Some statistics

14 submissions (3 undergrad., 11 grad.). Looked at 13 reports.

For problem 1:

1.1 (period). All **13** did it (1 person missed a factor of 2).

1.2 (scaling). **6** correct+**1** partial+**3** with a correct approach.

1.3-4 (integral): **6** students achieved the required relative accuracy of 10^{-6} for the oscillation period+**2** students nearly got it+**2** students used appropriate methods, but failed due to coding mistakes. Used **7** different methods, with the number of integration points needed from ~10 to ~10^{7}.

1.5 (low-A dependence): **8** correct fits. **6** correct theoretical calculations.

1.6 (large-A dependence): **9** correct.

1.7 (all-A fit): Only **1** student satisfied the requirements. **2** more chose a correct form, but failed to find the right parameters.

For problem 2:

2.1 (prove $S(E) \sim \int T(E')dE'$): **4** people did it correctly+**7** people had the right idea, but there are some issues with the proof

2.2 ($S(E)$): **3** people did it correctly+**4** people had various minor deficiencies+**1** person missed a factor of 2.

2.4 (levels): **1** person got the correct values+**6** people had minor deficiencies

2.6 (direct calculation of levels): **3** people attempted this, only **1** person got it right

1.1

$$\frac{1}{2}m\left(\frac{dx}{dt}\right)^2+U(x)=E$$

$$\frac{dx}{dt}=\sqrt{\frac{2}{m}[E-U(x)]}$$

$$\sqrt{\frac{m}{2[E-U(x)]}}\,dx=dt$$

Assume the potential is symmetric [U(-x)=U(x)]. Then the extreme points of the trajectory are ±A. Time it takes to go from -A to A is T/2.

$$\int_{-A}^{A}\sqrt{\frac{m}{2[E-U(x)]}}\,dx=\int_0^{T/2}dt=T/2$$

$$T(A)=\sqrt{2m}\int_{-A}^{A}\frac{dx}{\sqrt{E-U(x)}}=2\sqrt{2m}\int_0^{A}\frac{dx}{\sqrt{E-U(x)}}$$

At x=±A the velocity is zero, therefore E(A)=U(±A).

$$T(A)=2\sqrt{2m}\int_0^{A}\frac{dx}{\sqrt{U(A)-U(x)}}\qquad T(E)=2\sqrt{2m}\int_0^{A(E)}\frac{dx}{\sqrt{E-U(x)}}$$

1.2

$$T(E;m,\alpha,\beta)=C_1 T(C_2 E;2,1,1)$$

$$T(E;m,\alpha,\beta)=2\sqrt{2m}\int_0^{A(E,\alpha,\beta)}\frac{dx}{\sqrt{E-\alpha x^2-\beta x^4}}$$

$A(E,\alpha,\beta)$ is the positive solution of $\alpha A^2+\beta A^4=E$

You can check that for α,β ≥ 0 there are only 2 real solutions with the same absolute values and opposite signs.

$$C_1 T(C_2 E;2,1,1)=4C_1\int_0^{A(C_2 E,\alpha,\beta)}\frac{dy}{\sqrt{C_2 E-y^2-y^4}}$$

Need to make the coefficients of x^2 and x^4 equal. Do a variable change $x=Cy$

$$\alpha x^2=\alpha C^2 y^2 \qquad \beta x^4=\beta C^4 y^4 \qquad \alpha C^2=\beta C^4 \Rightarrow C=\sqrt{\alpha/\beta} \qquad x=\sqrt{\alpha/\beta}\,y$$

$$2\sqrt{2m}\int_0^{A(E,\alpha,\beta)}\frac{dx}{\sqrt{E-\alpha x^2-\beta x^4}}=2\sqrt{2m}\int_0^{\sqrt{\beta/\alpha}A(E,\alpha,\beta)}\frac{\sqrt{\alpha/\beta}\,dy}{\sqrt{E-\alpha\left(\frac{\alpha}{\beta}\right)y^2-\beta\left(\frac{\alpha}{\beta}\right)^2 y^4}}$$

$$=2\sqrt{2m}\int_0^{\sqrt{\beta/\alpha}A(E,\alpha,\beta)}\frac{\sqrt{\alpha/\beta}\,dy}{\sqrt{E-\left(\frac{\alpha^2}{\beta}\right)y^2-\left(\frac{\alpha^2}{\beta}\right)y^4}}=2\sqrt{2m}\int_0^{\sqrt{\beta/\alpha}A(E,\alpha,\beta)}\frac{\sqrt{\alpha/\beta}\,dy}{\frac{\alpha}{\sqrt{\beta}}\sqrt{\left(\frac{\beta}{\alpha^2}\right)E-y^2-y^4}}$$

