COMPUTER ASSISTED LOWER BOUNDS
FOR ATOMIC ENERGIES

LUIS A. SECO *

Abstract. For an atom of nuclear charge Z, the ground state energy is defined to be the lowest possible value of the energy Hamiltonian. We describe an algorithm to produce rigorous lower bounds for the ground state energy of atoms as well as its implementation.

0. Introduction.

The Hamiltonian for an atom of charge Z is

$$H = \sum_{i=1}^{Z} \left[\left(-\tfrac{1}{2}\Delta_{x_i}\right) - \frac{Z}{|x_i|} \right] + \frac{1}{2} \sum_{i \neq j} \frac{1}{|x_i - x_j|}$$

acting on

$$\mathcal{H} = \bigwedge_{i=1}^{Z} \left(L^2\left(\mathbf{R}^3\right) \otimes \mathbf{C}^2 \right) \tag{0.1}$$

The antisymmetric tensor product "$\wedge$" has to do with Pauli's exclusion principle, and $L^2\left(\mathbf{R}^3\right) \otimes \mathbf{C}^2$ is the set of states of one electron with two spins. We will refer to $\mathcal{H}$ as the space of antisymmetric wave functions. It is an important problem in Quantum Mechanics to compute good bounds for the ground state energy of the atom,

$$E = \inf_{\lambda \in Spec(H)} \lambda = \inf_{\substack{\psi \in \mathcal{H} \\ \|\psi\|_2 = 1}} \langle H\psi, \psi \rangle$$

Upper bounds to E can be obtained by restricting the infimum in the definition to a smaller class of functions. In Hartree-Fock method, for example, the infimum is taken over functions that can be written as antisymmetric products of one–electron functions. See [FF] for more information on upper bounds.

The problem of obtaining lower bounds is considerably more complicated, and was treated numerically before by Hertel, Lieb and Thirring in [HLT]. In this paper we will

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* Department of Mathematics, Princeton University. Supported by a Sloan Foundation Dissertation Fellowship

present very general ideas to improve the lower bounds they obtained that will moreover produce rigorous results. For complete information and refinements of this method, see [Se].

The basic idea of the method is to construct a radial function $V(|x|)$ and a constant C such that

$$\frac{1}{2}\sum_{i\neq j}\frac{1}{|x_i-x_j|}\geq\sum_{i=1}^{Z}V(|x_i|)-C. \tag{0.2}$$

which provides the operator inequality

$$H\geq\sum_{i=1}^{Z}\left(-\tfrac{1}{2}\Delta_{x_i}-\frac{Z}{|x_i|}+V(|x_i|)\right)-C$$

This implies that, if $\lambda_1<\cdots<\lambda_n<\cdots<0$ are the negative eigenvalues of

$$-\tfrac{1}{2}\Delta-\frac{Z}{|x|}+V(|x|)\overset{\text{def}}{=}H^{1\text{ electron}}$$

then

$$E\geq\begin{cases}2\displaystyle\sum_{i=1}^{Z/2}\lambda_i-C & Z\text{ even}\\[2ex] 2\displaystyle\sum_{i=1}^{(Z-1)/2}\lambda_i+\lambda_{(Z+1)/2}-C & Z\text{ odd}\end{cases}$$

The factor 2 appears because, by (0.1), eigenvalues come with multiplicity 2: one for each spin.

Separation of variables tells us then that the negative eigenvalues of $H^{1\text{ electron}}$ are the same as the negative eigenvalues of the ODE operator

$$-\tfrac{1}{2}u''-\left(\frac{Z}{r}-\frac{l(l+1)}{2r^2}-V(r)\right)u \tag{0.3}$$

acting on

$$\mathcal{H}_{\text{ODE}}=\left\{f:r^{-1}\cdot f(r)\in L^2[0,\infty)\right\}$$

for $l=0,1,2,\ldots$; every eigenvalue has multiplicity $2l+1$. For our eigenvalue problem, this space is equivalent to $L^2(0,\infty)$ with Dirichlet boundary conditions at 0 and ∞.

This ODE in general cannot be solved explicitly, but we will still be able to estimate its eigenvalues. For this, we will use computer assisted techniques, as will be explained in section 3.

