

ELASTIC SCATTERING OF FAST CHARGED PARTICLES IN A SINGLE CRYSTAL

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Scattering of fast charged particles in a single crystal is investigated as a function of the thickness. In a thin crystal in which the Born approximation is applicable over the crystal as a whole, the scattering is proportional to the square of the coherence length, which is determined exclusively by the kinematics of the process. In the case where perturbation theory is inapplicable to the entire crystal, the scattering decreases substantially as the result of the Glauber shadow effect. In this case a dynamic shortening of the coherence length occurs, which depends on the coupling constant of the potential and the kinematics of the process.

1. INTRODUCTION

IN interaction with atoms of matter, a fast charged particle transfers to the atom a transverse momentum of the order of the inverse screening radius $\kappa = me^2 Z^{1/3}$ ($\hbar = c = 1$), so that the characteristic deflection angles are $\vartheta \sim (\kappa/p) \ll 1$. In the longitudinal direction a momentum $\Delta p_{\parallel} \sim p\vartheta^2 \sim \kappa^2/p$ is transferred to the atom which decreases with increasing particle energy. Therefore in scattering of ultrarelativistic particles large longitudinal distances $(\Delta p_{\parallel})^{-1} \sim p\kappa^{-2}$ are important. As a result of this, in particular, the crystal structure of matter can manifest itself in the scattering even when the particle wavelength λ is much smaller than the lattice constant a , provided that the longitudinal transferred wavelength $(p\vartheta^2)^{-1} > a$.^[1,2] Ter-Mikaelyan^[1] has discussed this effect in detail on the assumption that perturbation theory is valid for scattering over the entire crystal. The condition for considering the potential of the entire crystal U as a perturbation, as is well known, has the form ($\beta = p/E$)

$$\frac{L}{a\beta} \int U_0(x, y, z) dx \ll 1, \quad (1.1)$$

where the x axis is directed along the motion of the particle, U_0 is the potential of an individual atom, and L is the crystal thickness along the x axis. It follows from Eq. (1.1) that the condition of applicability of perturbation theory substantially limits the crystal thickness. A discussion in terms of perturbation theory^[1] showed that atoms located at a length $(p\vartheta^2)^{-1}$ scatter coherently, the cross section increases by a factor L/a in comparison with an amorphous medium, and interference effects appear due to the change in direction of entry into the crystal. We can expect that the relations found will change when we go beyond the framework of perturbation theory. In the opposite case, for example, with increasing crystal thickness, the total cross section for elastic scattering in the crystal would become larger than the geometrical cross section. Actually, following Ter-Mikaelyan^[1], we can obtain the total cross section for elastic scattering in a crystal for particles incident parallel to one of the crystallographic axes

$$\sigma = \sigma_0(L/a)^2 N_{\perp}, \quad (1.2)$$

where σ_0 is the total cross section for elastic scattering by one isolated atom and N_{\perp} is the total number of atoms in a transverse plane; for

$$Ze^2 L/a > 1 \quad (1.3)$$

the cross section becomes greater than geometrical.

Preservation of this situation beyond the limits of applicability of perturbation theory would lead to an absurd result—the number of scattered particles could be greater than the number of incident particles. However, in (1.3) the results of refs. 1 and 2 are not valid, since in the case of (1.3) perturbation theory is inapplicable to scattering in the crystal as a whole^[3]. Therefore it is of interest to investigate the electromagnetic processes in a single crystal as a function of its thickness in the case in which the Born approximation is inapplicable. For this purpose it is convenient to use the well known high-energy approximation^[4,5], which is applicable for crystals which are not too thick. The condition of applicability of this approximation

$$L \ll p(\Delta p)^{-2} \quad (1.4)$$

for high energies is weaker than (1.1). Consideration shows that the scattering relations for fast particles in a single crystal change qualitatively as we go outside the framework of perturbation theory^[3]. This fact can be interpreted as follows.

Coulomb scattering at high energies can be considered as diffraction at the Coulomb center^[6]. As Glauber has shown in discussion of another problem^[5], the existence of the diffraction shadow weakens the scattering by other scatterers if part of the scatterer lies in the region of the diffraction shadow.

