

# ON A MODEL OF CONTINUOUS MEDIUM, TAKING INTO ACCOUNT THE MICROSTRUCTURE

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A method of constructing a continuous medium possessing certain discrete structural properties which is given here, is based on a micromodel of a linear chain. The method yields the spectrum of the initial discrete system with sufficient accuracy, even in the long wave approximation. The dynamics of the constructed continuous medium is described by the equations of displacement of the center of mass of a macrocell and by the equations of moments of various orders. The spectrum of this medium tends to the complete spectrum of a linear chain (for both, a simple and a complex chain) with increasing number of moments.

1. Let us consider a simple, linear chain with period  $a$ . Equations of motion are given by

$$ms_{\mu}'' = \sum_{\nu} C_{\mu\nu} (s_{\nu} - s_{\mu}) \quad \left( s_{\mu}'' \equiv \frac{d^2 s_{\mu}}{dt^2} \right) \quad (1.1)$$

where  $s_{\mu}$  is the displacement of the particle  $\mu$  from its equilibrium position and  $C_{\mu\nu}$  are force constants characterizing the interaction between the particles  $\mu$  and  $\nu$ . For two adjacent particles, these equations have the form

$$ms_{\mu}'' = C (s_{\mu-1} - 2s_{\mu} + s_{\mu+1}) \quad (1.2)$$

Another method of approach consists of forming macrocells from groups of  $N$  adjacent atoms; particle  $\mu$  will then belong to the  $r$ -th macrocell and will be assigned an index  $n$  such, that

$$\mu = N(r-1) + n, \quad x_{\mu} \equiv x_r^n = aN(r-1) + an \quad (1.3)$$

Then the system (1.2) can be rewritten as follows:

$$ms_r'' = C (s_r^{n+1} - 2s_r^n + s_r^{n-1}) \quad (n = 1, \dots, N) \quad (1.4)$$

$$(s_r^0 \equiv s_{r-1}^N, s_r^{N+1} \equiv s_{r+1}^1)$$

while the general system (1.1) will assume the form

$$ms_r'' = \sum_{nk} C_{nk}^{r,\nu} (s_{r\nu}^k - s_r^n) \quad (1.5)$$

It is known from [1] that using the normal modes of oscillation

$$s_r^n = A \exp i(kx_r^n - \omega t) \quad (1.6)$$

of Eqs. (1.1) we can find the spectral curve

$$\omega = \varphi(k), \quad 0 \leq k \leq 2\pi/a \quad (1.7)$$

Function  $\varphi(k)$  is even with respect to the axes  $k = 0, \pi/a, 2\pi/a, \dots$ . In particular, when we have (1.4) and  $N = 2$

$$\varphi(k) = \sqrt{4C/m} |\sin^{1/2} ka| \quad (1.8)$$

The spectral curve (1.7) can be constructed by specular reflections of the multivalued curve

$$\omega = \varphi_p(k_1), \quad 0 \leq k_1 \leq 2\pi/aN \quad (1.9)$$

defined on a shortened interval.

Let now the value  $k = k_p$  given by

$$k_p = \frac{2\pi p}{aN} - k_1 \quad (p = 2\nu), \quad k_p = \frac{2\pi p}{aN} + k_1 \quad (p = 2\nu + 1) \tag{1.10}$$

correspond to each value  $k_1$  from (1.9), with  $p$  fixed. Using these values for  $k_p$  we obtain from (1.6)

$$s_r^n = A \exp(i2\pi pn / N) \exp(i(\mp k_1 x_r^n - \omega t)) \tag{1.11}$$

Inserting now (1.11) into (1.5), we obtain a specific spectral curve (1.7) for each value of  $p$ . When  $k_1$  is connected with  $k_p$  by the relation (1.10), we can also use (1.9) to obtain the values of the frequencies  $\omega$  in (1.7) for any  $k_p$ , i. e. we have

$$\varphi(k_p) = \varphi_p(k_1), \quad 0 \leq k_1 \leq 2\pi / aN \quad (k_p = 2\pi p / aN \mp k_1) \tag{1.12}$$