1. The Potential. In order to obtain V and C in (0.2), we use an idea introduced in [FLl]; they wrote

$$\frac{1}{|x-y|} = \frac{1}{\pi}\int_{R>0}\int_{z\in\mathbf{R}^3} \chi_{B(z,R)}(x)\cdot\chi_{B(z,R)}(y)\,\frac{dz\,dR}{R^5}$$

where $\chi_{B(z,R)}$ is the characteristic function of the ball $B(z,R)$. This implies that

$$\frac{1}{2}\sum_{i\neq j}\frac{1}{|x_i-x_j|} = \frac{1}{2\pi}\int_{R>0}\int_{z\in\mathbf{R}^3} N(N-1)\frac{dzdR}{R^5}$$

where

$$N = N(x_1,\ldots,x_Z;z,R) = \sum_{i=1}^{Z}\chi_{B(z,R)}(x_i)$$

is the number of x_i that belong to $B(z,R)$.

Observe that given *any* function $\bar N = \bar N(z,R)$ defined in the space of all balls in $\mathbf{R}^3$ that takes values $k + 1/2$ with k a nonnegative integer, we have

$$N(N-1) = (N-\bar N)^2 + (2\bar N - 1)N - \bar N^2 \geq \frac{1}{4} + (2\bar N-1)N - \bar N^2$$

therefore,

$$\begin{aligned}\frac{1}{2}\sum_{i\neq j}\frac{1}{|x_i-x_j|} &\geq \frac{1}{2\pi}\sum_{i=1}^{Z}\iint(2\bar N-1)\chi_{B(z,R)}(x_i)\,\frac{dz\,dR}{R^5} - \frac{1}{2\pi}\iint\left(\bar N^2 - 1/4\right)\,\frac{dz\,dR}{R^5}\\ &= \sum_{i=1}^{Z}V(|x_i|) - C.\end{aligned}$$

with

$$\begin{aligned}V(|x|) &= \frac{1}{2\pi}\iint_{\substack{|z-x|<R\\ R>0}} 2(\bar N(z,R)-1)\,\frac{dz\,dR}{R^5}\\ C &= \frac{1}{2\pi}\iint\left(\bar N^2(z,R) - 1/4\right)\,\frac{dz\,dR}{R^5}.\end{aligned}$$

Note that whatever our choice of $\bar N(z,R)$ we obtain a lower bound; however, different choices of $\bar N$ will give different results, and it is important to make a good choice for $\bar N$. The way $\bar N$ is chosen is by selecting a charge density $\rho(x)\geq 0$, with $\int_{\mathbf{R}^3}\rho(x)dx = Z$ that we believe (but need not prove) is close to the real one, and then choose $\bar{N}$ according to the following rule:

Define functions $R_i(z)$, $1 \leq i \leq Z-1$, in such a way that

$$\int_{B(z,R_i(z))} \rho(x)dx = i.$$

Then, set

$$\bar{N}(z,R) = \begin{cases} 1/2 & \text{if } R < R_1(z) \\ i + 1/2 & \text{if } R_i(z) < R < R_{i+1}(z) \\ Z - 1/2 & \text{if } R > R_{Z-1}(z) \end{cases}$$

The freedom in choosing $\bar{N}$ then translates in the freedom to choose the R_i. This has as a consequence that we can make our potential V have the following properties:

1. If we take the R_i to be piecewise-linear functions in $|z|$, we can write the integrals over $\mathbf{R}_+^4$ in elementary terms that involve only sums of rational expressions of degree at most 5.

   Since we can approximate any such R_i by piecewise linear functions, this is not a severe restriction.

2. The potential is piecewise analytic, i. e., there exist finitely many points

   $$\infty > x_0 > x_1 > \cdots > x_n > 0$$

   such that V has a power series expansion around each x_i convergent in a disk that contains both x_{i-1} and x_{i+1}, and V agrees with this power series *to the left* of x_i. Globally, V has in general only 1 continuous derivative, (except at x_0 and x_n where it is merely continuous) and all discontinuities happen at the x_i. Moreover, the partition $\{x_i\}$ can be refined as needed. This will be useful, for example, to obtain small steps for the ODE solver.

3. V is constant around 0, i. e.

   $$V(x) = \text{ constant} \qquad 0 \leq x \leq x_n \tag{1.1}$$

4. Around ∞, V can be taken to have the special form

   $$V(x) = \frac{2\lambda k}{x} - \frac{l(l+1)}{x^2} \qquad x \geq x_0 \tag{1.2}$$

where λ is any positive number and k is a positive integer that depends on λ.

