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Some calculations on a parabolic differential equation with free boundary

by

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1. Introduction

A certain physical problem [1] led to the partial differential equation

$$\frac{\partial}{\partial\rho}\left(\frac{\partial q}{\partial\rho}+\frac{q}{\rho}\right)=\frac{\partial q}{\partial\tau} \tag{1.1}$$

with boundary conditions

$$\rho=1:\ q(1,\tau)=q_1>1\ ,\quad \rho=\rho_b(\tau):\ \ q(\rho_b(\tau),\tau)=1\ ,\quad \tau\geqslant 0\ .$$

and initial condition

$$\tau=0:\ q(\rho,0)=\text{ given function of }\rho,\ \rho_b(0)\leqslant\rho\leqslant 1.$$

The boundary curve $\rho_b(\tau)$ is not previously known but is determined by the ordinary differential equation

$$\left(\frac{\partial q}{\partial\rho}+\frac{q}{\rho}\right)_{\rho=\rho_b(\tau)}=-\frac{d\rho_b}{d\tau} \tag{1.2}$$

with initial condition

$\tau=0:\rho_b(0)$ = given value.

Similar problems - with the heat equation instead of (1.1) and the derivative $\partial q/\partial\rho$ prescribed for $\rho=1$ instead of the function itself - have been treated among others by Landau [2], Evans, Isaacson and MacDonald [3] and Douglas and Gallie [4].

In this report the method used to find approximate solutions and some further calculations connected with the physical problem are described. Since no existence, convergence and stability proofs are given, this is a report on a mathematical experiment rather than a contribution to numerical analysis.

2. Method of solution

The equations (1.1) and (1.2) were integrated simultaneously using a finite difference approximation. For this purpose a lattice in the $\rho\tau$-plane was constructed in the following way. The range $0 \leq \rho \leq 1$ was divided into N equal intervals of length $h = N^{-1}$; the discrete arguments ρ_i were defined by $\rho_i = 1 - ih$, $i = 0(1)N$. The intervals in the τ-direction were not aequidistant; the arguments τ_j were defined by $\rho_b(\tau_j) = \rho_j$ and were determined successively during the integration process. Putting $q_{i,j} = q(\rho_i, \tau_j)$ the initial and boundary conditions are on this lattice

$$\rho_b(0) = \rho_k, \tau_k = 0, \quad q_{i,k} = \text{given function}, \; 0 \leq i \leq k,$$
$$q_{0,j} = q_1, \quad q_{j,j} = 1, \quad j \geq k$$

and the required quantities are $q_{i,j}$ and τ_j, $j \geq k$, $0 \leq i \leq j$. A scaling suitable to simplify the formulas is

$$Z_i = N\rho_i = N - i, \quad u_j = N^2\tau_j.$$

The free boundary curve is represented by the lattice points (ρ_j, τ_j). It is determined by the values of τ_j. Suppose u_j and $q_{i,j}$, $i = 0(1)j$, are known for some j. Then u_{j+1} follows from the finite difference approximation of (1,2)

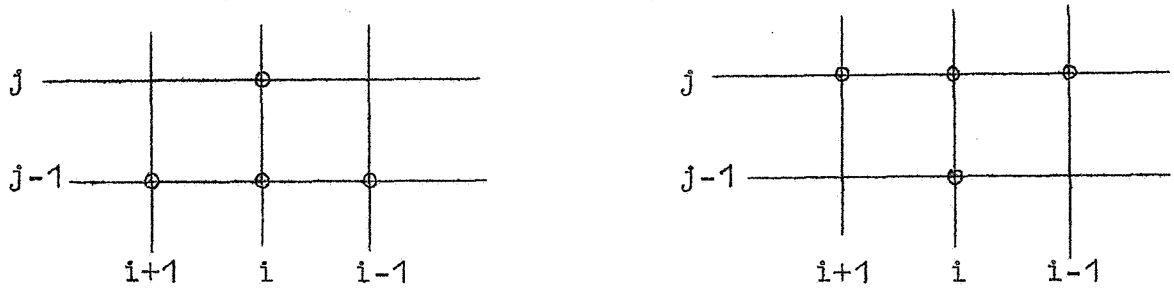
$$u_{j+1} = u_j + \left[\frac{1}{Z_j} + h\left(\frac{\partial q}{\partial \rho}\right)_{\rho_j,\tau_j}\right]^{-1} , \qquad (2.1)$$

wherein the derivative is calculated by means of a formula of Newton-type

$$h\left(\frac{\partial q}{\partial \rho}\right)_{\rho_j \tau_j} = - \sum_k \frac{1}{k} \nabla^k q_{j,j} \qquad . \qquad (2.2)$$

One obtains (2.1) from (1.2) by putting $-d\rho_b/d\tau = h/(\tau_{j+1} - \tau_j)$ As for the precision the "central" formula $-d\rho_b/d\tau = 2h/(\tau_{j+1} - \tau_{j-1})$ would be preferable but as could be expected it gave unstable results.

