

Newton's constant of gravitation and verified numerical quadrature

OLIVER HOLZMANN, BRUNO LANG, and HOLGER SCHÜTT

In this paper we describe the use of interval arithmetic in an experiment for determining G , Newton's constant of gravitation. Using an interval version of Gaussian quadrature, we bound the effects of numerical errors and of several tolerances in the physical experiment. This allowed to identify "critical" tolerances which must be reduced in order to obtain G with the desired accuracy.

Гравитационная постоянная Ньютона и верифицированная численная квадратура

О. ХОЛЬЦМАНН, Б. ЛАНГ, Х. ШЮТТ

Описывается использование интервальной арифметики в эксперименте по определению гравитационной постоянной Ньютона G . С помощью интервального варианта квадратуры Гаусса определяются границы численных погрешностей и некоторых допусков в физическом эксперименте. Таким образом, оказалось возможным найти критические допуски, величина которых должна быть уменьшена для достижения требуемой точности G .

1. Introduction

Of all the fundamental physical constants, the Newtonian constant of gravitation G is known with the least precision. The CODATA (Committee on Data for Science and Technology of the International Council of Scientific Unions) recommends the value $G = 6.67259 \cdot 10^{-11} \text{ m}^3\text{kg}^{-1}\text{s}^2$ with a relative uncertainty of $1.28 \cdot 10^{-4}$ [1]. Since gravitation is the most obvious physical force in everyday life and the dominant force in medium to very large distance ranges, much effort has been undertaken to determine this constant to a higher precision [4].

Several different experiments have been made in the last few years. Some of the results are claimed to have a relative error of less than 10^{-4} [2, 9]. However, since these results differ from each other by more than 10^{-3} , not all of them are correct. Therefore, care must be taken to monitor every possible error introduced in the physical experiment itself and in the following computations.

One of the experiments for determining G takes place at the University of Wuppertal [13, 14]. Its ultimate goal is to obtain a value for G with a relative uncertainty in the order of 10^{-5} . The project described in this paper was initiated to provide verified bounds for an important intermediate result in the computational part of the experiment and to investigate the sensitivity of this result to tolerances in the geometry of the experiment [5].

In the following section, we shortly summarize the physical background of the experiment. In Section 3 the goal of our project is specified. Then we briefly describe how the verified computations were done using Gaussian quadrature with result verification. In Section 5 we report the results.

2. Physical background

The experiment used in Wuppertal is sketched in Figure 1. Its main components are two massive cylinders (*field masses*) M_1 , M_2 made of brass and a pair of pendulums whose bodies P_1 , P_2 are positioned midway between the field masses. The four bodies are all aligned on a common axis of symmetry, and the field masses can be moved along this axis. When M_1 is moved from the “far” position (solid lines in Figure 1) to the “near” position (dotted lines) then its attractive force to both pendulums increases, causing them to move towards M_1 . As the force is inversely proportional to the square of the distance, P_1 is deflected more than P_2 , and the distance b between the pendulums increases by a small amount Δb . When both field masses move synchronously, Δb doubles. (The main reason for using two field masses is that some systematic errors almost cancel out due to the symmetry.)

Although the field masses are quite heavy (each weighing more than half a ton), the value Δb is tiny (approximately 12 nm). To be able to measure these small relative movements with high accuracy, the inner faces of the pendulums are spherical mirrors, so that together they work as a microwave resonator (*Fabry-Pérot resonator*). Thus, increasing the distance between the pendulums decreases the frequency of resonance, which in turn can be measured to very high accuracy.

The constant G is obtained by equating the measured value of Δb with a value computed as follows [5, 13].

According to Newton’s law of gravitation, a point mass m_1 is attracted by another point mass m_2 with the force

$$F = G \frac{m_1 m_2}{\|d\|^2} \cdot \hat{d}$$

where $d \in \mathbb{R}^3$ is the vector from the first mass m_1 to the second mass m_2 and $\hat{d} = d/\|d\|$. Therefore, the pendulum P_i is attracted by the field mass M_j with the force

$$F_{ij} = G \int_{P_i} \int_{M_j} \frac{\rho_i \rho_j d}{\|d\|^3} dV_j dV_i$$

where the integration is over the volumes of the bodies and ρ_i , ρ_j denote the density functions within the pendulum and the field mass, resp.