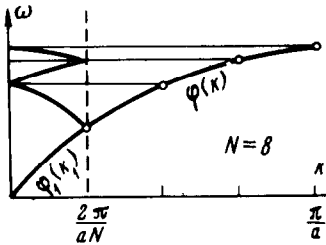


Fig. 1

These relations represent the law of specular reflection (see Fig. 1). When the fixed value of  $p$  is even, the curve  $\varphi_p(k_1)$  is reflected with respect to the axis  $\bar{k} = 2\pi / aN$  and transferred to the corresponding interval of the values of  $k_p$ . When  $p$  is odd, the curve  $\varphi_p(k_1)$  is transferred directly onto its interval of the values of  $k_p$ . We note that for odd values of  $N$ , the curve  $\varphi(k)$  transforms into itself on the interval

$$\frac{\pi}{a} \left(1 - \frac{1}{N}\right) \leq k_p \leq \frac{\pi}{a} \left(1 + \frac{1}{N}\right)$$

In this manner we construct the whole of the function  $\varphi(k)$  on the interval from 0 to  $2\pi / a$ .

This fact, although unessential in the study of discrete systems, becomes important when the couple-stress mechanics is constructed for continuous medium using long wave approximations. In the latter case the curves  $\varphi_p(k_1)$  on the interval  $0 \leq k_1 \leq 2\pi/aN$  can be replaced by the tangents to them at the point  $k_1 = 0$  if the number of particles included in a macrocell is sufficiently large.

Let us now replace the system of point functions  $s_r^n(t)$  with a system of  $N$  continuously differentiable functions  $s_n(x, t)$  of the coordinate and time coinciding with  $s_r^n$  at the points  $x = x_r^n$  and satisfying the system of equations obtained from (1.5) by the formal transition to the continuous form. We can see from (1.4), that in the particular case of a short-range interaction, these equations assume the form

$$ms_n'' = C[s_{n+1}(x+a) - 2s_n(x) + s_{n-1}(x-a)] \quad (n = 1, \dots, N) \tag{1.13}$$

$$s_0(x-a) \equiv s_N(x-a), \quad s_{N+1}(x+a) \equiv s_1(x+a)$$

Setting now  $s_r^n = A_n \exp i(kx_r^n - \omega t)$  (1.14)

$$s_n = B_n \exp i(kx - \omega t)$$

and inserting (1.14) into (1.4) and (1.13), respectively, we find that the corresponding secular equations coincide. This means that the spectrum of continuous medium described by Eqs. (1.13) and the spectrum of the initial linear chain coincide completely.

Let  $\nu$  denote the number of interacting particles. If we limit ourselves to second order derivatives in the expansion of  $s_i(x \pm \nu a)$  near the point  $x$  (long wave approximation), then the spectrum of (1.13) will obviously consist of the tangents to the corresponding curves  $\varphi_p(k_1)$  for  $k_1 = 0$  and, as shown above, the set of these tangent lines will tend to the complete spectrum of a discrete system with increasing number  $N$  of particles incorporated in the macrocell.

A continuous medium with a more accurate spectrum can be obtained in a similar manner proceeding from a complex linear chain whose cell consists of two different particles of masses  $m_1$  and  $m_2$  with a period  $a$ , and taking into account the interaction of the adjacent cells (\*). Equations of motion of such a system have the form

$$\begin{aligned}
 m_1 s_r^{1''} &= C_1 (s_r^2 - s_r^1) + C_2 (s_{r-1}^2 - s_r^1) + C_3 (s_{r+1}^1 - 2s_r^1 + s_{r-1}^1) + C_4 (s_{r-1}^2 - s_r^1) \quad (1.15) \\
 m_2 s_r^{2''} &= C_1 (s_r^1 - s_r^2) + C_2 (s_{r+1}^1 - s_r^2) + C_3 (s_{r+1}^2 - 2s_r^2 + s_{r-1}^2) + C_4 (s_{r-1}^1 - s_r^2)
 \end{aligned}$$

where  $r$ , as before, denotes the number of the cell and  $C_i$  ( $i = 1, 2, 3, 4$ ) are the constants of interaction. Let us combine the groups of  $N$  adjacent cells into macrocells and re-number the particles (in the place of  $r$  and  $n = 1, 2$  we introduce the macrocell number  $R$  and the number  $\mu = 1, 2 \dots 2N$ ) denoting a particle in the macrocell) so, that

$$\begin{aligned}
 2r + (n - 2) &= 2 N(R - 1) + \mu \quad (1.16) \\
 x_r^n &= ar + x^n, \quad x^1 = 0, \quad x^2 = b \\
 x_R^\mu &= aNR + x^\mu, \quad x^\mu = \begin{cases} 1/2 (\mu - 2) a + b, & \mu \text{ even} \\ 1/2 (\mu - 1) a, & \mu \text{ odd} \end{cases}
 \end{aligned}$$