The simplest difference analogue of (1.1) yields a relation between four points which can form an "explicite" or an "implicit" pattern as shown in fig. 1.



explicit

implicit

Fig. 1 Difference patterns

The explicit method is the most convenient one for integration since the unknown value of $q_{i,j}$ follows immediately from three known points (except for $q_{j-1,j}$). A great disadvantage of this method, however, is the danger of instability. In the analogous case of the heat-equation it is well-known that errorgrowth can occur for $r = \Delta\tau/(\Delta\rho)^2 > \frac{1}{2}$ and one may expect that in the present case a similar stability condition will hold. In this set-up the length of the τ-intervals cannot be freely chosen but varies with the slope of the function $\rho_b(\tau)$, in fact $\Delta\tau \approx h(d\rho_b/d\tau)^{-1}$ and thus $r \approx (h d\rho_b/d\tau)^{-1}$. For actual values $d\rho_b/d\tau = 2$, $h = 10^{-2}$ one finds $r \approx 50$ which is certainly too large; diminishing the interval h would only make the situation worse. Indeed an attempt to use the explicit method failed. For the implicit pattern the difference equation reads

$$\left(1 + \frac{1}{2Z_i}\right) q_{i-1,j} - \left(2 + \frac{1}{Z_i^2} + \frac{1}{\nabla u_j}\right) q_{i,j} + \left(1 - \frac{1}{2Z_i}\right) q_{i+1,j} = -\frac{1}{\nabla u_j} q_{i,j-1}, \tag{2.3}$$

$j \geqslant k + 1$, $i = 1(1)j-1$.

For a fixed j, (2.3) provides a system of j-1 linear equations in the j-1 unknowns $q_{i,j}$. This seems rather unpleasant; for $h = 10^{-2}$ one gets matrices of orders up to 100. These matrices, however, have such a simple shape that solution of the equations is not impracticable. Here the direct method of elimination and backsubstitution was used which in this case can be described by the set of recurrence formulas:

$$A_{i-1,j} = N_{i,j}^{-1}\left(1+\frac{1}{2Z_i}\right) \quad , (2,4)$$

$$B_{i-1,j} = N_{i,j}^{-1}\left[\left(1-\frac{1}{2Z_i}\right)B_{i,j} + \frac{q_{i,j-1}}{\nabla u_j}\right] \quad , (2.5)$$

$$N_{i,j} = 2 - \left(1-\frac{1}{2Z_i}\right)A_{i,j} + \frac{1}{Z_i^2} + \frac{1}{\nabla u_j} \quad . (2,6)$$

With the initial values $A_{j-1,j} = 0, B_{j-1,j} = 1$ the formulas (2,4) - (2.6) enable one to calculate $A_{i,j}$ and $B_{i,j}$ for $i = j-2(1)0$. Then the function values $q_{i,j}, i = 1(1)j$ follow from

$$q_{i+1,j} = A_{i,j}\, q_{i,j} + B_{i,j} \quad , \qquad (2.7)$$

starting with $q_{0,j} = q_1$.
After this calculation a new point of the boundary curve can be found and the next value of j can be dealt with.

3. Solution with free start

As a special case one may consider the solution where the boundary curve starts at $\rho_b(0) = 1$. At the starting point $\rho = 1, \tau = 0$ the function $q(\rho,\tau)$ is singular, its limiting value being dependent on the direction of approach. In the difference set-up one has $k = 0$; $q_{0,0}$ is not defined. The singularity causes some difficulty in calculating u_1 since $\partial q/\partial \rho$ is infinitely large at that point. One can use the formula $u_1 = \left[q_1 - 1 + 1/(N-1)\right]^{-1}$ as a crude estimate. However, an error in the value of u_1 is not very important since it has no influence on the $q_{i,j}$; the boundary curve as a whole suffers a shift in the τ-direction which is very small as the slope of the curve is nearly zero near the starting point.

