CONSTRUCTION OF A THERMODYNAMICALLY COMPLETE EQUATION OF STATE OF A NONIDEAL PLASMA BY MEANS OF DYNAMIC EXPERIMENTS

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We consider a method for constructing a thermodynamically-complete equation of state of optically dense media and of a plasma from the results of experiments with shock waves. An equation of state in the form E = E (P, V) is constructed on the basis of the conservation laws in the front of the shock wave and from the results of measurements of the shock-compression parameters. This equation is used to determine the temperature T = T (P, V) by integrating the differential equation representing the second law of thermodynamics. The accuracy is estimated by the Monte Carlo method with a computer. The method is verified with the model problem of determining the equation of state of a dense cesium plasma with a thermodynamic behavior described by the Debye theory in the grand canonical ensemble.

1. INTRODUCTION

ONE of the important present-day problems of plasma physics is the investigation of the thermodynamic properties of a nonideal plasma, in which the effects of interaction between the charged particles play the decisive role (see, for example, [1]). It is known that the development of a consistent statistical theory of such a system encounters considerable mathematical difficulties, connected with the need of calculating the partition function in general form. In the case of a weakly-nonideal plasma the ratio of the Coulomb energy of the interaction between the charged particles to their thermal energy is a small parameter, and the thermodynamic functions of such a system are calculated in the form of the first few terms of the expansion in this parameter.[2] If the plasma is strongly nonideal, the approach to the solution of this problem should apparently be the same as for ordinary liquids, namely, the construction of model theories and their verification with the aid of the experimental data.[1)] However, many difficulties, due to the need of producing high pressures and temperatures, arise in the development of the required experimental technique. In addition, with increasing density, the effects of the nonideal behavior increase, but on the other hand the radiation free path decreases, and the medium becomes optically opaque, making it impossible to use the well-developed optical diagnostics methods. The number of experiments on nonideal plasmas is therefore quite limited. In addition, in the interpretation of the existing experimental data it is necessary to introduce various theoretical assumptions, which in final analysis makes it difficult to separate the influence of the nonideal behavior on the thermodynamic functions.

Krasnikov and Lomakin[4] proposed a method of obtaining a nonideal plasma by compressing and heating cesium vapor in the front of a shock wave. Calculations show[5] that this results in sufficiently large values of the plasma nonideality parameter $\Gamma = e^2/kT\rho_D$ (ρ_D is the Debye screening radius).

Measurements of the velocity of the shock wave front and of the plasma density make it possible to determine, with the aid of the conservation laws, the equation of state in the form of the dependence of the internal energy E on the pressure P and on the specific volume V. However, the equation of state in this form is incomplete, since it does not contain the temperature, an important thermodynamic parameter. The latter cannot be measured at the given plasma densities by the traditional optical methods, owing to the small free path of the optical radiation.

In the present paper, using an idea proposed by Zel'dovich,[6] we consider a method of determining the equation of state of a plasma from experiments with shock waves, without limiting assumptions concerning the form of this equation. Particular attention is paid to the practical use of computers in this method. The exposition is presented in general form, which admits of direct application to investigations of matter with the aid of shock and detonation waves in condensed and gaseous media. The accuracy estimate is by the Monte Carlo method, with the probabilistic structure of the measurement process simulated with a computer. We consider the problem of determining the equation of state of a nonideal plasma with a thermodynamic behavior described by the Debye theory in the grand canonical ensemble of statistical mechanics.[4]

2. FORMULATION OF PROBLEM

We consider a medium whose state is determined completely by specifying two thermodynamic parameters such that any other parameter is a single-valued function of the chosen pair of variables. The form of this dependence (the equation of state) cannot be obtained on the basis of thermodynamic reasoning alone, and is determined either by the methods of statistical physics or experimentally. Since dense media do not lend themselves to a rigorous theoretical analysis, the decisive role is played in this case by experimental in-

[1)]Progress has recently been made in developing machine methods for investigation of nonideal media (see, for example, [3]).

vestigations. In particular, shock waves are used extensively for the experimental determination of the equation of state.[7]

When a steady-state shock discontinuity propagates through a medium, the initial states (labeled with the index zero) and the final states are connected by the Rankine-Hugoniot conditions

$$DV = V_0(D-u),\ V_0(P-P_0) = Du,$$
$$E - E_0 = {}^1/_2(P+P_0)(V_0 - V). \tag{1}$$

Here V is the specific volume, P the pressure, E the internal energy, D the velocity of the shock-wave front in the laboratory frame, and u the jump of the mass velocity on the discontinuity.

