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A System of Simultaneous Non-linear Equations in Three-Thousand Variables

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A very effective method is presented to solve a large set (~ 3000) of coupled transcendental equations numerically. We apply the method to calculate the mean production rates of nuclei in the statistical decay of highly excited heavy nuclei. For this case usually at most 40 iteration steps are needed to obtain a solution with a relative accuracy of $< 10^{-6}$. We demonstrate the method for the most severe case of a phase transition where the statistical fluctuations are large, causing our system of coupled mean-field equations to become unstable.

1. INTRODUCTION

We consider the problem of solving N real (transcendental) equations in N real unknowns in the case we know by some other (physical) arguments that only a few real solutions exist. A well-known method is Newton's, provided that the functions involved are differentiable. But there is one drawback: in Newton's method a $N \times N$ dimensional linear equation must be solved in a suitable neighborhood of the solution. This, of course, is difficult to implement in reasonable time if $N \sim 3000$. We therefore looked for other methods and tried Schechter's nonlinear successive overrelaxation process [1] especially recommended by Greenspan [3]. In Section 2 the mathematical background of Schechter's method is given together with an improvement that sometimes is very useful. In Section 3 this is applied to the physical problem of phase transitions in heavy nuclei.

2. MATHEMATICAL FOUNDATIONS

The method, essentially due to Schechter [1], is a generalization of the technique of successive overrelaxation (SOR) from linear to nonlinear systems, consider the system

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$$\begin{aligned} f_1(\mathbf{x}) &= f_1(x_1, x_2, \ldots, x_N) = 0 \\ f_2(\mathbf{x}) &= f_2(x_1, x_2, \ldots, x_N) = 0 \\ &\vdots \\ f_N(\mathbf{x}) &= f_N(x_1, x_2, \ldots, x_N) = 0 \end{aligned} \tag{2.1}$$

where f_i: $R^N \to R$ are N nonlinear functions in N variables. Let $f_{ii}(\mathbf{x}) = \partial f_i / \partial x_i \neq 0$. Given a system of indices $\{i_p\}$ which exhaust the set $\{1, 2, \ldots, N\} = Z_N$ infinitely often, a sequence of real numbers $\{\omega_p\}$, $p = 0, 1, 2, \ldots$, and a starting guess $\mathbf{x}_0$, Schechter's approximate relaxation process is defined by

$$\begin{aligned} i_p = k\text{:}\ x_k^{(p+1)} &= x_k^{(p)} - \omega_p \frac{f_k(x_1^{(p)}, x_2^{(p)}, \ldots, x_N^{(p)})}{f_{kk}(x_1^{(p)}, x_2^{(p)}, \ldots, x_N^{(p)})} \\ i_p \neq k\text{:}\ x_k^{(p+1)} &= x_k^{(p)} \end{aligned} \tag{2.2}$$

where ω_p is in the range

$$0 < \omega_p < 2.$$

The left-hand side of (2.1) may be written

$$\mathbf{f}\text{:}\ R^N \to R^N,$$

where $\mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_N(\mathbf{x}))$, $\mathbf{x} \in R^N$.

The theoretical, more interested reader will find a painstaking treatment of Schechter's method in the book of Meis and Marcowitz [2, Chap. III]. Recently Brewster and Kannan [7] have given a new proof for the convergence of Schechter's method. As they remark, if the range of the parameter ω_p is extended to $\omega_p > 2$, then convergence would still be possible. It should be noted that $\omega_p > 2$ in practical applications is only useful if $\mathbf{f}(\mathbf{x})$ is convex. Especially when the starting point is far away from the solution will a value $\omega_p > 2$ give rapid convergence. In contrast, the iteration process for a *concave* function $\mathbf{f}(\mathbf{x})$ with $\omega_p > 2$ will run away from the solution.

Despite the theoretical investigations, it is rarely possible to determine *a priori* when this method will converge to a solution of (2.1). The fact that a certain vector is a solution should *always* be verified by direct substitution into the given system. The most popular way for getting a sequence $\{\omega_p\}$ is to take $\omega_p = \omega$, constant for all p. A good choice for ω can be determined only by experimentation in the range $0 < \omega < 2$.

A second way to determine $\{\omega_p\}$ is to generate random numbers in the interval $I \subset [0, 2)$; this seems never before to have been taken into consideration. The advantage over the first method is that no search for a suitable ω is needed.