Then in place of (1.15) we have

$$\begin{aligned}
 m_{1,2} s_R^{\mu''} &= C_1 (s_R^{\mu \mp 1} - s_R^\mu) + C_2 (s_R^{\mu \mp 1} - s_R^\mu) + C_3 (s_R^{\mu+2} - 2s_R^\mu + \\
 &\quad + s_R^{\mu-2}) + C_4 (s_R^{\mu \pm 3} - s_R^\mu) \\
 \mu = 1, 2, \quad s_R^0 &\equiv s_{R-1}^{2N}, \quad s_R^{-1} \equiv s_{R-1}^{2N-1} \quad (1.17) \\
 \mu = 2N - 1, 2N, \quad s_R^{2N+1} &= s_{R-1}^1, \quad s_R^{2N+2} \equiv s_{R-1}^2
 \end{aligned}$$

Considering now the solution of (1.15) in the form of (1.6) where the wave vector is  $0 \leq k \leq 2 \pi / a$ , we obtain from (1.15) the spectral curves

$$\omega = \varphi_1(k), \quad \omega = \varphi_2(k) \quad (1.18)$$

The same frequencies can also be found using the method given above, from two multivalued curves defined on a shortened interval

$$\omega = \varphi_{1p}(k_1), \quad \omega = \varphi_{2p}(k_1), \quad 0 \leq k_1 \leq 2\pi / aN \quad (1.19)$$

provided that a corresponding value of  $k_p$  given by (1.10) is taken for each  $k_1$ , with the value of  $p$  fixed.

In this case the substitution of

$$s_r^n = A_n \exp i (\mp k_1 x_r^n - \omega t) \exp i \frac{2\pi p}{N} (\mu - 2N - 1) \quad (n = 1) \quad (1.20)$$

$$s_r^n = A_n \exp i (\mp k_1 x_r^n - \omega t) \exp i \frac{2\pi p}{N} \left( \frac{b}{a} - \frac{2N - \mu}{2} \right) \quad (n = 2)$$

into (1.15) yields the curves (1.19) such, that

$$\varphi_{1p}(k_1) = \varphi_1(k_p), \quad \varphi_{2p}(k_1) = \varphi_2(k_p) \quad (1.21)$$

i. e. the same law of specular reflection is observed in constructing  $\varphi_1$  and  $\varphi_2$  in terms of  $\varphi_{1p}$  and  $\varphi_{2p}$ . Passing further  $k_1$  the field, i. e. replacing  $s_r^n(t)$  with continuously differentiable  $s_\mu = s_\mu(x, t) |_{x=x_R^\mu} = s_R^\mu(t)$  we shall require that the latter satisfy the following system of equations:

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\*) This formulation is made for the sake of simplicity.

$$\begin{aligned}
 m_1 s_\mu'' &= C_1 [s_{\mu+1}^c(x+b) - s_\mu(x)] + C_2 [s_{\mu-1}(x-b+a) - s_\mu] + \\
 &+ C_3 [s_{\mu+2}(x+a) - 2s_\mu + s_{\mu-2}(x-a)] + C_4 [s_{\mu+3}(x+a+b) - s_\mu] \\
 &\mu = 1, 3 \dots 2N - 1 \tag{1.22} \\
 m_2 s_\mu'' &= C_1 [s_{\mu-1}(x-b) - s_\mu(x)] + C_2 [s_{\mu+1}(x+b-a) - s_\mu] + \\
 &+ C_3 [s_{\mu+2}(x+a) - 2s_\mu + s_{\mu-2}(x-a)] + C_4 [s_{\mu-3}(x-a-b) - s_\mu] \\
 &\mu = 2, 4 \dots 2N
 \end{aligned}$$

It is easily verified that the secular equations for (1.17) and (1.22) coincide. Consequently, for the continuous medium corresponding to a complex linear chain, the spectrum in the long wave approximation will also consist of tangents to  $\varphi_{1p}(k_1)$  and  $\varphi_{2p}(k_1)$  at the point  $k_1 = 0$ . When the values of  $N$  are large, the set of these tangents will describe the complete spectrum of the discrete system with sufficient accuracy. The present method can naturally be extended to spatially periodic structures. When the number of particles included in a macrocell becomes sufficiently large, the corresponding field equations of motion will reflect the dynamic microstructural properties of the medium.