2. The Functional Analysis. The underlying Banach space in this theory is the space of piecewise analytic functions, with a lower bound on the size of the domains of analyticity. The purpose of this section is to formalize definitions and set up the framework for computer assisted analysis in function space. For similar and more detailed analysis, see [Ra], [EKW], [EW], [Mo] and [KM], for example.

Consider the Banach space

$$H^1 = \left\{ f(z) \;\middle|\; f(z) = \sum_{n=0}^{\infty} a_n\, z^n, \quad \sum_{n=0}^{\infty} a_n < \infty \right\}$$

with norm

$$\|f\| = \sum_{n=0}^{\infty} |a_n|$$

This is a subspace of the set of analytic functions in the unit disk, that becomes a Banach Algebra with $\| \, \|$.

We consider a neighborhood basis consisting of sets of the form

$$\mathcal{U}(I_1, \ldots, I_N; C) = \left\{ f(z) = \sum_{n=0}^{\infty} a_n\, z^n \,\middle|\, a_n \in I_n, \quad 0 \le n \le N, \sum_{n=N+1}^{\infty} |a_n| \le C \right\} \tag{2.1}$$

where C is a positive real number and I_n are intervals in the real line. For the computer implementation, C will run over $\mathcal{R}$, the set of computer-representable numbers, and the intervals will be those with representable endpoints; we call denote as $\mathcal{I}$ the set of this intervals.

The reason why this is a convenient space to work in is because elementary operations, such as addition, product, integration, differentiation (composed with a slightly contracting dilation), evaluation at points in the domain of analyticity and integration of initial value problems in ordinary differential equations are expressible by elementary formulas in terms of this set of neighborhoods. The question is now how to perform these elementary computations in an exact way using a computer. For this we use interval arithmetic. Although this point is something that several articles in these Proceedings are going to discuss, here is a very brief account of the technique:

Let $\mathcal{R}$ be the set of computer representable numbers. Given any real number r, the idea is to work with an interval in which r is contained, $[r_1, r_2]$ with $r_1, r_2 \in \mathcal{R}$, and translate in terms of these intervals whatever manipulation we intend to do with real numbers. In this way, matters are reduced to obtaining upper and lower bounds for manipulations of representable numbers in terms of representable numbers. This is possible using the capabilities of a computer. Standard references for these ideas are [KM] and [Mo] .

Observe that if we have a function $f(z)$ which is analytic in some disk, $|z - z_0| < r$, then, for any $\tilde{r} < r$, if we define $\tilde{f}(\tilde{z}) = f(\frac{\tilde{z}-z_0}{\tilde{r}})$, then $\tilde{f} \in H^1$. This allows to translate analytic functions into functions in H^1 of the unit disk.

In the real analytic case, $H^1[a,b]$ will denote H^1 of the disc with center a and radius $|b-a|$.

In the previous section, we saw that we will have to deal with functions with are sums of rational expressions. It is immediate to produce neighborhoods of type (2.1) that contain these functions locally.

3. The ODE. In this section we will discuss how our ODE problem (0.3) can be dealt with using the functional analysis introduced in the previous section. This presentation is taylored to deal with our special problem, but it can be modified trivially, at the expanse of complication, to deal with more general problems.

We consider first the solution of initial value problems. Lemma 3.1 below takes care of the solutions of an IVP with analytic coefficients. Lemmas 3.2 and 3.3 take care of the expansion of the solutions at the singularities of the ODE, around 0 and ∞. All three lemmas can be proved by matching coefficients.

Lemma 3.1: *Consider the ODE:*

$$\left.\begin{aligned} u'' + qu &= 0 \\ u(0) &= u_0 \\ u'(0) &= u_1 \end{aligned}\right\}$$

where $q(x) \in \mathcal{U}\,(q_0, \cdots, q_N; \delta)$. Then, $u \in \mathcal{U}(u_0, \cdots, u_{N+2}; C)$ where

$$u_{n+2} = -\frac{1}{(n+2)(n+1)} \sum_{i=0}^{n} u_i q_{n-i} \qquad 0 \le n \le N$$

and

$$C \le \frac{\displaystyle\sum_{i=0}^{N+2} \Big\{ \sum_{k=N+1-i}^{N} \frac{|q_k|}{(k+i+2)(k+i+1)} + \frac{\delta}{(N+3+i)(N+2+i)} \Big\} |u_i|}{1 - \left(\displaystyle\sum_{k=0}^{N} \frac{|q_k|}{(k+N+5)(k+N+4)} + \frac{\delta}{(2N+6)(2N+5)} \right)}$$

And this scales trivially to deal with $q \in H^1[a,b]$ for any a and b.