The relations (1) written in this form are expressions of the general laws of the conservation of mass, momentum, and energy, and imply no assumptions whatever concerning the properties of the matter in question. The state of the medium behind the front of the shock wave is characterized by the quantities V, P, D, E, and u. By measuring any two of them and assuming the initial states E_0, V_0, and P_0 to be known, we can determine all the necessary hydrodynamic variables with the aid of (1). The easiest to measure accurately by standard methods is the shock-wave velocity D. The choice of the second measured parameter depends on the concrete experimental conditions. In the case of a cesium shock tube, it is possible to determine the specific volume V of the plasma from the absorption of soft x-radiation. In dynamic experiments with condensed media, the second parameter is usually the mass velocity u (for details see [7]). This makes it possible to obtain the value of the internal energy E = E (P, V) in each experiment. Performing similar measurements at different initial conditions and shock-wave intensities, we can determine the function E = E (P, V) in the P-V space region covered by the Hugoniot adiabats. However, the internal energy is not the thermodynamic potential with respect to the variables P and V and, consequently, it is impossible in this case to develop the complete thermodynamics of the investigated system. Characteristically, a dynamic experiment based on the registration of mechanical quantities yields direct information on the equation of state only in the incomplete caloric form E = E (P, V). The construction of the complete thermodynamics of the system is possible if, besides E = E (P, V), we know the temperature T = T (P, V).

In principle, such a connection can be established experimentally by measuring the temperature together with other hydrodynamic variables in each individual experiment. In most cases, however, a direct measurement of the temperature density entails fundamental difficulties. For example, for a dense cesium plasma, such measurements cannot be carried out because of the optical opacity and because of the screening of the emerging radiation by the molecular cesium vapor, which has an anomalously large cross section for the absorption of optical radiation.

A similar situation obtains in the investigation of condensed media with the aid of strong shock waves,[7,8] where the equation of state is determined from the shock-compression parameters. To find the temperature in these experiments it is necessary to use various semi-empirical models of the equation of state.

Ya. B. Zel'dovich[6] proposed the idea of determining the temperature of condensed media from shock-wave experiments and measurements of the states in adiabatic relaxation. Similar proposals were advanced in [9] as applied to the equation of state of detonation products. The gist of these considerations can be formulated as follows. By starting from the second law of thermodynamics and the experimentally known E = E (P, V) dependence, we readily obtain

$$\left[P + \left(\frac{\partial E}{\partial V}\right)_P\right]\frac{\partial T}{\partial P} - \left[\left(\frac{\partial E}{\partial P}\right)_V\right]\frac{\partial T}{\partial V} = T. \tag{2}$$

The solution of this linear inhomogeneous partial differential equation is the function T = T (P, V) of interest to us.

The solution (2) is constructed from the solution of the characteristic system of equations

$$\frac{dP}{dV} = -\frac{P + (\partial E/\partial V)_P}{(\partial E/\partial P)_V} = f_1(P, V), \tag{3}$$
$$\frac{dT}{dV} = -\frac{T}{(\partial E/\partial P)_V} = f_2(P, V). \tag{4}$$

It is easily seen that the characteristic equations coincide with the relations for the isentropes. In the case of a monatomic ideal gas, E = $^3/_2$PV, and Eqs. (3) and (4) can be integrated:

$$\frac{P}{P_0} = \left(\frac{V}{V_0}\right)^{-5/3}, \quad \frac{T}{T_0} = \left(\frac{V}{V_0}\right)^{-2/3},$$

which, naturally, coincides with the Poisson adiabats with exponent k = $^5/_3$.

Equations (3) and (4) are supplemented by the following boundary conditions: the temperature must be specified in a region where it can either be experimentally measured or reliably calculated by the methods of statistical physics.