2. The classical theory of elasticity based on the concepts of mean density, mean velocity and mean displacement together with those of stress and deformation tensors appears, from our point of view, to represent a long wave approximation, and can only yield information on the motion of the centers of mass of the macrocells. Couple-stress theory of elasticity on the other hand, introduces phenomenological field concepts (internal moments), thus giving a more complete description of the behavior of a solid body and, apparently, gives an entire and correct description of the behavior of a system of particles in the acoustic range of the spectrum [2]. However, the couple-stress theory of elasticity takes into account the oscillations which also pertain to the optical branch of the spectral curve [3]. It seems therefore appropriate to employ yet another approach to constructing the latter theory, containing a more accurate description of the motion of the macrocells.

Let us consider a complex linear chain of period  $l$ , each of its cells containing  $N$  different particles. We shall assume the interaction to be such, that the corresponding series and expansions of the potential energy converge. Equation of motion of the  $n$ -th particle in the  $r$ -th cell has the form

$$\begin{aligned}
 m_n s_r^n &= \sum_{p, k} C_{nk}^{r, r+p} (s_{r+p}^k - s_r^n) = C \sum_{r, k} \alpha_{nk}^{r, r+p} (s_{r+p}^k - s_r^n) \\
 C &\equiv C_1 r_2^r, \quad \alpha_1 r_2^r = 1
 \end{aligned} \tag{2.1}$$

Here  $\alpha_{nk}^{r, r+p}$  are the dimensionless interaction constants, possessing the following properties:

$$\begin{aligned}
 \alpha_{nk}^{r, r+p} &= \alpha_{kn}^{r+p, r}, \quad \alpha_{nn}^{r, r+p} = \alpha_{nn}^{r, r-p} \\
 \sum_{n, p} \alpha_{nk}^{r, r+p} &= \sum_{k, p} \alpha_{nk}^{r, r+p} = 0
 \end{aligned} \tag{2.2}$$

Instead of the absolute displacements  $s_r^n$  of each particle of the cell, we shall now consider the relative displacements  $u_r^n$  and the displacement  $s_r$  of the center of mass of the cell. The coordinate  $x_r$  of the center of mass of a cell is, as usually, given by

$$x_r = \frac{1}{M} \sum_{n=1}^N m_n x_r^n = \sum_{n=1}^N \mu_n x_r^n \tag{2.3}$$

$$M = \sum_{n=1}^N m_n, \quad \sum_{n=1}^N \mu_n = 1$$

Here  $x_r^n$  denotes the absolute coordinate of the  $n$ -th particle in the  $r$ -th cell. The absolute displacement  $s_r^n$  is given by

$$s_r^n = s_r + u_r^n, \quad s_r = x_r - X_r = x_r - \sum_{n=1}^N \mu_n X_r^n \tag{2.4}$$

where  $X_r^n$  is the equilibrium position of the  $n$ -th particle in the  $r$ -th cell. From (2.3) follows

$$\sum_{n=1}^N \mu_n u_r^n = 0 \tag{2.5}$$

Let us obtain a set of  $N - 1$  linearly independent variables for each  $r$ . We shall call them moments and assume them to be relative to the center of mass of the  $r$ -th cell

$$m_r^k = \sum_{n=1}^N \mu_n u_r^n (\xi^n)^k \quad (k = 0, 1, \dots, N - 1) \tag{2.6}$$

Here  $\xi^n$  is the equilibrium coordinate of the  $n$ -th particle relative to the center of mass of the cell (due to symmetry of the chain in its equilibrium position  $\xi^n$  is independent of the cell number). From (2.5) we see that  $m_r^0 = 0$ . Solving the set of linear equations (2.6) for  $\mu_n u_r^n$ , we obtain

$$u_r^n = \frac{1}{\mu_n} \sum_{k=1}^{N-1} \beta_{nk} m_r^k \tag{2.7}$$

The matrices  $\beta_{nk}$  are minors of the determinant related to  $D$

$$D = \begin{vmatrix} 1 & 1 & \dots & 1 & 1 \\ \xi^1 & \xi^2 & \dots & \xi^{N-1} & \xi^N \\ (\xi^1)^2 & (\xi^2)^2 & \dots & (\xi^{N-1})^2 & (\xi^N)^2 \\ \dots & \dots & \dots & \dots & \dots \\ (\xi^1)^{N-1} & (\xi^2)^{N-1} & \dots & (\xi^{N-1})^{N-1} & (\xi^N)^{N-1} \end{vmatrix} \tag{2.8}$$