An analytical approximation in the neighbourhood of the singular point $\rho=1, \tau=0$, is obtained by cancelling the term q/ρ in (1.1) and (1.2). The derivative $\partial q/\partial\rho$ grows indefinitely for $\tau \to 0$ since $\partial q/\partial\rho \approx (q_1-1)/[1-\rho_b(\tau)]$. Hence for $1-\rho_b(\tau) \ll q_1-1$, i.e. $\tau \approx 0$, one has $q/\rho \ll \partial q/\partial\rho$.
The equations (1.1) and (1.2) modified in this way have according to Pippard [5] the solution

$$q(\rho,\tau) = q_1 - \sqrt{\pi}\,\beta\, e^{\beta^2} \operatorname{erf} \frac{1-\rho}{2\sqrt{\tau}} \tag{3.1}$$

$$\rho_b(\tau) = 1 - 2\beta\sqrt{\tau} \tag{3.2}$$

where β has to be solved from the equation

$$q_1 - 1 = \sqrt{\pi}\,\beta\, e^{\beta^2} \operatorname{erf}\beta \tag{3.3}$$

and erf x is the error function $\operatorname{erf} x = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-\xi^2)\,d\xi$.
It is seen that the variables ρ and τ occur in $q(\rho,\tau)$ only as the single "Similarity variable" $(1-\rho)/\sqrt{\tau}$.
An investigation was made of the dependence of the results on the integration step h. As a test case the time τ_N which satisfies $\rho_b(\tau_N)=0$ was determined for some values of h with the parameter q_1 = 1,5. The results are plotted in fig. 2. The two curves (which have the same limiting value for $h \to 0$) relate to a different number of differences retained in (2.2):

(a) $h\left(\frac{\partial q}{\partial\rho}\right)_{\rho_j,\tau_j} = -\nabla q_{j,j} = q_{j-1,j} - 1$

(b) $h\left(\frac{\partial q}{\partial\rho}\right)_{\rho_j,\tau_j} = -\left(\nabla + \frac{\nabla^2}{2}\right) q_{j,j} = -\frac{1}{2} q_{j-2,j} + 2q_{j-1,j} - \frac{3}{2}$

The function $q(\rho,\tau)$ is much less dependent on h than the boundary curve.

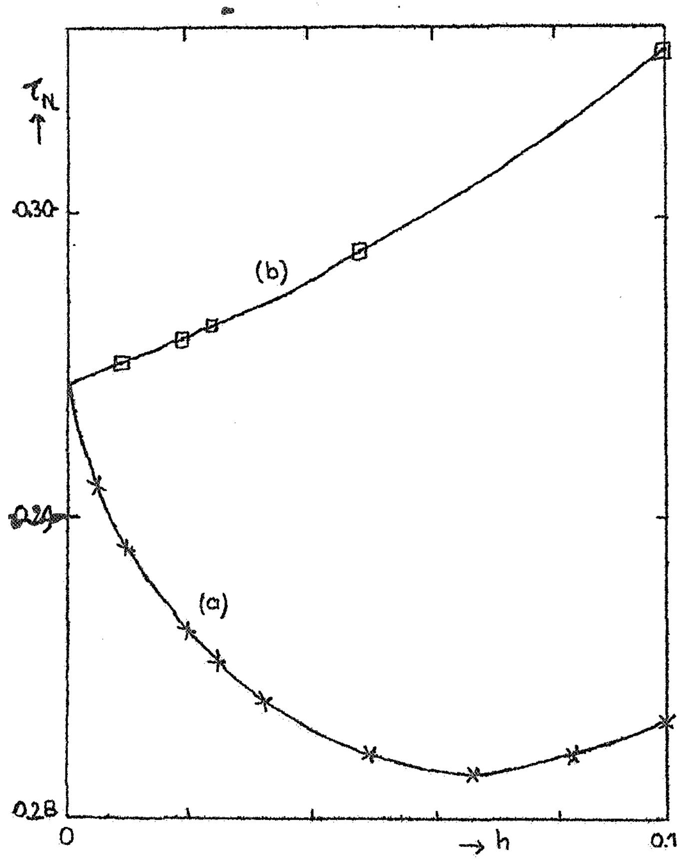


Fig. 2 Dependence on h.