Lemma 3.2: *Consider the ODE*

$$u'' + \left(\frac{2\lambda k}{r} - \lambda^2\right) u = 0$$

for k a positive integer. Then, the only solution of the ODE that vanishes at ∞ is

$$u = e^{-\lambda r} \sum_{n=0}^{k} a_n r^n$$

where a_k is an arbitrary constant, and

$$a_n = a_{n+1} \frac{n(n+1)}{2\lambda(n-k)} \qquad n \leq k-1$$

Lemma 3.3: *Consider the ODE*

$$u'' + \left(a + \frac{b}{r} - \frac{n(n+1)}{r^2}\right) u = 0$$

for n a positive integer. Then, the only solution of the ODE that vanishes at 0 is

$$u = \sum_{k=n+1}^{\infty} u_k r^k$$

where u_{n+1} is an arbitrary constant, and

$$\begin{aligned} u_{n+2} &= -\frac{b \cdot u_{n+1}}{(n+2)(n+1) - n(n+1)} \\ u_{k+2} &= -\frac{b \cdot u_{k+1} - a \cdot u_k}{(k+2)(k+1) - n(n+1)} \qquad k \geq n+1 \end{aligned}$$

$$\sum_{k > N+2} |u_k| \leq \frac{\dfrac{|b \cdot u_{N+2}| + |a \cdot u_{N+1}|}{(N+3)(N+2) - n(n+1)} + \dfrac{|a \cdot u_{N+2}|}{(N+4)(N+3) - n(n+1)}}{1 - \dfrac{|b|}{(N+4)(N+3) - n(n+1)} - \dfrac{|a|}{(N+5)(N+4) - n(n+1)}}$$

We now pass to discuss how to use these lemmas to the problem of the localization of eigenvalues.

A crucial device in the study of eigenvalue problems is the "*match*" function, $M(\lambda)$ associated with the ODE operator $-u'' - q \cdot u$ acting on $\mathcal{H}_{\text{ODE}}$. It is defined as follows:

given $\lambda > 0$, $-\lambda^2$ is a negative eigenvalue iff

$$u'' + (q - \lambda^2) \cdot u = 0$$

has a solution in $\mathcal{H}_{\text{ODE}}$. Take any point y, and consider u_0, a solution of the ODE which vanishes at 0, and u_∞, a solution that vanishes at ∞. Then, define

$$M(\lambda) = \frac{u_0'(y) \cdot u_\infty(y) - u_0(y) \cdot u_\infty'(y)}{\sqrt{u_0^2(y) + {u_0'}^2(y)} \cdot \sqrt{u_\infty^2(y) + {u_\infty'}^2(y)}}.$$

Then, $-\lambda^2$ is an eigenvalue iff $M(\lambda) = 0$. The eigenvalues of the ODE thus correspond to the zeroes of M.

For our analysis we will use a computer bound for M, $\mathcal{M} : \mathcal{R} \to \mathcal{I}$, that will satisfy the property that for any representable r,

$$M(r) \in \mathcal{M}(r). \tag{3.1}$$

One possible way of implementing $\mathcal{M}$ is as follows: First, define the "phase" of a function u to be the point in the unit circle given by

$$\Phi_u(x) = \frac{\big(u'(x), u(x)\big)}{\sqrt{u(x)^2 + u'(x)^2}}.$$

Note that the phase is invariant under multiplication of u by a nonzero constant, and it is only defined for functions that do not vanish to order two: since the functions we will be working with will be nonzero solutions of an ODE problem, their phase is defined. Note also that

$$M(\lambda) = \det\left(\Phi_{u_0}(y), \Phi_{u_\infty}(y)\right)$$

For positive $\lambda \in \mathcal{R}$ the eigenvalue problem we need to solve is

$$\left.\begin{array}{r} \frac{1}{2}u'' + p(x)u = 0 \\ u(0) = u(\infty) = 0 \end{array}\right\}$$

where

$$p(x) = \frac{Z}{x} - \frac{l(l+1)}{2x^2} - V(x) - \lambda^2 \tag{3.2}$$

From section 1, we have a finite set of real numbers, $x_0 > x_1 > \cdots > x_n > 0$ such that the coefficients of the ODE are in $H^1[x_i, x_{i+1}]$ for $0 \leq i \leq n-1$, and (1.1) and (1.2) say that the ODE takes the special form dealt with in lemmas 3.2 and 3.3 around 0 and ∞. Elsewhere, it takes the form dealt with in Lemma 3.1.