Mechanical meaning of the moments introduced above can be ascertained from the kinetic energy expressions  $T_r$  and from the moment of momentum of various orders  $Q_r^k$  of the cell. On the grounds of (2.6) we have

$$T_r = \frac{M}{2} \left[ \sum_{n,k} b_{nk} m_r^n m_r^{k*} + s_r^* \right], \quad b_{nk} = \sum_{i=1}^N \frac{\beta_{in} \beta_{ik}}{\mu_i} \tag{2.9}$$

$$Q_r^k = \sum_{i=1}^N m_i u_r^{i*} (\xi^i)^k = M m_r^{k*}$$

Expression for the kinetic energy density in terms of an additional parameter ("micro-distortion") which usually appears in the couple-stress theory of elasticity, follows from (2.9) on the transition to the field functions, with only the first moment taken into account,

Using (2.3) and (2.4) we obtain an equation for  $s_r$  by performing summation of (2.1) over  $n$  and taking into account (2.6) with (2.7)

$$\begin{aligned}
 Ms_r'' &= CF_r \\
 F_r &= \sum'_p \left[ \alpha^{r, r+p} (s_{r+p} - s_r) + \sum_{k=1}^{N-1} (\alpha_k^{r, r+p} m_{r+p}^k - \alpha_k^{r+p, r} m_r^k) \right] \\
 \alpha^{r, r+p} &= \sum_{n, k=1}^N \alpha_{n, k}^{r, r+p}, \quad \alpha_k^{r, r+p} = \sum_{n, l=1}^N \alpha_{nl}^{r, r+p} \frac{\beta_{lk}}{\mu_l}
 \end{aligned} \tag{2.10}$$

Equations for  $m_r^k$  are obtained by multiplying (2.1) by  $(\xi^n)^k$ , summing over  $n$  and utilizing (2.6), (2.7) and (2.10)  $Mm_r^{k''} = C\Phi_r^k$

$$\begin{aligned}
 \Phi_r^k &= \sum'_p \gamma_k^{r, r+p} (s_{r+p} - s_r) + \sum_{q=1}^{N-1} m_r^q \rho_{qk}^r + \sum'_{p, q} \gamma_{qk}^{r, r+p} m_{r+p}^q \\
 \gamma_k^{r, r+p} &= \sum_{n, l=1}^N \alpha_{nl}^{r, r+p} \left[ (\xi^n)^k - \sum_{q=1}^{N-1} \mu^q (\xi^q)^k \right]
 \end{aligned} \tag{2.11}$$

$$\gamma_{qk}^{r, r+p} = \sum_{i, j=1}^N \alpha_{ij}^{r, r+p} \frac{\beta_{jq}}{\mu_j} \left[ (\xi^i)^k - \sum_{n=1}^{N-1} \mu_n (\xi^n)^q \delta_{qk} \right]$$

$$\rho_{qk}^r = \sum_{i, j=1}^N \alpha_{ij}^{r, r+p} \frac{\beta_{jq}}{\mu_j} [(\xi^i)^k - (\xi^j)^k] - \sum'_p \alpha_{ij}^{r, r+p} \frac{\beta_{jk}}{\mu_j} \left[ (\xi^j)^k - \sum_{n=1}^{N-1} \mu_n (\xi^n)^q \delta_{qk} \right]$$

Here  $\delta_{qk}$  is the Kronecker delta, while the prime accompanying the summation sign denotes summation over all  $p$  except  $p = 0$ .

