scattering plane.

With regard to the special representation chosen in (5) it is useful to decompose the scalar product $\mathbf{n} \cdot \mathbf{s}$ as follows

$$\mathbf{n} \cdot \mathbf{s} = n_z s_z + n_- s_+ + n_+ s_- \quad (22)$$

where $n_z = \mathbf{n} \cdot \mathbf{h}$, $n_\pm = \frac{1}{2}(n_x \pm i n_y)$ and $s_\pm = s_x \pm i s_y$. With the well known matrix elements of s_z, s_+, s_- we get

$$(\mathbf{n} \cdot \mathbf{s})_{MM'} = (\mathbf{n} \cdot \mathbf{h}) M \delta_{MM'} + n_- \delta_{MM'+1} + n_+ \delta_{MM'-1}. \quad (23)$$

All subscripts have to be $\pm \frac{1}{2}$. From Eqs. (13, 20, 23) we obtain the following cross sections

$$\sigma_{MM'}(E, \mathbf{e}, \mathbf{e}', \mathbf{h}) = |a_0 + a_1 \mathbf{n} \cdot \mathbf{h} M|^2 \delta_{MM'} + \frac{1}{4} (\mathbf{n} \cdot \mathbf{n} - (\mathbf{n} \cdot \mathbf{h})^2) |a_1|^2 [\delta_{MM'+1} + \delta_{MM'-1}]. \quad (24)$$

The first term of the r.h.s. of Eq. (24) describes "fully elastic" scattering, the second term is responsible for transitions between the magnetic substates and is important for spin relaxation phenomena. Equation (24) explicitly shows how these special WUB-cross sections depend on scattering geometry and quantization axis.

Finally, as an application of the WUB-equation (12), supplemented by a flow term $\mathbf{e} \cdot \partial / \partial \mathbf{M} / \partial \mathbf{x}$, with the \mathbf{h} -dependent cross sections (24), the heat conduction in the high field limit can be treated. As one infers easily from the first Chapman-Enskog- or the moment equations, indeed only the part of the distribution matrix diagonal in the magnetic quantum numbers is relevant.

For the expansion of the distribution function the following vectors are used:

$$\Phi_\mu^q = \sqrt{3} e_\mu, \quad (25)$$

the average of which is proportional to the heat flux q_μ and

$$\Phi_{\mu, MM}^a = \sqrt{12} M (\mathbf{e} \times \mathbf{h})_\mu \quad (26)$$

the average of which describes a special kind of nonequilibrium velocity-spin-correlation ("azimuthal polarization") typical of spin-1/2-particles. The vectors (25) and (26) are orthogonal and normalized — with respect to the equilibrium distribution $f_0 = N_0 / 8\pi$ (N_0 = equilibrium number den-

sity of the Lorentzian gas; $\sum_M f_0 d^3e = N_0$) — according to

$$\langle \Phi_\mu^q \Phi_\nu^q \rangle_0 = \delta_{\mu\nu}, \quad \langle \Phi_\mu^a \Phi_\nu^a \rangle_0 = \delta_{\mu\nu} - h_\mu h_\nu. \quad (27)$$

With standard techniques (e.g. Chapman-Enskog or the moment method) one obtains for small nonsphericity of the interaction [i.e. $|a_1| \ll |a_0|$ in Eq. (20)] the following expression for the heat flux in the high field limit:

$$q_\mu^\infty = -\lambda_{\text{iso}} [\delta_{\mu\nu} + \omega_{\mu\lambda}^{qa} \omega_{\lambda\nu}^{qa} / (\omega_{\text{sph}}^q \omega_{\text{sph}}^a)] \nabla_\nu T. \quad (28)$$

Here, $\lambda_{\text{iso}} = 5 N_0 k_B^2 T_0 / 2 m \omega_{\text{sph}}^q$ is the heat conductivity for a purely spherical potential. The relaxation coefficients of heat flux and azimuthal polarization in spherical approximation, ω_{sph}^q and ω_{sph}^a , are solely determined by the cross section $\sigma_0 = |a_0|^2$:

$$\omega_{\text{sph}}^q = \omega_{\text{sph}}^a = 2\pi n c \int \sigma_0 (1 - \cos \vartheta) \sin \vartheta d\vartheta, \quad (29)$$

where $\vartheta = \arccos(\mathbf{e} \cdot \mathbf{e}')$ is the angle of deflection. The r.h.s. of (29) also determines the particle diffusion coefficient¹⁰; the heat conduction of the Lorentzian gas consists in "diffusion of energy".

For the calculation of the cross coupling coefficients $\omega_{\mu\lambda}^{qa}, \omega_{\lambda\nu}^{qa}$ which are 2nd rank tensors, the full cross section (24) must be used:

$$\omega_{\mu\lambda}^{qa}(\mathbf{h}) = (3 n c / 4 \pi) \sum_{M, M'} \iint \sigma_{MM'}(E, \mathbf{e}, \mathbf{e}', \mathbf{h}) \cdot (\mathbf{e}_\mu - \mathbf{e}_\mu') M (\mathbf{e} \times \mathbf{h})_\lambda d^2e d^2e'. \quad (30)$$

By inserting (24) into (30) one obtains

$$\omega_{\mu\lambda}^{qa}(\mathbf{h}) = \omega^{qa}(\delta_{\mu\lambda} - h_\mu h_\lambda), \quad (31)$$

where

$$\omega^{qa} = -\pi n c \int \operatorname{Re}(a_0^* a_1) (1 - \cos^2 \vartheta) \sin \vartheta \, d\vartheta. \quad (32)$$

Use of (28), (31) and of the Onsager symmetry

$$\omega_{\lambda r}^{aq} = -\omega_{r\lambda}^{qa} \quad (33)$$

yields the high field heat conductivity tensor

$$\lambda_{\mu\nu}^\infty = \lambda_{\text{iso}} [\delta_{\mu\nu} (1 - A^{qa}) + h_\mu h_\nu A^{qa}], \quad (34)$$

with

$$A^{qa} = (\omega^{qa})^2 / (\omega_{\text{sph}}^q \omega_{\text{sph}}^a) > 0. \quad (35)$$

From (34) one can immediately extract the heat conductivities parallel and perpendicular to the applied field:

$$\lambda_{\parallel}^\infty = \lambda_{\text{iso}}; \quad \lambda_{\perp}^\infty = \lambda_{\text{iso}} (1 - A^{qa}).$$

It should be noticed, however, that the quantities $\Delta\lambda_{\parallel} = \lambda_{\parallel}^\infty - \lambda(H=0)$ and $\Delta\lambda_{\perp}$ determined in the Senftleben-Beenakker experiments cannot be obtained from the WUB-equation (12); the original kinetic equation (1) has to be used to fix the field free value $\lambda(H=0)$. The same is true for the transverse heat conductivity⁷ in the whole range.

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