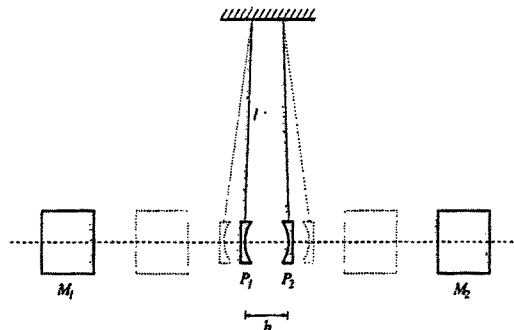


Figure 1. The principle of the experiment. Solid and dotted lines denote the “far” and “near” position, resp. (the movement of the pendulums is extremely over-emphasized). The common symmetry axis is shown as a dashed line

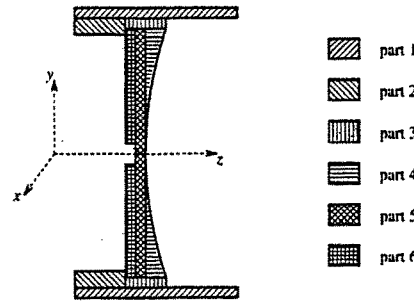


Figure 2. Decomposition of the pendulum's body into six parts

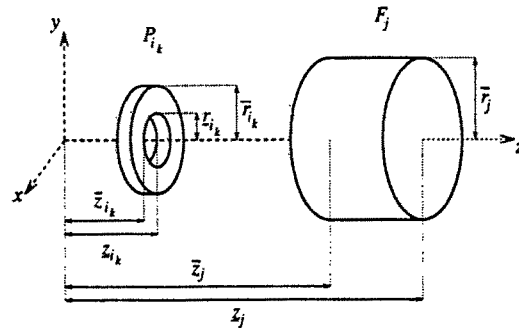


Figure 3. Coordinate system used in the integration

To facilitate the integration, the pendulum is decomposed into six simpler shaped parts P_{i_k} , see Figure 2. Thus we have $F_{ij} = \sum_{k=1}^6 F_{i_k j}$, where

$$F_{i_k j} = G \int_{P_{i_k}} \int_{M_j} \frac{\rho_i \rho_j d}{||d||^3} dV_j dV_{i_k}.$$

Making use of the common axis of symmetry, we introduce cylindrical coordinates (see Figure 3):

$$P_{i_k} = \{(r_i \cos \varphi_i, r_i \sin \varphi_i, z_i) : r_i \in [r_{i_k}, \bar{r}_{i_k}], \varphi_i \in [0, 2\pi], z_i \in [z_{i_k}, \bar{z}_{i_k}]\},$$

$$M_j = \{(r_j \cos \varphi_j, r_j \sin \varphi_j, z_j) : r_j \in [0, \bar{r}_j], \varphi_j \in [0, 2\pi], z_j \in [z_j, \bar{z}_j]\}.$$

Note that for part 4 from Figure 2, \bar{z}_{i_k} is a function of r_i . Then, the volume integral becomes

$$F_{i_k j} = G \int_{r_{i_k}}^{\bar{r}_{i_k}} \int_0^{2\pi} \int_{z_{i_k}}^{\bar{z}_{i_k}(r_i)} \int_0^{\bar{r}_j} \int_0^{2\pi} \int_{z_j}^{\bar{z}_j} \frac{\rho_i \rho_j d}{||d||^3} r_i r_j dz_j d\varphi_j dr_j dz_i d\varphi_i dr_i$$

where $d = (r_j \cos \varphi_j - r_i \cos \varphi_i, r_j \sin \varphi_j - r_i \sin \varphi_i, z_j - z_i)$. Substituting $\varphi = \varphi_i - \varphi_j$ and $\phi = \varphi_i + \varphi_j$ one obtains

$$F_{i_k j} = \frac{G}{2} \int_{r_{i_k}}^{\bar{r}_{i_k}} \int_0^{\bar{r}_j} \int_0^{2\pi} \int_{z_{i_k}}^{\bar{z}_{i_k}} \int_{z_j}^{\bar{z}_j} \int_0^{4\pi} \frac{\rho_i \rho_j d}{||d||^3} r_i r_j d\phi dz_j dz_i d\varphi dr_j dr_i \quad (1)$$

with

$$d = \begin{pmatrix} r_j \cos \frac{\phi - \varphi}{2} - r_i \cos \frac{\phi + \varphi}{2} \\ r_j \sin \frac{\phi - \varphi}{2} - r_i \sin \frac{\phi + \varphi}{2} \\ z_j - z_i \end{pmatrix} \quad (2)$$

and

$$\|d\| = \sqrt{r_j^2 + r_i^2 - 2r_j r_i \cos \varphi + (z_j - z_i)^2}. \quad (3)$$