The sequence $\{i_p\}$ that covers Z_N infinitely often is in practice just the sequence $1, 2, \ldots, N, 1, 2, \ldots$, but it may be better to prefer some directions in R^N, for example, $N = 4$ and the sequence 1, 1, 1, 2, 3, 4, 4, 4, 1, 1, 1, ... This, of course, depends

heavily on the structure of (2.1). Consider the following example given by Brown [4, p. 310, Example 2]:

$$f_1(x_1, x_2) = x_1^2 - x_2 - 1,$$
$$f_2(x_1, x_2) = (x_1 - 2)^2 + (x_2 - 0.5)^2 - 1. \tag{2.3}$$

The system has roots at

$$\mathbf{r} = (1.54634288, 1.39117631),$$
$$\mathbf{s} = (1.06734609, 0.139227667).$$

The starting guess was (0.1, 2.0) and a little bit of experimentation showed that $\omega = 1.5$ was a good choice. Then (2.2) converged to $\mathbf{r}$ in 29 iteration. Newton's method and Brown's method converge to $\mathbf{s}$ in 24 and 10 iterations. If $\{\omega_p\}$ are taken to be random numbers in $I = [1, 2]$ then 30 or 60 iterations are needed to get the same result. The number of iterations depends on the initial value of the random number generator if the number of steps in (2.2) is small. To get the solution $\mathbf{s}$ we used the inner product deflation method described by Brown [4, p. 331]. We defined the following new system of equations,

$$g_i(x_1, x_2) = f_i(x_1, x_2) \cdot \langle \mathbf{e}, \mathbf{x} - \mathbf{r} \rangle^{-1} \qquad (i = 1, 2) \tag{2.4}$$

where $\mathbf{e} = (1, 1)$ is the unit vector and $\langle \cdot, \cdot \rangle$ denotes the inner product. The starting guess was unchanged but the value of ω was changed drastically to 0.4. Then $\mathbf{s}$ was found in about 50 iterations.

3. Application to Phase-Transitions in Finite Nuclei

The decay of heavy nuclei after bombardment by ultrarelativistic protons ($E_p > 10$ GeV) can be described by a statistical model (Gross *et al.* [5]). It is assumed that every open multi-fragment decay channel is equally populated. In this picture the dissociation of the nuclei into various fragments is equivalent to the equilibrium of a finite system of nucleons under short range forces (nuclear) and long range forces (Coulomb). The short range forces lead to a condensation of the nucleons into drops (nuclei) which coexist with a free-nucleon gas. Such a system has a complicated phase structure. It is found that there is a pronounced and sharp phase transition of first order (Sa and Gross [6]). The phase transition points can be most easily determined in a mean field approximation.

The Coulomb interaction of a fragment i with the rest of the system in a given decay-channel α is

$$V_i^{\text{Coul}} = Z_i \sum_{k \neq i} n_k^{\alpha} \frac{Z_k e^2}{|\mathbf{r}_i - \mathbf{r}_k|}, \tag{3.1}$$

where n_k^α gives the number (0, 1) of fragment nuclei $k \neq i$ together with nucleus i in the channel α, Z_i is the proton number of nucleus i and $\mathbf{r}_i$ its position. In the mean field approximation one replaces n_k^α by its average value in all channels $\langle n_k \rangle_i$. This is further approximated by the single-particle distribution $\langle n_k \rangle$:

$$\begin{aligned} \langle n_k \rangle_i &= \langle n_k \rangle \alpha_i \qquad \text{for} \quad Z_i + Z_k \leqslant Z_{\text{total}} \\ &= 0 \qquad\qquad\quad \text{for} \quad Z_i + Z_k > Z_{\text{total}}. \end{aligned} \tag{3.2}$$

α_i is determined by the charge conservation

$$\sum_{k \neq i} Z_k \langle n_k \rangle_i = Z_{\text{total}} - Z_i. \tag{3.3}$$

In [5] it is shown that the mean number of nuclei $\langle n_i \rangle$ of kind i is then determined by the following coupled set of N nonlinear equations

$$\begin{aligned} \langle n_i \rangle &= g_i(\langle n_1 \rangle, \ldots, \langle n_N \rangle) \\ g_i(\langle n_1 \rangle, \ldots, \langle n_N \rangle) &= \exp[\gamma_i + \beta\{\mu_N N_i + \mu_z Z_i \\ &\qquad - V_i^{\text{Coul}}(\langle n_1 \rangle, \ldots, \langle n_N \rangle\}] \end{aligned} \tag{3.4}$$

with

$$\exp(\gamma_i) = \left(\frac{M_i T}{2\pi\hbar^2}\right)^{3/2} \Omega \cdot \xi_i(\beta) \exp[\beta B_i] \tag{3.5}$$

$$\beta = \frac{1}{T}. \tag{3.6}$$

Here M_i is the mass, N_i the neutron number, ξ_i the number of internal states excited, B_i the binding energy of the fragment-nucleus i, T is the temperature and Ω the volume of the system at the point of decay.