If the position of the isentrope in the P-V plane is known theoretically or experimentally, then (4) is integrated along the isentrope:

$$T = T_0 \exp\left\{-\int_{V_0}^{V}\left(\frac{\partial E}{\partial P}\right)_V^{-1} dV\right\}.$$

From the solution (3) and (4) we determine T = T (P, V), which, together with the relation E = E (P, V) completes the problem of constructing the thermodynamically-complete equation of state of a substance from shock-wave experiments in optically dense media.

3. CONSTRUCTION OF THE ENERGY SURFACE E = E (P, V)

Disregarding the concrete experimental procedure for determining the parameters of the medium in shock compression, we shall assume that there is a certain number N of experimental points $\{E_i, V_i, P_i\}_{i=1}^{N}$, arbitrarily distributed in the P-V plane. To construct the analytic function E = E (P, V) from these data, it is necessary to solve the problem of regression analysis for a function of two independent variables. For the usual considerations we use the least-squares method for the construction of the regression surface (see the Appendix).

Considering the case of a two-dimensional parabolic approximation, we construct the equation of state in the form

$$E(P, V)=\sum_{k+l\leq q}\sum e_{kl}V^kP^l. \qquad (5)$$

The degree q of the polynomial should satisfy the condition $\frac{1}{2}(q+1)(q+2) \leq N$. To find the coefficients e_{kl} of the polynomial, it is necessary to solve the system of normal equations (A.3). This raises the difficulties that are well known from the one-dimensional analog of the problem and connected with the poor validity of the matrix of the system of normal equations at large values of N and q.[10] In this case there are no effective numerical methods of solving the system of linear equations with a near-zero determinant, since the rounding-off errors in computer calculations greatly distort the results, and the obtained solution of (A.3) is highly inaccurate.

These difficulties can be avoided by changing over to Chebyshev orthogonal polynomials[11] (see the Appendix), by regrouping the terms in (5) in such a way, that the condition of orthogonality between the individual groups is satisfied. The matrix of the normal system is transformed into a diagonal matrix and can be easily and rapidly inverted without great loss of accuracy. The calculation of the approximating polynomial in accordance with this algorithm reduces to multiple taking of the scalar product with subsequent reduction of similar terms, yielding the solution in the form (5).

The degree q of the polynomial is chosen by analyzing the experimental data. An increase of the degree of the approximated polynomial leads to a decrease of the best-approximation element (A.2), but at the expense of increasing the variance of this polynomial.[12] It is necessary to increase consecutively the degree q, re-estimating each time the newly appearing terms in accordance with the Fisher statistical significance criteria.[12]

This is particularly conveniently done for orthogonal polynomials because of their property of inclusion with respect to the degrees, according to which a polynomial of degree q can be calculated by using the results obtained in the preceding step for $q-1$.

By constructing the equation of state in the form (5) in this manner from the experimental data, it is possible to calculate the right-hand sides of the system (3) and (4) and to integrate it in accordance with some explicit numerical scheme.

In the present paper, the system (3) and (4) was integrated by the Adams scheme; the initial sections of the isentropes were calculated by the Runge-Kutta method.

4. ESTIMATE OF THE ACCURACY BY THE MONTE CARLO METHOD

The decisive question in the use of this method is that of the accuracy with which the temperature can be determined from the experimentally known relation $E = E(P, V)$.

In view of the complicated dependence of the solution of (2) on the experimental data (the approximation (5) and the solution of the characteristic system (3) and (4)), it is advantageous to use the Monte Carlo method for an estimate of the accuracy. (It should be noted that the estimate "by the maximum" would be too high, since the errors in computer calculations are random and cancel out in part[10].) Essentially similar considerations are used in the calculation of queueing systems, in determining the quality and reliability of complicated systems, etc.[15]

Each measurement result is influenced by a large number of unaccounted-for random facts that act independently. The result itself is therefore a random quantity which, as is well known, can be described by a corresponding distribution specified on a set of realizations. Using the usual considerations based on the Lyapunov theorem, we arrive at a normal law for the error distribution density.

According to the principles of mathematical statistics,[14] when speaking of experimental data it is necessary not only to consider the results obtained in the given experiment for a certain combination of random factors, but also to bear in mind the entire aggregate of possible results, which could be obtained for a different combination of causes of random errors. It is customary to regard the results of the first experiment as a sample (realization) out of the general aggregate of all possible results at a fixed complex of external conditions.