If we assume radial density profiles (i.e., that ρ_i and ρ_j are functions of r_i and r_j , resp.), then the innermost integral can be evaluated explicitly. In particular, its x and y components are zero. Therefore, only the z component of $F_{i,kj}$ must be computed:

$$F_{i,kj} = 2\pi G \int_{r_{i,k}}^{\bar{r}_{i,k}} \rho_i r_i \int_0^{\bar{r}_j} \rho_j r_j \int_0^{2\pi} \int_{\bar{z}_{i,k}}^{\bar{z}_j} \frac{z_j - z_i}{\sqrt{a + (z_j - z_i)^2}^3} dz_j dz_i d\varphi dr_j dr_i \quad (4)$$

where $a = r_j^2 + r_i^2 - 2r_j r_i \cos \varphi \geq 0$. Again, the innermost integration can be done analytically:

$$F_{i,kj} = 2\pi G \int_{r_{i,k}}^{\bar{r}_{i,k}} \rho_i r_i \int_0^{\bar{r}_j} \rho_j r_j \int_0^{2\pi} \int_{\bar{z}_{i,k}}^{\bar{z}_j} f(r_i, r_j, \varphi, z_i) dz_i d\varphi dr_j dr_i \quad (5)$$

with $f(r_i, r_j, \varphi, z_i) = 1/\sqrt{a + (z_j - z_i)^2} - 1/\sqrt{a + (\bar{z}_j - z_i)^2}$. For *non-verified* numerical evaluation (see the remark in Section 4) with a Gaussian quadrature method, the integrals can be further simplified with the substitutions $x = z_j - z_i$ and $y = \bar{z}_j - z_i$ and the indefinite integral

$$\int \frac{1}{\sqrt{a + x^2}} dx = \log(x + \sqrt{a + x^2}) + C. \quad (6)$$

Thus, computing $F_{i,kj}$ amounts to numerically evaluating a triple integral.

In a final step, Δb is obtained from the $F_{i,kj}$ values. The two masses generate the force

$$F_i = \sum_{j=1}^2 \sum_{k=1}^6 F_{i,kj}$$

on the pendulum P_i , resulting in the pendulum's deflection from the rest position:

$$\Delta z_i = \frac{F_i}{m_i \omega_i^2}.$$

Here, m_i and $\omega_i = \sqrt{g/l_i}$ denote the pendulum's mass and frequency, resp. Therefore, placing the field masses at a certain position "pos" increases the distance of the pendulums by

$$\Delta b(\text{pos}) = \Delta z_1(\text{pos}) + \Delta z_2(\text{pos})$$

as compared to having no field masses. Moving the field masses from the "far" to the "near" position causes the distance to change by

$$\Delta b = \Delta b(\text{near}) - \Delta b(\text{far}). \quad (7)$$

Note that 48 integrations $F_{i,kj}$ are necessary to compute this value Δb which, together with the measured value, yields G .

3. The goal of the project

It is clear from the previous section that Δb must be measured and computed to high accuracy to yield G with small relative uncertainty. In the experiment, Δb can be measured with a relative error well below 10^{-4} . Therefore, the error in the computed value should not be significantly larger. This error consists of two components:

- Numerical errors: Using a quadrature formula yields only approximations to the exact values of the integrals. In addition, rounding errors are made during the computations.
- Geometrical errors: The arguments of Section 2 made heavy use of the alignment of all four bodies on a common axis of symmetry. In practice, this perfect geometry cannot be achieved. In addition, the dimensions of the bodies are only known within certain tolerances.

Interval arithmetic provides adequate means to capture both categories of uncertainty. The goal of this project was to use interval arithmetic to answer (if possible) the following questions:

- Assuming a perfect geometry, can we guarantee a relative (numerical) error $\leq 10^{-5}$?
- Are the tolerances in the geometry small enough to guarantee a relative error $\leq 10^{-5}$?
In particular, tolerances in the following dimensions were to be investigated:
 - the radii and heights of the field masses M_j ,
 - the dimensions of the pendulums,
 - the distance of the field masses from each other,
 - the displacement of the pair of pendulums from the midpoint
 - * along the axis of symmetry and
 - * perpendicular to this axis,
 - a twisted resonator, and
 - tilted field masses.