$$T(E;m,\alpha,\beta)=2\sqrt{2m}\int_0^{\sqrt{\beta/\alpha}A(E,\alpha,\beta)}\frac{\sqrt{\alpha/\beta}\,dy}{\frac{\alpha}{\sqrt{\beta}}\sqrt{\frac{\beta}{\alpha^2}E-y^2-y^4}}$$

$$=2\sqrt{\frac{2m}{\alpha}}\int_0^{\sqrt{\beta/\alpha}A(E,\alpha,\beta)}\frac{dy}{\sqrt{\frac{\beta}{\alpha^2}E-y^2-y^4}}=2\sqrt{\frac{2m}{\alpha}}\int_0^{A\left(\frac{\beta}{\alpha^2}E,1,1\right)}\frac{dy}{\sqrt{\frac{\beta}{\alpha^2}E-y^2-y^4}}$$

$$\alpha[A(E,\alpha,\beta)]^2+\beta[A(E,\alpha,\beta)]^4=E$$

$$1\times[\sqrt{\beta/\alpha}A(E,\alpha,\beta)]^2+1\times[\sqrt{\beta/\alpha}A(E,\alpha,\beta)]^4=$$

$$\frac{\beta}{\alpha^2}\left\{\alpha[A(E,\alpha,\beta)]^2+\beta[A(E,\alpha,\beta)]^4\right\}$$

$$\sqrt{\beta/\alpha}A(E,\alpha,\beta)=A\left(\frac{\beta}{\alpha^2}E,1,1\right)$$

$$C_1T(C_2E;2,1,1)=4C_1\int_0^{A(C_2E,\alpha,\beta)}\frac{dy}{\sqrt{C_2E-y^2-y^4}}$$

$$C_1=\sqrt{\frac{m}{2\alpha}};\ C_2=\frac{\beta}{\alpha^2}$$

1.3. Integration

$$T(A)=4\int_0^A \frac{dy}{\sqrt{A^2+A^4-y^2-y^4}}=|y=Az|=4\int_0^1 \frac{A\,dz}{\sqrt{A^2(1-z^2)+A^4(1-z^4)}}$$

$$=4\int_0^1 \frac{dz}{\sqrt{1-z^2}\sqrt{1+A^2(1+z^2)}}=4\int_0^1 \frac{dz}{\sqrt{1-z}\sqrt{1+z}\sqrt{1+A^2(1+z^2)}}$$

Complication: the integrand diverges at z=1 as $1/\sqrt{1-z}$

As we have seen in the previous homework, even a milder singularity like

$\sqrt{1-z}$ increases the error of the trapezoidal method from $O(h^2)$ to $O(h^{3/2})$

A stronger singularity will, of course, be much worse. Trapezoidal cannot be used, unless we remove the end point. We can use the midpoint method. For the subinterval next to the singularity, the exact value is

$$\int_{1-h}^1 \frac{dz}{\sqrt{1-z}}=2\sqrt{1-z}\Big|_{1-h}^1=2\sqrt{h}.$$ Midpoint gives $$\frac{1}{\sqrt{1-(1-h/2)}}h=\sqrt{2h}.$$

The difference is $O(h^{1/2})$. To achieve accuracy of 10^{-6}, will need to use about 10^{12} integration points.

For this reason, straightforward Romberg integration (aka Richardson extrapolation) will not work. Assumes that the error is

$$E(h) = C_1 h^2 + C_2 h^4 + \ldots$$

Then the error of (9/8)I(h/3)-(1/8)I(h) is O(h^4).

But this is only true for integrands without singularities. In our case,

$$E(h) = C_1 h^{1/2} + C_2 h^{3/2} + C_3 h^{5/2} + \ldots$$

$$I(h) = I(0) + C_1 h^{1/2} + O\left(h^{3/2}\right)$$

$$I(h/3) = I(0) + C_1 (h/3)^{1/2} + O\left(h^{3/2}\right)$$

$$\frac{9}{8} I(h/3) - \frac{1}{8} I(h) = I(0) + \frac{3\sqrt{3}-8}{8} h^{1/2} + O\left(h^{3/2}\right)$$

The error is still O($h^{1/2}$). "Modified Romberg" $\dfrac{\sqrt{3}\, I(h/3) - I(h)}{\sqrt{3}-1}$ has error O($h^{3/2}$), would require ~ 10^4 nodes.

After 2 stages, $\dfrac{9\, I(h/9) - 4\sqrt{3}\, I(h/3) + I(h)}{9 - 4\sqrt{3} + 1}$ has error O($h^{5/2}$) (~200 nodes).

Moreover, pretty much all integration schemes with equidistant points designed for regular integrands will be equally bad, no matter how high order they are. Repeat the same calculation for any super-sophisticated open Newton-Cotes scheme from Numerical Recipes – get the same result.