In the case under consideration, the Monte Carlo method consists of simulating the probability structure of the measurement process by reviewing the possible combinations of random factors that lead to the experimental error, and determining the influence of this error on the solution in question with the aid of a computer. A specified experimental file $\{E_i, V_i, P_i\}_{i=1}^N$ is set in correspondence with a "statistical file" $\{\widetilde{E}_i, V_i, P_i\}_{i=1}^N$, where E_i are random quantities with a normal distribution density $f(\widetilde{E}_i)$ having a mean value E_i and a variance $\sigma_i = \Delta_i/3$ (99.9% confidence probability, Δ_i is the error of the i-th experiment):

$$f(\widetilde{E}_i)=\frac{1}{\sqrt{2\pi}\,\sigma_i}\exp\left\{-\frac{(E_i-\widetilde{E}_i)^2}{2\sigma_i^2}\right\}. \qquad (6)$$

Such a rearrangement of the files is effected by a generator of pseudorandom numbers distributed in accordance with the law (6).

$\{E_i, V_i, P_i\}_{i=1}^N$ is used to construct the equation of state in the form (5), which is used in turn to solve the system of characteristic equations (3) and (4). The results are the isentropes $\widetilde{P}_S = \widetilde{P}_S(V)$ and $\widetilde{T}_S = \widetilde{T}_S(V)$, which are also random quantities with a certain distribution function. The mean value $\mu_\xi(V)$ and the variance $\sigma_\xi(V)$ are calculated in accordance with the formulas (ξ = P, T)

$$\mu_\xi(V)=\frac{1}{\alpha}\sum_{i=1}^{\alpha}\widetilde{\zeta}_i(V),\quad \sigma_\xi(V)=\left\{\frac{1}{\alpha-1}\sum_{i=1}\left[\widetilde{\zeta}_i(V)-\mu_\xi(V)\right]\right\}^{1/2}. \qquad (7)$$

If the number of realizations α used to estimate the sought quantities is sufficiently large, then by virtue of the law of large numbers the estimates (7) acquare a statistical stability (the order of magnitude of the variance of (7) is $1/\alpha$).

As a result of the calculations we obtain the relations

$$\mu_{P,T}=\Phi_\mu(V, \Delta_i, \{E_i, V_i, P_i\}_{i=1}^N),$$

$$\sigma_{P,T}=\Phi_\sigma(V, \Delta_i, \{E_i, V_i, P_i\}_{i=1}^N),$$

which describe the influence of the experimental errors on the accuracy with which the temperature is determined along the isentrope. We note that the solution is

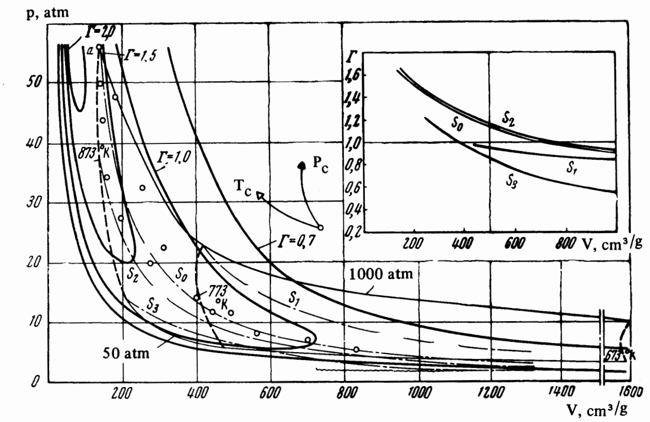

FIG. 1. P-V state diagram of a cesium plasma produced behind the front of a shock wave. The heavy solid curves correspond to a constant value of $\Gamma = e^2/kT\rho_D$ (ρ_D is the Debye radius); dashed curves—Hugoniot adiabats (the initial temperatures are indicated alongside); the light solid curves correspond to a constant pressure of the propelling gas; the dash-dot curves are the isentrope characteristics; O—points of the file $\{E_i, V_i, P_i\}_{i=1}^N$ N = 15. In the inset we have the value of the nonideality parameter along the characteristics.

influenced not only by the experimental errors themselves, but also by the distribution of the experimental points in the P-V plane. This method of estimating makes it possible to determine the accuracy of the solution for an arbitrary set of errors Δ_i, and for an arbitrary character of distribution of the experimental points in the P-V plane.