If the scatterers are located in a string along the motion of the particle, the superposition of the shadows from several "semitransparent" scatterers forms a "black" shadow and substantially weakens the participation in the scattering of the shadowed scatterers. The coherence length in which the scattering amplitudes from the different scatterers add effectively already cannot be determined by purely mathematical reasoning in this case, as in perturbation theory, but is determined by the dynamics of the process. We discuss below the elastic scattering of fast charged particles in a single crystal in the case where perturbation theory is inapplicable.

2. SCATTERING BY A DIATOMIC MOLECULE

The main features of the effect considered are conveniently studied at first in the simplest example—scattering by a diatomic molecule.

Let the atoms be located at the points $\mathbf{r} = 0$ and $\mathbf{r} = \mathbf{a}$, and the potential of the molecule have the form

$$U_2(\mathbf{r}) = Ze \left\{ \frac{1}{r} \exp(-\kappa r) + \frac{1}{|\mathbf{r} - \mathbf{a}|} \exp(-\kappa |\mathbf{r} - \mathbf{a}|) \right\}. \quad (2.1)$$

If the angle ϑ_0 between the particle momentum \mathbf{p} and the molecule axis \mathbf{a} is small and the condition

$$a \ll p\kappa^{-2} \quad (2.2)$$

is satisfied, the amplitude of scattering by the molecule $f_2(\mathbf{q})$ can be related to the amplitude of scattering by one atom $f_1(\mathbf{q})$ by the equation^[4,5]

$$f_2(\mathbf{q}) = f_1(\mathbf{q}) + f_1(\mathbf{q}) \exp(i\mathbf{q}_\perp \mathbf{a}_\perp) + \frac{i}{2\pi p} \int d^2 s_\perp f_1(s_\perp) f_1(\mathbf{q}_\perp - s_\perp) \exp(is_\perp \mathbf{a}_\perp), \quad (2.3)$$

where \mathbf{a}_\perp is the component of \mathbf{a} perpendicular to \mathbf{p} . Using the optical theorem, we express the cross section for scattering by two centers σ_2 in terms of the single-center cross section σ_1 :

$$\sigma_2 = 2\sigma_1 + \frac{2}{p} \operatorname{Re} \int d^2 s_\perp f_1(s_\perp) f_1(-s_\perp) \exp(is_\perp \mathbf{a}_\perp). \quad (2.4)$$

The real part of the amplitude for scattering by the atom can be represented in the form

$$\operatorname{Re} f_1(\mathbf{q}) = \alpha p (q^2 + \kappa^2)^{-1},$$

and the imaginary part in view of the unitarity condition can be written as

$$\operatorname{Im} f_1(\mathbf{q}) = \frac{i}{4\pi p} \int d^2 l_\perp f_1(l_\perp) f_1^*(l_\perp - \mathbf{q}_\perp).$$

Using the above, we can easily carry out the integration in (2.4), obtaining

$$\sigma_2 = 2\sigma_1 + 2\sigma_1 [(a\kappa\vartheta_0) K_1(a\kappa\vartheta_0)] - \sigma_1 \frac{\alpha^2}{4} \exp\left[-\frac{1}{4}(a\kappa\vartheta_0)^2\right], \quad (2.5)$$

where $K_1(x)$ is the Macdonald function. If the direction of motion of the incident particle coincides with the axis of the molecule ($\vartheta_0 = 0$), then

$$\sigma_2 = 4\sigma_1 - \sigma_1 \alpha^2 / 4. \quad (2.6)$$

In the Born approximation the second term should be dropped, and the result coincides with that obtained by Ter-Mikaelyan^[1]. Departure from perturbation theory leads to weakening of the scattering, and the weakening increases with increasing coupling constant α . The weakening of the scattering can be interpreted as the result of incidence of the second atom in the region of the diffraction shadow from the first atom. With increasing α the shadow becomes deeper and the scattering cross section decreases.