With the aid of Lemma 3.2, we can determine a neighborhood of type (2.1) of $H^1[x_0, \infty]$ that contains u_∞. This allows us to obtain intervals that contain $u_\infty(x_0)$ and $u'_\infty(x_0)$ and we can therefore give bounds for $\Phi_{u_\infty}(x_0)$.

With the aid of Lemma 3.1, we can solve the initial value problem at x_0, thus obtaining another neighborhood of type (2.1) of $H^1[x_0, x_1]$ that contains u_∞, and again obtain intervals that contain $\Phi_{u_\infty}(x_1)$.

Repeating this argument, we can obtain bounds for $\Phi_{u_\infty}(x_n)$.

With the aid of Lemma 3.3, we can determine bounds for $\Phi_{u_0}(x_n)$.

Then, we define

$$\mathcal{M}(\lambda) = \det\left(\Phi_{u_0}(x_n), \Phi_{u_\infty}(x_n)\right).$$

where the determinant is taken in the interval arithmetic sense. It is just clear that $M(\lambda) \in \mathcal{M}(\lambda)$ for $y = x_n$.

The idea now is to create heuristic (e.g. using numerical analysis) representable numbers

$$\lambda_1^{\mathrm{up}} > \lambda_1^{\mathrm{dn}} > \lambda_2^{\mathrm{up}} > \lambda_2^{\mathrm{dn}} > \cdots \lambda_k^{\mathrm{up}} > \lambda_k^{\mathrm{dn}} > 0$$

and then compute $\mathcal{M}(\lambda_i^{\mathrm{up,\ dn}})$.

If we can prove that

$$\begin{aligned} &\mathcal{M}(\lambda_i^{\mathrm{up}}) > 0 \quad \mathcal{M}(\lambda_i^{\mathrm{dn}}) < 0 \quad i = 1, 3, \ldots \\ &\mathcal{M}(\lambda_i^{\mathrm{up}}) < 0 \quad \mathcal{M}(\lambda_i^{\mathrm{dn}}) > 0 \quad i = 2, 4, \ldots \end{aligned} \tag{3.3}$$

using (3.1) and the fact that M is continuous we would have proved that each interval $\lambda_i^* = (\lambda_i^{\mathrm{dn}}, \lambda_i^{\mathrm{dn}})$ contains at least one eigenvalue.

This previous procedure does not work if we substitute the phase by simply the vector $(u(x), u'(x))$; the reason is that interval arithmetic estimates are far to conservative and the bounds we obtain are very bad after a few steps. The reason why the previous algorithm proves good bounds for the eigenvalues has to do with the fact that the solution of this particular ODE is of the form $e^{-\lambda x}$ with a factor with only polynomial growth. As a consequence, the normalizing factor in the phase has a contractive effect that makes the bounds more stable. In other words, if you look at the time flow

$$T_t\left(\Phi_u(x)\right) = \Phi_u(x+t)$$

for the particular ODE we are working with, the phase of the eigenfunctions are almost always in the unstable manifold, and expansion of the phase backward in time gives good answers. If the phase were in the stable manifold, then this procedure would be stable expanding forward in time. In general, however, one sided shooting is not enough, and you need to consider the projection into the stable and unstable manifolds separately. For this important generalization see [LR].

The fact that (3.3) holds thus tells us that there are negative eigenvalues $-\lambda^2$, with $\lambda_i \in \lambda_i^*$, $i = 1, \cdots, k$, with eigenfunctions u_k, but we still have to show that we didn't miss any eigenvalue, that is, that if $-\lambda^2$ is a negative eigenvalue and $-\lambda^2 \leq -\lambda_k^2$ then $\lambda = \lambda_i$ for some i; in other words, λ_k really is the k'th eigenvalue. In order to do this, we use the fact that ours is a Sturm-Liouville problem. Therefore if a certain eigenfunction u_k has $k-1$ zeroes, then its eigenvalue *is* the k'th one. Hence, there are no other eigenvalues between $-\lambda_1^2$ and $-\lambda_k^2$.