In fig. 3 the behaviour of the solutions is shown qualitatively by the lines of q = Const. in the $\rho\tau$-plane. The occurrence of the nodal point D in the curve q = 1 is an indication for the deviation from the analytical approximation (3.1). This point shifts to the right as q_1 approaches to 1.
Apparently the difference approximation for (1.1) breaks down in the neighbourhood of the point F which seems to be singular just as the starting point S.

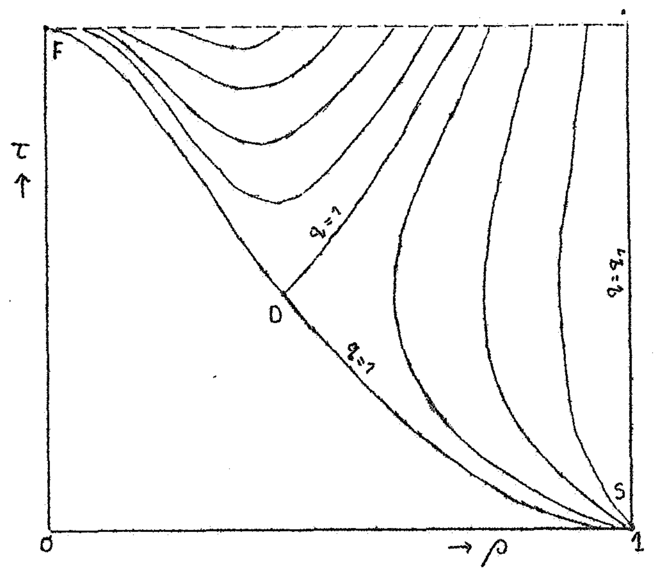


Fig. 3. Solution with free start

4. Periodical solution

In another case also interesting from a physical point of view the initial field $q(\rho,0)$ is such that for a certain value of τ , say τf , it is reproduced in the interval $\rho_b(0)\leqslant\rho\leqslant 1$, thus $q(\rho,\tau f)\equiv q(\rho,0), \rho_b(0)\leqslant\rho\leqslant 1$.
For that value of τ the boundary has reached the value $\rho_b(\tau f)$; in the range $\rho_b(\tau f)\leqslant\rho\leqslant\rho_b(0)$ a minimum $q(\rho,\tau f)=q_r<1$ occurs. One is interested in the relation between q_r and the mean value of $\frac{1}{2q_1}\left(\frac{\partial q}{\partial\rho}+\frac{q}{\rho}\right)_{\rho=1}$ over a period $0\leqslant\tau\leqslant\tau f$ for several values of the parameter q_1.

For the mean value mentioned above one can derive an expression not containing the derivative $\partial q/\partial\rho$, so that it is more suitable for numerical calculations. One finds using (1.1) and (1.2)

$$\tau f\,\overline{\left(\frac{\partial q}{\partial \rho}+\frac{q}{\rho}\right)}_{\rho=1} = \int_0^{\tau f}\left(\frac{\partial q}{\partial \rho}+\frac{q}{\rho}\right)_{\rho=1} d\tau$$

$$= \int_0^{\tau f}\left[\left(\frac{\partial q}{\partial \rho}+\frac{q}{\rho}\right)_{\rho=\rho_b(\tau)} + \int_{\rho_b(\tau)}^{1}\frac{\partial}{\partial \rho}\left(\frac{\partial q}{\partial \rho}+\frac{q}{\rho}\right)d\rho\right]d\tau$$

$$= \int_0^{\tau f}\left[-\frac{d\rho_b}{d\tau} + \int_{\rho_b(\tau)}^{1}\frac{\partial q}{\partial \tau}\,d\rho\right]d\tau$$

$$= -\rho_b(\tau f)+\rho_b(0)+\int_0^{\tau f}\left[\int_{\rho_b(\tau)}^{1}\frac{\partial q}{\partial \tau}\,d\rho\right]d\tau\,,$$

Inspection of fig. 4 shows that by interchange of the integrations with respect to ρ an τ the boundaries modify as follows:

$$\int_0^{\tau f} d\tau \int_{\rho_b(\tau)}^{1} d\rho = \int_{\rho_b(0)}^{1} d\rho \int_0^{\tau f} d\tau + \int_{\rho_b(\tau f)}^{\rho_b(0)} d\rho \int_{\tau_b(\rho)}^{\tau f} d\tau\,,$$

where $\tau_b(\rho)$ is the inverse function of $\rho_b(\tau)$.