Equations of motion of a one-dimensional continuous medium are obtained from (2.10) and (2.11), using the procedure described in Sect. 1 and taking into account the fact that the functions  $s_r$  and  $m_k^r$  are given at the points  $x_r$ , while  $s_r^n$  are given at different points  $x_r^n$  for some fixed value of  $r$ . Limiting ourselves to the second derivatives, we can write the equations of motion for  $s(x, t)$  and  $m_k(x, t)$  in the form

$$\begin{aligned}
 s'' &= \frac{C}{l\rho} \left[ \alpha s'' + \sum_{k=1}^{N-1} \rho_{k1} m_k + \rho_{k2} m_k' + \rho_{k3} m_k'' \right] \\
 m_k'' &= \frac{C}{l\rho} \left[ \alpha_{k1} s' + \alpha_{k2} s'' + \sum_{q=1}^{N-1} \rho_{kq1} m_q + \rho_{kq2} m_q' + \rho_{kq3} m_q'' \right] \\
 &\quad \left( \rho \equiv \frac{M}{l}, \quad m_k' \equiv \frac{\partial m_k}{\partial x} \right) \\
 \alpha &\equiv \frac{l^2}{2} \sum_{p, i, j} \alpha_{ij}^{\circ p} p^2, \quad \rho_{k1} \equiv - \sum_{i, j=1}^N \alpha_{ij}^{\circ} \left( \frac{\beta_{jk}}{\mu_j} - \frac{\beta_{ik}}{\mu_i} \right) \\
 \rho_{k2} &\equiv l \sum_{\substack{p > 0 \\ i, j}} p \alpha_{ij}^{\circ p} \left( \frac{\beta_{jk}}{\mu_j} - \frac{\beta_{ik}}{\mu_i} \right), \quad \rho_{k3} \equiv \frac{l^2}{2} \sum_{p, i, j} p^2 \alpha_{ij}^{\circ p} \frac{\beta_{jk}}{\mu_j} \\
 \alpha_{k1} &\equiv l \sum_{p > 0, ij} p \alpha_{ij}^{\circ p} [(\xi^i)^k - (\xi^j)^k]
 \end{aligned} \tag{2.13}$$

$$\alpha_{k2} \equiv \frac{l^2}{2} \sum_{p, i, j} p^2 \alpha_{ij}^{\circ p} \left[ (\xi^i)^k - \sum_{n=1}^{N-1} \mu_n (\xi^n)^k \right]$$

$$\rho_{kq1} \equiv \sum_{i, j} (\xi^i)^k \frac{\beta_{jk}}{\mu_j} \left[ \alpha_{ij}^{\circ} - \sum_p \alpha_{ij}^{\circ p} \right]$$

$$\rho_{kq2} \equiv l \sum_{p, i, j} p \alpha_{ij}^{\circ p} \frac{\beta_{jq}}{\mu_j} \left[ (\xi^i)^k - \sum_{n=1}^{N-1} \mu_n (\xi^n)^q \delta_{qk} \right]$$

$$\rho_{kq3} \equiv \frac{l^2}{2} \sum_{p, j, i} p^2 \alpha_{ij}^{\circ p} \frac{\beta_{jq}}{\mu_j} \left[ (\xi^i)^k - \sum_n \mu_n (\xi^n)^q \delta_{qk} \right]$$

Assumption that  $N$  denotes a set of identical particles or identical cells, does not lead to any significant simplification of Eqs. (2.13). Additional conditions will however be imposed on the constants of interaction appearing in these equations. In this case we shall have a continuous medium constructed with the help of macrocells. In the long wave approximation this medium will be described by equations of displacement of the center of mass of the cell and by equations of moments of various order. Increase in the number of particles in a macrocell will lead to the sharpening of the spectrum of the initial discrete system. If the macrocell coincides with the real cell of the discrete system, we note that we can draw conclusions from (2.13) concerning both, the acoustic and optical oscillations of the system at small  $k$  only. In order to make the spectrum more precise, at least two cells of the initial chain must be included into the macrocell.

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### THE PROPAGATION OF WEAK DISCONTINUITIES IN THE SYSTEMS OF EQUATIONS OF MAGNETOGASDYNAMICS

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We consider the problem of weak discontinuities in quasi-linear hyperbolic systems and obtain transport equations for the case when the characteristic surfaces of the system have constant multiplicity. We also investigate weak discontinuities in magnetogasdynamics for the case when the characteristic surface is adjacent to a region of rest.

Authors of [1] deal with the problem of propagation of weak discontinuities in linear hyperbolic systems when the unknown functions of the system and their derivatives up