In order to confirm the interpretation proposed, let us consider the limiting case of strong coupling—diffraction by two impenetrable spheres of radius R_0 located at the points $\mathbf{r} = 0$ and $\mathbf{r} = \mathbf{a}$, where $a \ll pR_0^2$ and the angle ϑ_0 between the incident-particle momentum \mathbf{p} and \mathbf{a} is small. In this case the total scattering cross section is

$$\sigma_{\text{tot}} = \sigma_1 \left\{ 1 + \frac{2}{\pi} [\arcsin(aR_0^{-1} \sin\vartheta_0) + aR_0^{-1} \sin\vartheta_0 \times (1 - (aR_0^{-1} \sin\vartheta_0)^2)^{1/2}] \Theta(1 - aR_0^{-1} \sin\vartheta_0) + \Theta(aR_0^{-1} \sin\vartheta_0 - 1) \right\}, \quad (2.7)$$

where

$$\Theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0 \end{cases} \quad \sigma_1 = 2\pi R_0^2.$$

Thus, in the case discussed of diffraction scattering, the shadow effect^[4] has completely suppressed the interference. This leads to the result that at zero entrance angle $\vartheta_0 = 0$ the total scattering cross section is equal to the cross section for scattering by a single center, and the second center does not participate in the scattering, since it is in the region of the diffraction shadow.

3. SCATTERING BY A STRING OF ATOMS

If perturbation theory is applicable for scattering by an isolated atom, then the shadowing of the next atom is small. However, in scattering by a linear string of atoms the superposition of relatively weak shadows from several atoms can lead to a deep shadow^[3]. In fact, for $N \ll p/\kappa^2 a$ the effective coupling constant is NZe^2 , which should lead to a substantial shadow effect on the scattering process. Therefore it is interesting to consider elastic scattering in the case of motion of a particle along the string axis. Let N atoms be located at the points $\mathbf{R}_n = n\mathbf{a}$ ($n = 0, 1, 2, \dots, N-1$) and $Na \ll p\kappa^{-2}$. In this case the high-energy approximation^[4] is valid, from which an explicit form follows for the amplitude of scattering of a particle by the entire chain of atoms:

$$f_N(\mathbf{q}) = ip \int_0^\infty J_0(qb) b db \left\{ 1 - \exp\left[-\frac{i}{\beta} \int_{-\infty}^{+\infty} U(\mathbf{b}, x) dx\right] \right\}, \quad (3.1)$$

where $J_0(x)$ is a Bessel function and

$$U(\mathbf{r}) = \sum_n U_0(\mathbf{r} - \mathbf{R}_n)$$

where the summation is carried out over all the atoms of the string. The applicability of Eq. (3.1) is limited to not too large scattering angles

$$\vartheta < (\kappa/p)^{1/2}. \quad (3.2)$$

It should be noted that condition (3.2) permits using (3.1) over practically the entire region of effective angles. The potential of an individual atom is the screened Coulomb potential, so that

$$U(\mathbf{r}) = \sum_{n=0}^{N-1} \frac{\alpha}{|\mathbf{r} - \mathbf{R}_n|} \exp(-\kappa |\mathbf{r} - \mathbf{R}_n|), \quad (3.3)$$

where $\alpha \equiv Ze^2$.

Substitution of (3.3) into (3.1) and integration gives

$$f_N(\mathbf{q}) = ip \int_0^\infty J_0(qb) b db \left\{ 1 - \exp\left[-i \frac{2N\alpha}{\beta} K_0(b\kappa)\right] \right\}. \quad (3.4)$$

Let us discuss first the case of a rather long string for which

$$\alpha^{-1} \ll N \ll (p/\kappa)(\kappa a)^{-1}. \quad (3.5)$$

In this case we can use asymptotic methods to evaluate the integral. In fact, using the stationary-phase method^[7] we can calculate the explicit form of (3.4). Thus, for

$$\mathcal{L} \equiv \frac{q}{\kappa} \ln \frac{N\alpha}{\beta} < 1$$

we obtain

$$f_N(\mathbf{q}) = i \frac{p}{\kappa} \left[\ln \left(2N\alpha \frac{\sqrt{V\pi}}{\beta} \right) + i \frac{\pi}{2} \right].$$

$$\times \left\{ q^{-1} J_1 \left[\frac{q}{\kappa} \ln \left(2N\alpha\gamma \frac{\sqrt{\pi}}{\beta} \right) + i \frac{\pi}{2} \right] \right\}, \quad (3.6)$$

where $\gamma = e^C \approx 1.781\dots$ and C is Euler's constant.