5. DETERMINATION OF THE EQUATION OF STATE OF A DEBYE PLASMA

Using the parameters of a real shock tube intended for the production and investigation of a dense cesium plasma (for details see [15]), let us consider the model problem of determining the equation of state of a nonideal plasma produced behind the front of the shock wave in experiments with the aid of the setup. The nonideality of the cesium plasma is taken into account within the framework of the Debye theory in the grand canonical ensemble. In considering this problem, we can carry out an exhaustive verification of the method, since we are able in this case to compare the results with the relation T = T(P, V) known from the Debye theory. For the present analysis, it is important to establish whether the characteristics lie entirely in that region of the P-V plane which is covered by the experiment.

To construct the regions of interest to us, we undertook the calculation of the propagation of shock waves in cesium vapor under conditions characteristic of a pneumatic shock tube with external heating[5] 2). Figure 1 shows the results of these calculations in the P-V plane. The dashed lines denote the shock adiabats characterized by the heater temperature T_c, which determines the pressure of the saturated cesium vapor (the state ahead of the shock-wave front). The turning-back of these curves is connected with processes of cesium ionization behind the shock-wave front.[8] The heavy lines correspond to a constant value of the nonideality parameter Γ. The light curves correspond to a constant value of the initial pressure P_c of the propelling gas (He), which is necessary to attain a given state behind the front of the shock wave. Assuming the maximum permissible pressures P_c = 1000 atm for shock tubes of the diaphragm type, we obtain an upper limit of the experimentally attainable region. The lower limit is determined by processes of radiative cooling of the stopper and apparently corresponds to a cesium pressure ~1 atm.[16]

By varying the initial heating T_c (by changing the initial conditions) we are able to change over from one shock adiabat to another. On the other hand, by changing the initial pressures of the propelling gas P_c (by varying the intensity of the shock wave), we move along a fixed adiabat. Thus, on the diagram of states of the cesium plasma there is a coordinate grid T_c, P_c such that any state from the experimentally attainable region can be obtained by a suitable choice of the parameters of the experimental setup.

By using the relation E = E(P, V) determined from the Debye theory in a grand ensemble from the system (3) and (4), we draw the characteristics S_c, which henceforth are regarded as "standard," since the representation (5) was not used for their construction.

It is seen from Fig. 1 that the isentropes lie entirely in the experimental region, so that the proposed method can be used to determine the equation of state of a nonideal plasma from experiments with shock waves in cesium vapor.

The initial data were chosen for $\Gamma \lesssim 1$. In this region, the initial data were specified in accordance with the Debye theory in the grand ensemble, bearing in mind the results of model calculations by the method of molecular dynamics[17] and the fact that the terms $\sim n^2 \ln n$ in the expansion of the thermodynamic potential for a singly ionized plasma vanish by virtue of the charge symmetry. The characteristics were drawn from this region into the strongly nonideal region, and the right-hand sides of the system (3) and (4) were calculated from the known relation E = E(P, V). We note that, unlike the Hugoniot adiabats, the parameter Γ increases monotonically along the characteristic (Fig. 1, inset). The solution at the end of the isentrope at the point a was compared with the Debye P-V-T dependence. In essence, this served to verify the correctness of the method in the case when the E(P, V) dependence is unknown. The very slight difference (~0.3% in T) can be attributed to errors in the numerical integration of (3) and to inaccuracies of the iterations in the program for calculating the Debye relation E = E(P, V).

In order to reveal the nonideality effects most rapidly in the experiment, it is natural to place the experimental points in the vicinity of the proposed isentrope. The P_c-T_c coordinate grid makes it possible to choose in suitable fashion the parameters of the experimental setup.

To verify the procedure described above for constructing the equation of state and to estimate the expected error, we used points $\{E_i, V_i, P_i\}_{i=1}^{15}$ randomly distributed over the P-V plane (Fig. 1), chosen on the basis of the assumption that the Debye theory is valid in the entire region under consideration. By specifying these points in accordance with the exact Debye rela-

2) Experiments performed in the region of small nonidealities confirm the results of these calculations.