4. Gaussian quadrature with result verification

There exist a number of algorithms for numerical integration with result verification (see, e.g., [7]). The sophisticated integration program [11] turned out to be not fully adequate for our particular application because its *adaptive* part took an excessive number of recursive subdivisions in order to achieve the prescribed accuracy. Instead, we used multidimensional Gaussian quadrature [8, 12] with inclusion of the remainder term, preceded by a *static* subdivision of the integration domain [3], to enclose the multiple integrals that arise in the computation of $F_{i,kj}$.

The following enclosures are needed to evaluate an n -dimensional $m \times m \times \dots \times m$ point Gaussian quadrature formula (a *product* of n one-dimensional m point formulae) with result verification.

- Enclosures $[x_i]$, $[A_i]$, and $[e]$ for the nodes, weights, and the norming factor in the remainder term, resp., of the *one-dimensional* m point quadrature formula. These enclosures were provided by Ulrike Storck [10].

- Enclosures for the range of f over the small boxes $\mathbf{x}_I = [x_{i_1}] \times [x_{i_2}] \times \cdots \times [x_{i_n}]$ that contain the nodes of the multidimensional Gaussian formula. These were obtained using the “natural” (“naive”) interval evaluation of f .
- Enclosures $[D_i^{2m}]$ for the range of the partial derivatives $\partial^{2m} f / \partial x_i^{2m}$ over the whole domain of integration. These were computed at runtime using the `mitaylor` module by Ulrike Storck, which works with automatic differentiation.

In order to reduce the diameter of the resulting enclosure for the integral, the integration domain was split. In the following, the shorthand $\text{Gauss}(s, m)$ indicates that the domain of integration was subdivided into s parts *along each axis* (that is, into s^n subdomains) and that an $m \times m \times \cdots \times m$ point Gaussian quadrature formula was used on each subdomain.

Remark. The last simplification (6) of the integrals in Section 2 cannot be made in the context of interval evaluation and automatic differentiation. This representation of the indefinite integral is only valid if $a > 0$. But a is zero on two line segments on the boundary of the integration domain D (both given by the relations $r_i = r_j$ and $\cos \varphi = 1$). There we have $\int x^{-1} dx = \log x + C$. Thus, the right hand side of (6) is not a valid representation of the integrand over the whole domain D . This fact goes unnoticed in (non-verified) Gaussian quadrature, because the nodes of the Gaussian formula are chosen from the interior of D . For the interval evaluation of the partial derivatives, however, the boundary of D is included in the computations. Therefore, we had to use the quadruple integral (5) to enclose F_{ikj} .

5. Numerical results

The computations were done on a SUN SPARCstation 10 using Pascal-XSC [6]. We first considered the effect of numerical errors alone. Then, the influence of various tolerances in the geometry of the experiment was investigated, where the ranges of these tolerances were provided by the experimental physicists. If not explicitly stated otherwise, both—geometrical and numerical—errors are captured in the following results.

As pointed out in Section 3, geometrical tolerances are considered “adequate” if they do not cause the relative uncertainty $\varepsilon_{\Delta b}$ in Δb to exceed 10^{-5} .

5.1. Perfect geometry

For the reasons given in Section 4, the simplification (6) could not be made when interval arithmetic and automatic differentiation were used. Instead, we had to compute the quadruple integrals (5) even when a perfect alignment of the bodies was assumed. With $\text{Gauss}(2, 7)$ we obtained the inclusion

$$\Delta b \in [11.839672, 11.839691] \text{ nm}$$

implying $\varepsilon_{\Delta b} < 10^{-6}$. Thus, the numerical errors alone do not obstruct the desired accuracy.