In order to check that u_k has $k-1$ zeroes, note first of all the following corollary to comparison theorems for Sturm-Liouville problems:

Lemma 3.4: *Let u be any solution of*

$$\tfrac{1}{2}u'' - \left(V(x) + \frac{l(l+1)}{2x^2} - \frac{Z}{x} + \lambda^2\right) u = 0$$

on $[a,b]$, with $0 < a < b < \infty$, with V decreasing. Then, if

$$b - a \leq \pi \left(\frac{2Z}{b} - 2V(a) - \frac{l(l+1)}{a^2} - 2\lambda^2\right)_+^{-1/2}$$

then u cannot have two zeros in $[a,b]$.

Since our potential (3.2) is bounded above, we can arrange from the start that our partition $x_0, \cdots, x_n$ is fine enough so every interval (x_i, x_{i-1}) satisfies the hypothesis of this lemma. Also, for $l \neq 0$, since p is negative around 0 and ∞, we can take x_0 sufficiently big and x_n sufficiently close to 0 so $p(x_0)$ and $p(x_n)$ are both negative, and therefore u_k has no zeros in $(0, x_n)$ and (x_0, ∞); the special case $l = 0$ can be dealt with a trivial refinement of Lemma 3.4.

So, everything is reduced to counting the zeros of u_k in (x_n, x_0). For this, consider $u_\infty^{\rm up}$ and $u_\infty^{\rm dn}$, the solutions of the ODE with parameters $\lambda_k^{\rm up}$ and $\lambda_k^{\rm dn}$ respectively which are 0 at ∞. Again, comparison theorems tell us that the number of zeros of u_∞ in (x_n, x_0) is bounded between the number of zeros in (x_n, x_0) of $u_\infty^{\rm up}$ and $u_\infty^{\rm dn}$, and thus, it suffices to check that they both have $k-1$ zeros. In order to check this, note that Lemma 3.4 guarantees that the number of zeros of $u_\infty^{\rm up}$ and $u_\infty^{\rm dn}$ in (x_n, x_0) are (essentially) the same as the number of sign changes in the sequences $\{u_\infty^{\rm up}(x_i)\}_{i=0}^n$ and $\{u_\infty^{\rm dn}(x_i)\}_{i=0}^n$ respectively. From the ODE solver, we have good bounds for these sequences, hence the number of sign changes can be just counted, and if in both cases it is $k-1$, there are no more eigenvalues.

It is clear that with the control we have over the solutions of ODE's it is possible to bound the number of zeros without using Sturm-Liouville theory, but comparison theorems simplify the algorithm enormously.

4. The Results. The previous algorithm was carried out using as charge density guess an approximation to Thomas-Fermi density introduced in [Ti]. Once we solve the ODE's, the solutions give us another charge density in a trivial way, and this provides an iterative procedure that produces lower bounds for the ground state energy of atoms.

The following is a sample of results that can be obtained with this method for some values of the atomic charge Z: E_{lb} stands for the lower bounds obtained by the previous method; E_{ub} stands for known numerical —non rigorous— upper bounds to the energy obtained using Hartree-Fock's method (see [FF]).

Z	E_{lb}	E_{ub}	error (%)
10	−138.90	−128.54	7.74
20	−707.75	−676.75	4.47
30	−1,853.60	−1,777.84	4.17
40	−3,661.60	−3,538.99	3.40
50	−6,217.81	−6,022.93	3.18
60	−9,560.54	−9,283.88	2.98
70	−13,719.54	−13,391.45	2.45
80	−18,812.97	−18,408.99	2.20

The computer programs were written in **C**, and run on a SUN 3/60 workstation. The interval arithmetic package was supplied to me by D. Rana, and is the one he used in [Ra]. The program was divided into parts with a more general scope in mind than this particular problem, and most of them apply to more general situations. Execution time for the heuristics is of about two days for the largest atom, and the rigorous part takes about a month. A feature of the program is that most of the memory allocation is done during execution, and disposed of when no longer needed. This is done for two reasons: one, is to allow the degree of the Taylor expansions to be chosen adaptatively, and second, because it requires too much memory otherwise. Freeing memory, the program uses about 3Mb of memory, and without freeing memory it cannot run after a few hours.

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