The mean numbers $\langle n_i \rangle$ and the chemical potentials μ_N, μ_Z must be determined from Eqs. (3.4) and the constraints

$$\begin{aligned} \sum N_i \langle n_i \rangle &= N_{\text{total}}, \\ \sum Z_i \langle n_i \rangle &= Z_{\text{total}}. \end{aligned} \tag{3.7}$$

The set of Eqs. (3.4) are coupled via the Coulomb interaction $V_i^{\text{Coul}}(\langle n_1 \rangle, \ldots, \langle n_N \rangle)$. In the decay of an uranium nucleus about 3000 different nuclei, i can be formed. In this case (3.4) is a set of 3000 coupled nonlinear equations. It is difficult to solve this by an ordinary Newton method because we have to solve a

3000×3000 dimensional linear equation at each iteration. Very effectively, we used the method of successive overrelaxation discussed in Section 2. We set

$$\begin{aligned} x_i &= \langle n_i \rangle \\ f_i(x_1, \ldots, x_N) &= g_i(\langle n_1 \rangle, \ldots, \langle n_N \rangle) - \langle n_i \rangle. \end{aligned} \tag{3.8}$$

With $\omega = 0.6$ we were able to solve the set (3.4) within about forty (!) iterations and obtained a solution $\overline{\langle n_i \rangle}$ such that for most of the parameters Ω, T we have

$$\eta = \sum_i \left\{ \frac{\overline{\langle n_i \rangle} - g_i(\overline{\langle n_1 \rangle}, \ldots, \overline{\langle n_N \rangle})}{g_i(\overline{\langle n_1 \rangle}, \ldots, \overline{\langle n_N \rangle})} \right\}^2 < 10^{-6}. \tag{3.9}$$

The equations were ordered according to descending fragment masses $A_i = Z_i + N_i$. This has the advantage that the first equations needed only a few $\langle n_k \rangle$ because of the triangular conditions (3.2). The starting values of $\langle n_i \rangle$ were calculated by assuming a pure binary (fission) decay. I.e., in formula (3.2) we set $\langle n_k \rangle_i = 1$ for $Z_k + Z_i = Z_{\text{total}}$, $N_k + N_i = N_{\text{total}}$, and zero otherwise.

There were characteristic regions in Ω, T, where the set of Eqs. (3.4) converged very slowly or not at all. This happened in the neighborhood of the phase-transition

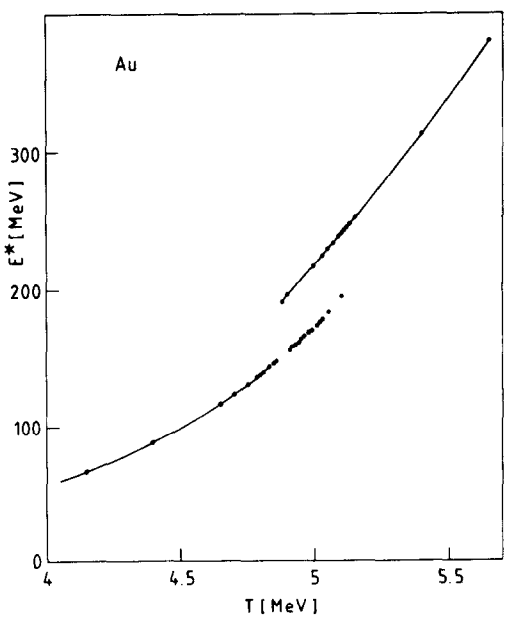

FIG. 1. Excitation energy of an *Au*-system at $\sim \frac{1}{3}$ normal nuclear density as a function of the temperature T. At about $T \sim 5$ MeV the system has a phase transition of first order with a latent heat of ~ 46 MeV. Here the system of equations becomes unstable and two solutions are obtained. The lines are to guide the eye. The solutions which we found are indicated by dots. The accuracy of the energy is of the order of 10^{-3} everywhere.