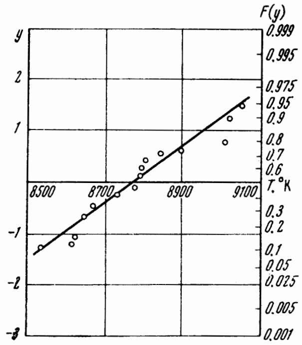

FIG. 2

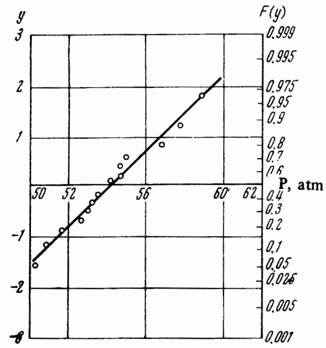

FIG. 3

FIG. 2. Normal character of the distribution for $\widetilde{T}_s(V)$ [11]:

$$F=\int_{-\infty}^{y(F)}\frac{1}{\sqrt{2\pi}}e^{-s^2/2}\,ds$$

FIG. 3. Normal character of the distribution for $\widetilde{P}_s(V)$.

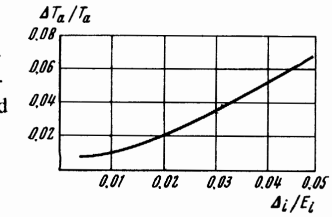

FIG. 4. Dependence of the solution error on the error in the experimental data for the point a indicated in Fig. 1. Equal-accuracy measurements.

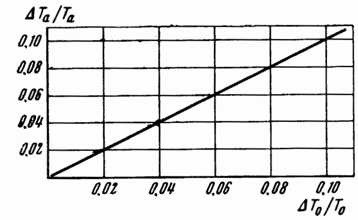

FIG. 5. Dependence of the solution error on the error in the initial data for the point a indicated in Fig. 1.

tions and comparing the results of the calculation with the "standard" characteristics, we determine the errors resulting from the approximation (5). We shall determine the influence of the experimental errors on the solution by the Monte Carlo method (Sec. 4). The normal character of the distribution of $\widetilde{P}_s$ and $\widetilde{T}_s$ on the end of the isentrope at the point a was verified with the "probability plot" (Figs. 2 and 3). We see that the distribution of $\widetilde{P}_s$ and $\widetilde{T}_s$ is close to normal, so that to determine the numerical characteristics of the random quantities it suffices to use the estimates (7). A comparison of the mathematical expectations with the "standard" values shows that the estimate (7) is not biased, so that the method does not introduce any noticeable systematic errors. Figure 4 shows plots of the errors at the point a against the errors of the file of the initial data, assuming equal-accuracy measurements. The influence of the errors in the initial data is shown in Fig. 5.

Let us estimate the order of magnitude of the expected error. By measuring the front velocity D with photomultipliers, accurate to $\sim 0.5\%$, and the specific volume V by transmission of soft x-rays, accurate to $\sim 0.5\%$, we obtain from (1)[18]

$$\frac{\delta E}{E-E_0}=\frac{\delta D}{D}+\left(\frac{V}{V_0-V}\right)\frac{\delta V}{V}.$$

The term in the parentheses is of the order of the degree of compression in the shock wave, and in our conditions has a value $\frac{1}{7}-\frac{1}{8}$. Therefore E is determined with accuracy on the order of 1–1.5%, corresponding to a contribution of $\approx 2\%$ or less to the solution if the number of experimental points is sufficiently large. This accuracy is fully adequate to reveal the influence of the nonideality effects of interest to us on the thermodynamic functions of the plasma.

We note that the described method is universal: it can be used to construct the equation of state of any medium from shock-wave experiments. The equations of state of condensed media obtained by this method are presently being readied for publication.

The authors consider it their pleasant duty to thank Yu. V. Kondrat'ev and B. N. Lomakin for help with the work, and also V. M. Ievlev, L. V. Al'tshuler, A. A. Vedenov, and A. I. Starostin for useful discussions.