5.2. Tolerances in the dimensions of the field masses

The tolerances for the diameter and height of each field mass are ± 0.3 mm. Since the mass of M_j is known with a relative precision $\approx 10^{-6}$ it can be considered constant. Therefore, changes Δh_j in the height were compensated by appropriately changing the diameter. The biggest

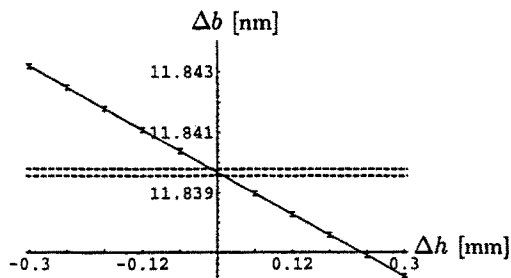


Figure 4. Variation of the height of the field masses. The error bars show the resulting intervals for the eleven equidistant values of Δh which were considered, while the dashed horizontal lines indicate the “acceptable” area (the relative uncertainty $\varepsilon_{\Delta b}$ in Δb is $< 10^{-5}$). The line connecting the midpoints of the intervals *approximates* the (seemingly almost linear) functional dependence of Δb on Δh

deviations in Δb occurred when both cylinders were altered in the same way, i.e., $\text{sign } \Delta h_1 = \text{sign } \Delta h_2$. For this reason we will only report the results obtained with $\Delta h_1 = \Delta h_2 =: \Delta h$.

The computations with Gauss(2,6) for the quadruple integrals (5) revealed a big influence of Δh on Δb , see Figure 4. Only for $\Delta h = 0$ the desired bound $\varepsilon_{\Delta b} < 10^{-5}$ can be guaranteed; for all other values of Δh that we have tried in our experiments (see Figure 4), the error Δb varies by more than this amount. A second set of runs with $\Delta h \in [-0.04, 0.04]$ mm showed that the height of the field masses must be known to ± 0.01 mm in order to have $\varepsilon_{\Delta b} < 10^{-5}$.

5.3. Tolerances in the dimensions of the pendulum bodies

Due to a high precision manufacturing process, the tolerances in the dimensions of the pendulum bodies are only $\pm 1 \mu\text{m}$. In contrast, their masses are not known with comparable precision. Therefore, the volume and the mass of the bodies were changed for the computation. More precisely, the boundaries were uniformly offset towards the interior (“shrink”) or exterior (“blow up”).

Again, the quadruple integrals (5) were evaluated with Gauss(2,7). (With a six point formula, the small deviations of Δb were completely shadowed by the widths of the resulting intervals.)

The precision of the pendulums seems to be sufficient, as $\varepsilon_{\Delta b} < 7.5 \cdot 10^{-6}$ over the whole range of tolerance.

5.4. Tolerance in the distance of the field masses

An optical procedure was used to measure the distance d from one field mass to the other with a tolerance of $\pm 20 \mu\text{m}$. As in Section 5.3, Gauss(2,7) was used to evaluate the quadruple integrals (5).

The computations revealed that the tolerance must be reduced to $\pm 5 \mu\text{m}$ in order to guarantee $\varepsilon_{\Delta b} < 10^{-5}$, see Figure 5. This tolerance must also cover the effects of thermic

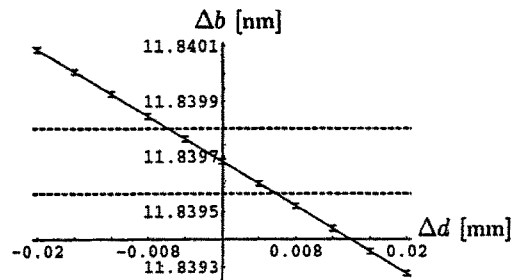


Figure 5. Tolerance in the distance of the field masses from each other

expansion on the transport mechanism which is used to move the field masses. Therefore, either the temperature or the distance must be monitored permanently.

5.5. Displacement of the pendulums

Since the pendulums are placed in a vacuum tank it is difficult to determine their exact position, e.g., with respect to the field masses. Therefore, the tolerance for the offset of the pair of pendulums from the midpoint is quite large: ± 1.0 mm.

We first considered a displacement Δz along the axis of symmetry. The computations with Gauss(2,7) for the quadruple integrals (5) yielded $\varepsilon_{\Delta b} \lesssim 10^{-5}$ over the whole range, see Figure 6. Thus, the big tolerance is acceptable.

Note that Δb attains its minimum not at $\Delta z = 0$ (i.e., when the pair of pendulums is placed exactly midway between the field masses), but at a small offset. This asymmetry comes from the fact that the field masses differ slightly, as do the masses of the pendulums.