In the case $\mathcal{L} > 1$ the stationary-phase method gives the following expression for the scattering amplitude.

$$f_N(q) = -i \frac{p}{\kappa} \left(\ln \frac{2N\alpha\kappa}{\beta q} \right)^{1/2} \exp \left[-i \frac{q}{\kappa} \ln \frac{2N\alpha\kappa}{\beta q} \right] / q. \quad (3.7)$$

Using the optical theorem and Eqs. (3.4) or (3.6), we can determine the total cross section for elastic scattering by a long string of atoms for the condition (3.5),

$$\sigma = \frac{2\pi}{\kappa^2} \left\{ (\ln A)^2 + (\ln A) \left[\frac{3}{4} + 2 \operatorname{ci}(1) - \frac{\sin A}{A} \right] \right\}, \quad (3.8)$$

where $\operatorname{ci}(x)$ is the cosine integral, and

$$A = 2 \frac{Ze^2}{\beta} N \left[\pi/2 \ln \left(2N \frac{Ze^2}{\beta} \right) \right]^{1/2}.$$

The total cross section for elastic scattering (3.8) can be obtained also as the result of integration of the square of the modulus of the scattering amplitude (3.6) over angle. The structure of the formulas obtained is similar to that of the formulas for diffraction by a semitransparent object. This similarity confirms the interpretation of the results as the consequence of superposition of shadows from several atoms. The "blackness" of the total shadow (and consequently also the transparency of the chain) is determined by the parameter $N\alpha$. In the limiting case $N\alpha \gg 1$ to which Eqs. (3.6)–(3.8) refer, the string becomes practically opaque for particles incident parallel to its axis. The dependence of the scattering cross section on the number of particles becomes very weak—the parameter $N\alpha$ enters into the result only in the argument of a logarithm. This is explained by the fact that the atoms at the end of the chain which fall in the deep shadow region play practically no part in the scattering.

If the amplitudes for scattering of a particle by different atoms located in a segment of this string of length l are effectively added, then the length l can be called the coherence length. For N atoms located in a coherence length, the scattering cross section is

$$d\sigma_N(\vartheta) = d\sigma_1(\vartheta) (l/a)^2$$

(for $L \equiv Na < l$ it is necessary to replace l by L), where a is the distance between atoms and $d\sigma_1$ is the scattering cross section of a single atom. In perturbation theory the coherence length is determined by kinematic considerations and is equal to $(p\vartheta^2)^{-1}$. However, generally speaking, the coherence length is determined by the dynamic relations. In the case discussed we can conclude that the coherence length is shortened, $l \sim a/\alpha$, i.e., atoms located up to the place of formation of the black shadow take part in the scattering. In other words, the length $l \sim a/\alpha$ represents that length in which the coherently scattering atoms form a potential with an effective interaction strength of the order of unity.

It should be emphasized that the results obtained for the total and differential scattering cross sections (3.6)–(3.8) are practically independent of the specific form of the atomic potential—the results depend exclusively on the effective interaction radius κ^{-1} .

In the opposite limiting case, $N\alpha \ll 1$, the cross section for scattering by a string of atoms can be discussed on the basis of perturbation theory. Expanding

the exponent in Eq. (3.4) in series, we obtain results which agree with ref. 1, i.e., are proportional to $(L/a)^2$.

In the intermediate case, $\alpha N \sim 1$, the integral (3.4) was calculated numerically. Using Eq. (3.4) and the optical theorem, we can represent the total scattering cross section in the form

$$\sigma = \frac{4\pi}{\kappa^2} \operatorname{Re} \int_0^\infty dx x (1 - \exp[-i \cdot 2A_0 K_0(x)]), \quad (3.9)$$

where $A_0 \equiv N\alpha/\beta$ is a parameter characterizing the coupling constant. By numerical integration methods we obtained the following dependence of the total cross section on the parameter A_0 :

$$\frac{\sigma}{4\pi/\kappa^2} = \varphi(A_0).$$

For A_0 equal to 0.1, 0.2, 0.6, 1, 2, 4, 8, 10, 20, 40, 10^2 , and 10^3 , the numerical values of the function $\varphi(A_0)$ are respectively 0.995×10^{-2} , 0.390×10^{-1} , 0.292, 0.630, 1.41, 2.58, 4.15, 4.74, 6.86, 9.40, 13.4, and 26.9.

It follows from the values given that for small A_0 the total cross section is proportional to A_0^2 , and for large A_0 it is described by Eq. (3.8).