Several possibilities:

1. Variable transformation to remove the singularity.

2. Special methods for singular integrands.

3. Non-equidistant integration nodes (higher density near the singularity).

Variable transformation

$$T(A)=4\int_0^1 \frac{dz}{\sqrt{1-z^2}\sqrt{1+A^2(1+z^2)}}=4\int_0^1 \frac{dz}{\sqrt{1-z}\sqrt{1+z}\sqrt{1+A^2(1+z^2)}}$$

In principle, any z(u) that is parabolic near z=1 will remove the singularity. But still, not all are equally good.

2 people used $z=1-u^2$.

$$T(A)=4\int_0^1 \frac{2u\,du}{u\sqrt{(2-u^2)[1+A^2(1+(1-u^2)^2)]}}=8\int_0^1 \frac{du}{\sqrt{(2-u^2)[1+A^2(1+(1-u^2)^2)]}}$$

Now, any scheme for regular integrands can be used. One person used the trapezoidal rule. $O(h^2)$ – about 10^3 integration points should suffice, although the person used 10^6 points.

The other person used a more sophisticated rule taken from Numerical Recipes:

$$\int_{x_1}^{x_N} f(x)\,dx = h\left[\frac{55}{24}f_2 - \frac{1}{6}f_3 + \frac{11}{8}f_4 + f_5 + f_6 + f_7 + \right.$$

$$\left. \ldots + f_{N-5} + f_{N-4} + \frac{11}{8}f_{N-3} - \frac{1}{6}f_{N-2} + \frac{55}{24}f_{N-1}\right] + O\left(1/N^4\right)$$

So this is $O(h^4)$ and, if implemented properly, should have given the required accuracy with < 100 integration nodes. Unfortunately, because of a coding error, the error was $O(h)$ and > 10^6 nodes were required.

```
 TINTGRLU = width*(  55/24*( TRANSVALU(x_1+width,x_0,x_nP1) +
&TRANSVALU(x_n-width,x_0,x_nP1) ) -
&1/6*( TRANSVALU(x_1+2*width,x_0,x_nP1) +
&TRANSVALU(x_n-2*width,x_0,x_nP1) ) +
&11/8*( TRANSVALU(x_1+3*width,x_0,x_nP1) +
&TRANSVALU(x_n-3*width,x_0,x_nP1) ) )
```

What is wrong with this?

Another, better transformation:

$$z = \sin u$$

$$T(A) = 4\int_0^1 \frac{dz}{\sqrt{1-z^2}\sqrt{1+A^2(1+z^2)}} = 4\int_0^{\pi/2} \frac{\cos u\, du}{\sqrt{1-\sin^2 u}\sqrt{1+A^2(1+\sin^2 u)}}$$

$$= 4\int_0^{\pi/2} \frac{du}{\sqrt{1+A^2(1+\sin^2 u)}}$$

The great thing about this is even for something as simple as the trapezoidal rule the error decays exponentially (faster than any power law) with N!

```
 2 4.035240833326511
 3 4.004538069827917
 4 4.004311446177784
 5 4.004309538933383
 6 4.004309521992798
 7 4.004309521837695
 8 4.004309521836241
 9 4.004309521836223
10 4.004309521836221
```

N = 5 is sufficient! Why is this so?

Simpson would work, too, because it is a linear combination of the trapezoidal rules for h and h/2, but there is no good reason to use it, since a simpler trapezoidal rule is extremely successful.

4 people tried to use either trapezoidal or Simpson or both with this transformation, but only 1 succeeded!

In one case it was a simple typo.

In one other case, a combination of a typo and a more serious issue:

```
h=2.d0*pi/1.d4
T= fx(A,0.d0)
x=0.d0 +h

do
if ((x).ge.pi*2.d0) exit
write(*,*) x/(2.d0*pi), T*h
T=T+fx(x,A)
x=x+h

end do
```

This is unreliable, because of round-off (annotation pointing to the line `if ((x).ge.pi*2.d0) exit`)

10000 intervals

0.99950000000013417	4.0022721130040182
0.99960000000013416	4.0027164002016047
0.99970000000013426	4.0031606877938319
0.99980000000013425	4.0036049756930030
0.99990000000013424	4.0040492638114218

20000 intervals

0.99974999999966396	4.0032908165096073
0.99979999999966396	4.0035129605194859
0.99984999999966384	4.0037351045786949
0.99989999999966384	4.0039572486762722
0.99994999999966372	4.0041793928012552
0.99999999999966371	4.0044015369426820

```
float simp(double m)
 {double h,sum1,sum2,n;
   int i;
   h= 0.0001; /* set stepsize */
   n=(PI/2)/h;
   sum1 = 0; sum2 = 0; /* initialization */
   for (i = 1; i < n; i+=2) sum1+=f(0+i*h,m);/* odd
points */
   for (i = 2; i < n; i+=2) sum2+=f(0+i*h,m);/*  even
points */
   return h*(4*sum1 + 2*sum2 + f(0,m) + f(PI/2,m))/3; /*
include first and last
points and return answer */
  }
```

There should be an integer number of steps!