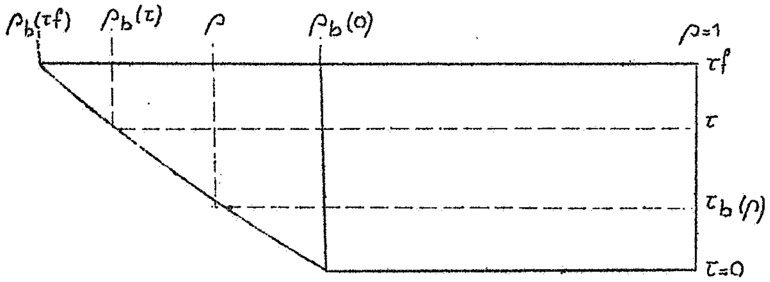


Fig. 4 Integration boundaries

Using this result one proceeds as follows:

$$\tau f\,\overline{\left(\frac{\partial q}{\partial \rho}+\frac{q}{\rho}\right)}_{\rho=1} = -\rho_b(\tau f)+\rho_b(0)+\int_{\rho_b(0)}^{1}\left[q(\rho,\tau f)-q(\rho,0)\right]d\rho\,+$$

$$+\int_{\rho_b(\tau f)}^{\rho_b(0)}\left[q(\rho,\tau f)-q(\rho,\tau_b(\rho))\right]d\rho.$$

Since by assumption $q(\rho,\tau f)\equiv q(\rho,0)$ in the range $\rho_b(0)\leqslant\rho\leqslant 1$ and $q(\rho,\tau_b(\rho))=1$ because of the boundary conditions this expression reduces to one single integral and one obtains the relation

$$\frac{1}{2q_1}\overline{\left(\frac{\partial q}{\partial \rho}+\frac{q}{\rho}\right)}_{\rho=1} \doteq \frac{1}{2q_1\tau f}\int_{\rho_b(\tau f)}^{\rho_b(0)} q(\rho,\tau f)d\rho\,. \qquad (4.1)$$

In the limiting case $q_r \rightarrow 1$ one gets $\tau f \rightarrow 0$ while both $\rho_b(0)$ and $\rho_b(\tau f)$ tend to a value ρ^* .For small values of τf one can put $\partial q/\partial \tau = 0$ in equation (1.1) since for the periodical solution $\int_0^{\tau f}\frac{\partial q}{\partial \tau}d\tau = 0$ holds exactly.

Taking the boundary conditions into account the solution of (1.1) then becomes

$$q = (1-\rho^{*2})^{-1}\left[(q_1-\rho^*)\rho + (1-q_1\rho^*)\rho^*\rho^{-1}\right].$$

The value of ρ^* now follows from the condition $\partial q/\partial \rho = 0$ at $\rho = \rho^*$, caused by the presence of the nodal point D of the curve q = 1 as shown in fig. 5.

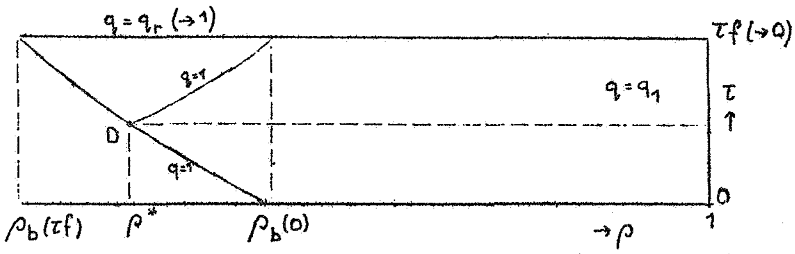


Fig. 5. Periodical solution with $q_r \rightarrow 1$

One finds $\rho^* = q_1 - (q_1^2-1)^{1/2}$ and the wanted quantity turns out to be

$$\frac{1}{2q_1}\overline{\left(\frac{\partial q}{\partial \rho}+\frac{q}{\rho}\right)}_{\rho=1} = \frac{1}{2q_1}\left(\frac{\partial q}{\partial \rho}+\frac{q}{\rho}\right)_{\rho=1} = \frac{q_1-\rho^*}{q_1(1-\rho^{*2})} =$$