For investigating offsets perpendicular to the axis of the field masses, it is sufficient to consider a single direction (e.g., the x direction). In contrast to all previous arrangements of the bodies, the force now has nonzero components in the z and x directions, and the coordinate systems in the cylindrical parameterizations of P_{ik} and M_j do not coincide. Therefore, the distance d and its norm in (1) slightly differ from (2) and (3), resp.

Let us first consider the computation of the (dominating) z component of the force. Now the innermost of the six integrals can no longer be evaluated explicitly. But still the integration over the height of the field mass can be done similarly to the transition from (4) to (5). Since

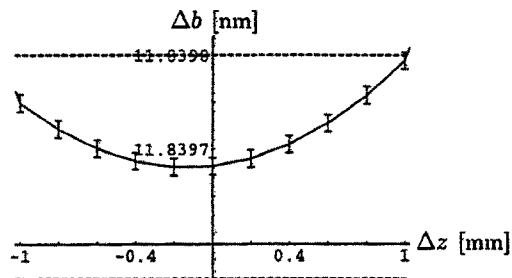


Figure 6. Displacement of the pair of pendulums along the axis of symmetry

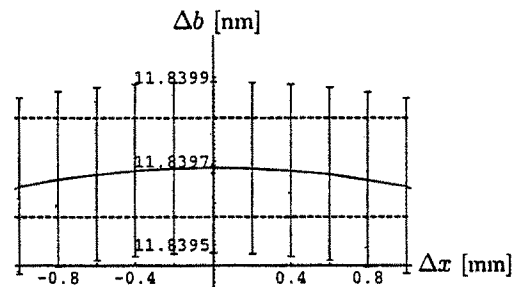


Figure 7. Displacement of the pair of pendulums perpendicularly to the axis of symmetry

the integration over z_i cannot be done analytically in the context of result verification (see the remark in Section 4), a five-dimensional integral must be evaluated numerically. Here, the limits of our integration algorithm were reached. While the midpoints of the resulting intervals for Δb clearly fulfill the desired relation $\varepsilon_{\Delta b} < 10^{-5}$ (see Figure 7), the intervals are too wide to allow guaranteeing this bound. But as the bound is exceeded only by a small factor and the computations with Gauss(2,6) already took some days, we did not switch to a higher order formula.

For the computation of the x component of the force, the situation seems even worse because the full six-dimensional integral must be computed numerically. Fortunately, though, a “cheap” four point formula was sufficient to prove that this component does not cause relative changes $> 10^{-5}$ in Δb . (On the other hand, the results did not even allow to determine the *direction* of the pendulums’ movement.)

5.6. Twisted pendulums and tilted field masses

With these changes in the geometry, different coordinate systems must be chosen for the pendulums and the field masses, which means that none of the six integrals in (1) can be solved analytically. In addition, all three components of the force may be nonzero. A rough estimate for the computation time yielded some *months*, if reasonably narrow guaranteed bounds are required.

Therefore, the computations for these two tolerances were done with a lower order quadrature formula and *without inclusion of the remainder term*. The results suggest (but do not prove) that the orientation of the pendulums and of the field masses is known with an adequate precision.

6. Conclusions

By using interval arithmetic we were able to give guaranteed bounds for the effect of rounding errors and of geometrical tolerances to the computed value Δb . Some of these effects had already been estimated (using standard Gaussian integration from a numerical library), and their magnitude could be confirmed. For other effects (e.g., numerical errors and tolerances in the dimensions of the field masses) no quantitative estimates were known before.

We could identify some tolerances that must be reduced substantially in order to obtain the ultimately desired relative accuracy $\approx 10^{-5}$ for G . In particular, it became clear that

the temperature must be controlled to ± 0.2 degrees centigrade. But it must be emphasized that even with the current values of these tolerances the accuracy for G is comparable to experiments made at other sites.

For the effect of a few tolerances no guaranteed bounds could be computed because the six-dimensional integration takes too much time. A parallel implementation is planned to alleviate this problem.

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O. HOLZMANN, B. LANG
Bergische Universität GH Wuppertal
Fachbereich Mathematik
Gastr. 20, 42097 Wuppertal
Germany
E-mail: {oholzma, lang}@math.uni-wuppertal.de

H. SCHÜTT
Bergische Universität GH Wuppertal
Fachbereich Physik
Gastr. 20, 42097 Wuppertal
Germany
E-mail: schuett@wpos4.physik.uni-wuppertal.de