APPENDIX

TWO-DIMENSIONAL APPROXIMATION

Knowing the set $\{f_i, x_i, y_i\}_{i=1}^{N}$ with accuracy determined by the weights $p_i = 1/\sigma_i$ (σ_i is the absolute error), let us consider a model that is linear in the parameters:

$$P_m=\sum_{k=1}^{m}C_k\varphi_k(x,y),\tag{A.1}$$

$\{\varphi_k(x, y)\}_{k=1}^{m}$ is a certain chosen system of linearly independent functions. The system of conditional equations takes the form

$$S_i=f_i-P_m(x,y),\quad i=1,2,\ldots,N.$$

Let us estimate the parameters C_k in (A.1). To this end, we require that the best-approximation element

$$S=\sum_{i=1}^{N}p_i^2S_i^2\tag{A.2}$$

be minimal with respect to the variables C_k. The condition for this is $\partial S/\partial C_k = 0$, and leads to the system of normal equations:

$$\begin{gathered}[\varphi_1,\varphi_1]C_1+[\varphi_1,\varphi_2]C_2+\ldots+[\varphi_1,\varphi_m]C_m-[\varphi_1,f]=0,\\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\\ [\varphi_m,\varphi_1]C_1+[\varphi_m,\varphi_2]C_2+\ldots+[\varphi_m,\varphi_m]C_m-[\varphi_m,f]=0,\end{gathered}\tag{A.3}$$

where $[\varphi_k, \varphi_l] = \sum_{i=1}^{N} p_i\varphi_k(x_i, y_i)\varphi_l(x_i, y_i)$ denotes the scalar product of the functions φ_k and φ_l on the set N. The solution of (A.3) is the sought set of quantities C_k in (A.1). In view of its symmetry, the system (A.3) is solved with a computer by the square-root method. The Gram determinant of (A.3) differs from zero because the $\varphi_k(x, y)$ are linearly independent.

We chose for φ_k the power-law functions:

$$\varphi_1=1,\quad\varphi_2=x,\quad\varphi_3=y,\quad\varphi_4=x^2,\ldots;$$
$$C_1=C_{00},\quad C_2=C_{10},\quad C_3=C_{01},\quad C_4=C_{20},\ldots,$$

which leads to (5).

To change over to orthogonal polynomials we consider besides $\{\varphi_k(x, y)\}_{k=1}^m$ their linear combinations

$$\psi_i = \sum_{j=1}^m \alpha_{ij}\varphi_j(x, y). \quad (A.4)$$

We seek the solution of the problem in the form

$$P_m(x, y) = \sum_{i=1}^m b_i\psi_i(x, y), \quad (A.5)$$

which leads to the system (A.3). The functions ψ_i are chosen to be mutually orthogonal:

$$[\psi_i, \psi_j] = A_{ij}\delta_{ij}, \quad (A.6)$$

where δ_j is the Kronecker symbol and A_{ij} is a nonnegative number. The system (A.3) will have a diagonal matrix

$$\left\| \begin{matrix} \sum\psi_1^2 & \cdots & 0 \\ & \sum\psi_2^2 & \\ \cdots & \cdots & \cdots \\ 0 & \cdots & \sum\psi_m^2 \end{matrix} \right\|.$$

Expression (A.5) takes the form

$$P_m(x, y) = \sum \frac{[\psi_i, f]}{[\psi_i, \psi_i]}\psi_i(x, y).$$

To find the connection between ψ_i and φ_i we use (A.6), defining α_{ij} by means of the formula

$$\alpha_{ij} = \begin{cases} 1, & i = j \\ 0, & i > j \end{cases}.$$

We obtain the recurrence relation

$$\psi_k = \varphi_k + \sum_{j=1}^{k-1} \alpha_{kj}\psi_k,$$

$$\alpha_{kj} = -\frac{[\varphi_k, \psi_j]}{[\psi_j, \psi_j]}.$$

Thus, all the coefficients of (A.4) have been determined.

The foregoing algorithms were used to compile computer programs with which to find the coefficients e_{ij} of (5) for specified $\{f_i, x_i, y_i\}_{i=1}^N$. The maximum degree of the polynomial was determined by the capacity of the operating memory of the computer, and amounts to q = 10 (66 coefficients) for computers of the M-20 and BESM-4 types.

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