$$= \frac{1}{2}\left[1+(1-q_1^{-2})^{1/2}\right]. \qquad (4.2)$$

The periodical solutions were obtained numerically by means of a procedure of iterative kind. A fixed value $\rho_b(0)=\rho_k$ was assumed ($\rho_k > \rho^*$ according to fig. 5) and the initial field $q_{i,k}$, $0 \leq i \leq k$, satisfying the requirement of periodicity, was determined as follows. An approximation $q_{i,k}^{(n)}$ being known, the field is integrated with the method of section 2 up to a time $\tau f^{(n)}$ defined by $q^{(n)}(\rho_k, \tau f^{(n)}) = 1$. Since as a rule τf is not one of the discrete argument values, interpolation between two adjacent values τ_l and τ_{l+1} is necessary. The situation is illustrated in fig. 6. With $q_{k,l} = 1+a$, $q_{k,l+1} = 1-b$ one gets by linear interpolation $\tau f = (a+b)^{-1}(a\tau_{l+1} + b\tau_l)$.
The next approximation is defined by $q_{i,k}^{(n+1)} = q^{(n)}(\rho_i, \tau f^{(n)})$; it follows from interpolation between $q_{i,l}^{(n)}$ and $q_{i,l+1}^{(n)}$. A suitable first estimate $q_{i,k}^{(0)}$ is supplied by the field for $\tau = \tau_k$ of the solution with free start, defined in section 3, which is acting in this manner as a "transient phenomenon".
In the cases investigatedone or two iterations were sufficient to obtain the periodic solution within the required accuracy.

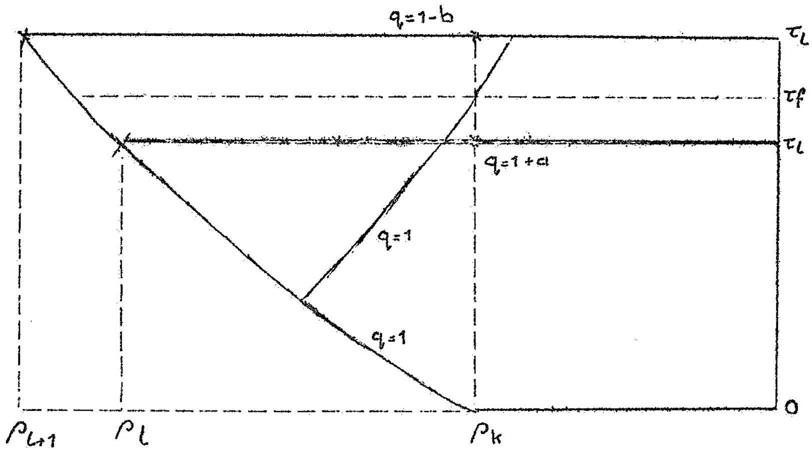


Fig. 6. Interpolation for periodical solution.

After this the value of $\int_{\rho_b(\tau f)}^{\rho_b(0)} q(\rho, \tau f)\, d\rho$ was found by interpolation between $\int_{\rho_l}^{\rho_k}$ and $\int_{\rho_{l+1}}^{\rho_k}$ which integrals were evaluated by aid of Simpson's rule.
Finally the value of q_r was found by interpolation between $q_{min}(\rho, \tau_l)$ and $q_{min}(\rho, \tau_{l+1})$. These minima were calculated

by aid of the formula

$$q_{min} = q_m - \frac{1}{2}\frac{(\delta q_m)^2}{\delta^2 q_m} = q_m - \frac{1}{8}\frac{(q_{m+1} - q_{m-1})^2}{q_{m+1} - 2q_m + q_{m-1}} ,$$

where q_m is the smallest of the discrete values for the τ concerned. This formula is obtained from the three-point interpolation formula.

5. Results

The integrations were performed on the electronic computer ARMAC of the "Mathematisch Centrum" for the parameter values $q_1 = 1.1(0.1)1.5$ with the interval $h = 0.02$ using first and second differences in (2.2). The solutions with free start (section 3) were calculated with the crude estimate for u_1 This was possible since in a test case with $q_1 = 1.5$ and $h = 0.001$ a good agreement between the solution with crude start and the analytical approximation (3.1) appeared. The periodical solutions (section 4) were calculated for three or four values of q_r. Some features of these solutions are communicated in a paper dealing with the physical theory that gave rise to the above calculations [6].

The calculations described in this report were carried out at the request of Professor C.J. Gorter of the Kamerlingh Onnes Laboratorium at Leiden. The autor was glad to receive many important hints from Professor A. van Wijngaarden.
The complicated ARMAC-programme for this work was drawn up by Miss G.C.F.E. Alleda.

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