4. SCATTERING IN A SINGLE CRYSTAL

Let us consider now a single crystal bounded by the planes $x = 0$ and $x = L$, assuming $L \ll p\kappa^{-2}$. The number of atoms in a string coinciding with the direction of motion of the particle will depend on the direction of incidence of the particle. Let us first consider the case in which the particle is incident along the crystallographic x axis. In this case the formulas for the cross section in a single crystal differ from (3.4)–(3.8) only in the fact that the result still involves the number of atoms of the crystal in the yz plane, N_\perp ; this is due to the fact that scattering occurs independently in the different strings, since the transverse effective dimensions, which are important for scattering, are determined by the radius of action of the potential κ^{-1} . Thus, we obtain from Eqs. (3.6) and (3.8) the coherent part of the cross section

$$\frac{d\sigma}{d\Omega} = \frac{N_\perp}{\kappa^2} \ln^2 \left(2 \frac{N\alpha}{\beta} \gamma \sqrt{\pi} \right) \frac{J_1^2 [2p \sin(\vartheta/2) \kappa^{-1} \ln(2N\alpha\gamma\sqrt{\pi}/\beta)]}{4 \sin^2(\vartheta/2)}, \quad (4.1)$$

$$\sigma = 2N_\perp \frac{\pi}{\kappa^2} \ln^2 \left(2 \frac{N\alpha}{\beta} \gamma \sqrt{\pi} \right). \quad (4.2)$$

It is important that Eqs. (4.1)–(4.2) are valid only in the case in which we can neglect the effect of thermal vibrations of the atoms of the crystal lattice. This places an upper limit on the longitudinal dimension $L_\parallel = Na_x$ of the crystal by the condition

$$L \ll \frac{a_0 \kappa^2 \ln^2(N\alpha\gamma\sqrt{\pi}/\beta)}{a^2 \bar{u}^2}, \quad (4.3)$$

where \bar{u}^2 is the mean square thermal displacement of the atom. As the direction of incidence of the particle changes, the number of atoms along the direction of incidence N_\parallel varies with the entrance angle ϑ_0 . In the limiting case $N(\vartheta_0)\alpha \gg 1$ the cross section varies weakly as a function of the entrance angle, and in the opposite limiting case $N(\vartheta_0)\alpha \ll 1$ it varies rapidly in accordance with the results of Ter-Mikaelyan^[1].

As the entrance angle ϑ_0 changes, the directions along which the greatest number of atoms $N(\vartheta_0)$ are

located alternate with directions along which a small number of atoms are located. Therefore the interference nature of the scattering cross section is preserved as the entrance angle varies. However, the peaks in the scattering cross section will be substantially smaller than predicted by Ter-Mikaelyan's theory^[1] in the case where $N(\vartheta_0)\alpha \gg 1$. The minima in the scattering cross section correspond to the case $N(\vartheta_0)\alpha \ll 1$ and therefore do not change essentially. The Ter-Mikaelyan interference effect is preserved in pure form only in sufficiently thin single crystals whose thickness is limited by use of the Born approximation: $L \ll a/Ze^2$. A detailed discussion of the interference effect with inclusion of the shadow effect will be given separately.

Thus, excursion beyond the limits of perturbation theory qualitatively changes the nature of fast charged particle scattering in a single crystal.

5. SCATTERING AT LARGE ANGLES

The expressions obtained above for the scattering amplitude are valid in the region of small scattering angles. It follows from Eq. (3.7) that the amplitude falls off with increasing momentum transfer as q^{-1} . However, this change in amplitude occurs only up to angles $\vartheta \lesssim \sqrt{\kappa/p}$. For further increase of the scattering angle the effective impact parameters decrease and the amplitude $f(q)$ falls more rapidly. Therefore it is of interest to study the dependence of the coherence length on momentum transfer. We will write the expression for the scattering amplitude of fast particles at not too small angles ($\vartheta > \sqrt{\kappa/p}$) in the high-energy approximation^[4]

$$f(q) = -\frac{E}{2\pi} \int d^3r \exp(-iqr) U(r) \times \exp \left\{ -\frac{i}{\beta} \left[\int_0^{\infty} ds U(r - n_1 s) + \int_0^{\infty} ds U(r + n_2 s) \right] \right\} \quad (5.1)$$

where $n_1 \equiv p_1/p$, $n_2 \equiv p_2/p$.