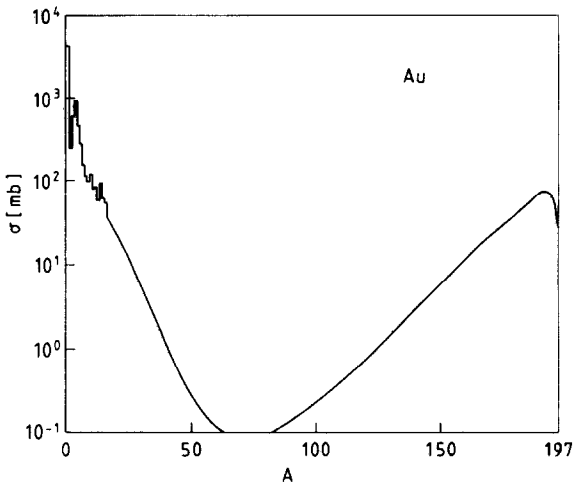

FIG. 2. Distributions of the fragment masses in absolute cross sections at $T = 4.86$ MeV. The mean multiplicities $\langle n_i \rangle$ defined in the text can be obtained by dividing the cross section by the total cross section $\sigma = 46 \cdot A^{0.69} = 1.76 \cdot 10^3$ [mb]. I.e., the $\langle n_i \rangle$ vary between $5 \cdot 10^{-5}$ and ~ 2. The accuracy obtained in 80 steps is $\eta = 7.8 \cdot 10^{-6}$. This type of mass distribution is characteristic for the lower branch (lower phase) in Fig. 1. It varies only smoothly along the lower curve.

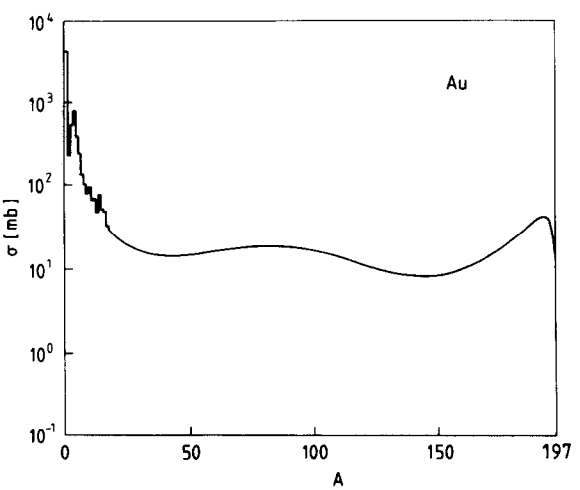

FIG. 3. The same as in Fig. 2 but now with $T = 4.88$ MeV. Observe the sharp change of the distribution for medium masses by about 3 orders of magnitude. The accuracy obtained in 80 steps is $\eta = 1.5 \cdot 10^{-3}$. This type of mass distribution is characteristic for the upper branch (upper phase) in Fig. 1. It varies only smoothly along the upper curve.

points of the system. Here our physical system has large fluctuations [6] and a mean field calculation tends to become unstable. Very often, a random ensemble for ω out of $I=(0.3, 1.3)$ produced fast convergence in these cases also. To illustrate the power of our method at such a most difficult point, we present the results for values of Ω, T close to a phase-transition point for the decay of an Au-system (see Fig. 1). At temperatures between $T\sim 4.86$ MeV and ~ 5.1 MeV and at a density of about $\frac{1}{4}-\frac{1}{9}$ the normal nuclear density (the parameters r_0 defined in [5] are chosen as $r_{0c}=2.45$ fm, $r_0=1.5$ fm) the mean excitation energy E^* jumps by ~ 46 MeV. The mass distribution of the fragments, which is deeply U-shaped and varies only slowly for all $T<4.86$ MeV, jumps to one which has a "fission peak" at about half the mass of the system for $T>5.1$ MeV (Figs. 2, 3). The latent heat is connected to a sudden opening of the "fission" channel. The physical implications of these phase transitions are further discussed in [5, 6]. From the point of view of the numerical method it is interesting that, even within the range of the phase transition, we could get a convergence to one of the two possible solutions or both in about 80 steps up to an accuracy $\eta\sim 10^{-3}$.

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