We will calculate the explicit form of the amplitude $f(q)$ for scattering angles $\vartheta > \sqrt{\kappa/p}$ in the case where the incident-particle momentum is parallel to the axis of an atomic string of length L :

$$f(q) = f_0(q) \sum_a \exp \left\{ i \left[\frac{q^2}{2p} X_a + \frac{2a}{\beta} \frac{X_a}{a} \ln \frac{\kappa Y}{q} \right] \right\} \times \exp \left\{ i\pi \left(1 + i \frac{\alpha}{\beta} \frac{X_a}{a} \right) \right\} \left\{ \Gamma \left(1 + i \frac{\alpha}{\beta} \frac{X_a}{a} \right) \right\}^2, \quad (5.2)$$

where $\Gamma(z)$ is the Γ function, X_a is coordinate of the atom at a and $f_0(q)$ is the amplitude for scattering by a single isolated atom.

For effective addition of the amplitudes for scattering by different atoms, both the kinematic and dynamic conditions for constructive interference must be satisfied. Therefore the coherence length is determined by the lesser of the two lengths, taking into account these conditions,

$$l \sim \min \{l_k, l_d\}. \quad (5.3)$$

Summation over the atoms of the string permits us to find

$$l_k = \frac{2p}{|p_1 - p_2|^2}, \quad l_d = a \left[\frac{Ze^2}{\beta} \ln \frac{|p_1 - p_2|}{\kappa} \right]^{-1}. \quad (5.4)$$

As we should expect, both l_k and l_d decrease with increasing momentum transfer. In addition, it must be emphasized that for $Ze^2 \rightarrow 1$, intense scattering occurs already at the first atom, giving a deep shadow, and the remaining atoms hardly take part in the interference.

In the case where $2p/|p_1 - p_2|^2 < a$, scattering by the atoms of the string occurs independently, and if perturbation theory is valid, i.e., $LZe^2/a < 1$, then the probabilities of electromagnetic processes are proportional to the string length L . If perturbation theory is inapplicable, $LZe^2/a > 1$, then the cross section for scattering at large angles is proportional to the number of atoms located in the dynamic length (5.4), i.e.,

$$\frac{d\sigma}{d\Omega} \sim \left[\frac{Ze^2}{\beta} \ln \frac{|p_1 - p_2|}{\kappa} \right]^{-1}. \quad (5.5)$$

The expression (5.2) obtained for the scattering amplitude permits a quantitative description of the shadow effects occurring in scattering of fast charged particles in single crystals^[5].

It is easy to calculate by means of Eq. (5.2) the mean square deviation angle of a particle after traversal of a thin single-crystal layer of thickness L . For thin layers in the case of particle incidence along a crystallographic axis, $L \ll a\beta/Ze^2$, we have the formula

$$\langle \vartheta^2 \rangle = 4\pi N_{\perp} (2Ze^2/p\beta)^2 \ln(210Z^{-1/2}) (L/a)^2, \quad (5.6)$$

which agrees with the result obtained by Ter-Mikaelyan^[1].

For thicker layers with thickness

$$a\beta/Ze^2 \ll L \ll p\kappa^{-2} \quad (5.7)$$

the mean square deviation angle is no longer dependent on the thickness of the layer and is determined by the relation

$$\langle \vartheta^2 \rangle \approx 4\pi N_{\perp} (2Ze^2/p\beta)^2 \{ \ln \ln(210Z^{-1/2}) \} \xi, \quad (5.8)$$

where $\xi = (\beta/2Ze^2)^2$ if $Ze^2/\beta \ll 1$ and $\xi = 1$ for $Ze^2/\beta \gg 1$.

It must be emphasized that the use of perturbation theory for charged particle scattering in a single crystal in the thickness range (5.7) leads to a result exaggerated by a factor $(L/l_d)^2$, as the result of the dynamic shortening of the coherence length in the region where perturbation theory is inapplicable.

The results obtained refer to the case of particle incidence strictly along a crystallographic axis. In the general case of interference scattering in a single crystal the effect of dynamic shortening of the coherence length limits the cross-section value in directions coinciding with the crystallographic axes.

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