2 people have used the Clenshaw-Curtis method with the z=sin u transformation

The error should also be exponentially small, just because it often is for regular integrands.

Again, overkill, because even the trapezoidal method works well, and Clenshaw-Curtis is more complicated, because it requires calculation of the weights.

For the $z=1-u^2$ transformation, actually is beneficial, because the error is exponential when the error of the trapezoidal etc. is not.

1 of the 2 people made a simple mistake making the accuracy quadratic instead of exponential.

There is no need to compute the nodes and the weights for every A – they are all the same!

Special methods for singular integrands

We have considered a series of Gauss methods for $\int_a^b W(x) f(x)\,dx$

For N nodes, are exact when f(x) is a polynomial of degree up to 2N-1.
Often the error is exponentially small in N.

Often, the nodes and weights are not given explicitly and need to be found by solving an algebraic equation.

But for a particular case when $W(x) = \frac{1}{\sqrt{1-x^2}}$, there is an explicit and very simple form:

$$\int_{-1}^{1} \frac{f(x)\,dx}{\sqrt{1-x^2}} \approx \frac{\pi}{N} \sum_{j=0}^{N} f(x_j), \quad x_j = \cos\left(\frac{\pi(2j-1)}{2N}\right)$$

Gauss-Chebyshev method

$$T(A) = 4\int_0^1 \frac{dz}{\sqrt{1-z^2}\sqrt{1+A^2(1+z^2)}} = 2\int_{-1}^{1} \frac{dz}{\sqrt{1-z^2}\sqrt{1+A^2(1+z^2)}}$$

Indeed, exponentially accurate. Only **1** person used it.

In fact, this method is equivalent to the midpoint method applied to the integral transformed using z=sin v. Midpoint is exponentially accurate, because it is a linear combination of two trapezoidal rules with h and 2h.

$$\int_{-1}^{1} \frac{f(z)\,dz}{\sqrt{1-z^2}} = \int_{-\pi/2}^{\pi/2} f(\sin u) \approx \frac{\pi}{N} \sum_{j=1}^{N} f\left(\sin[\pi/2 - \pi(j-1/2)/N]\right)$$

$$= \frac{\pi}{N} \sum_{j=1}^{N} f\left(\cos\left[\frac{\pi(2j-1)}{2N}\right]\right)$$

Another very interesting method ("modified midpoint", although I would call it modified trapezoidal):

The usual trapezoidal method is $\int_{x_0}^{x_N} \frac{dx}{f(x)} \approx \frac{h}{2} \sum_{j=1}^{N} \left[\frac{1}{f(x_{j-1})} + \frac{1}{f(x_j)} \right]$

The modified method is $\int_{x_0}^{x_N} \frac{dx}{f(x)} \approx 2h \sum_{j=1}^{N} \left[\frac{1}{f(x_{j-1}) + f(x_j)} \right]$

For $f(x) = x^{\nu}$: $\int_{x_{j-1}}^{x_j} \frac{dx}{x^{\nu}} = \frac{x_j^{1-\nu} - x_{j-1}^{1-\nu}}{1-\nu}$ vs. $\frac{2(x_j - x_{j-1})}{x_j^{\nu} + x_{j-1}^{\nu}}$

When $\nu = 1/2$: $2\left(x_j^{1/2} - x_{j-1}^{1/2}\right)$ vs. $\frac{2(x_j - x_{j-1})}{x_j^{1/2} + x_{j-1}^{1/2}}$ These are equal.

The equality only holds for ν=1/2 – the method is specific to the 1/√ singularity

In our case, the expansion of the integrand is $C_1 x^{-1/2} + C_2 x^{1/2} + \ldots$ The first term is treated exactly, but for the second term the error is like for the trapezoidal rule, i.e., $O(h^{3/2})$. The person who used this method did a wrong estimate. Need ~30000 integration points.

Non-equidistant integration nodes (without additional transformations)

More nodes where the contribution to the integral (and the error) is the largest, i.e., near the singularity.

Trapezoidal rule with Chebyshev nodes $x_j = \cos(\pi j / N)$

Subinterval adjacent to the singularity has width $h \sim 1/N^2$. So the “standard” error $O(h^{1/2})$ will be $O(1/N)$. Need about 10^6 nodes. It may be possible to play tricks, e.g., “modified trapezoidal” should give the usual “non-singular” $O(1/N^2)$ error.

Gauss-Legendre

It's a great method, often with an exponentially small error, **but** for regular integrands. The only advantage for our singular problem is that it also places more nodes near the boundaries (where the singularities are), which again gives the $O(1/N)$ error, but at a significantly higher cost, because there are no explicit expressions for the nodes – they need to be calculated by a root-finding procedure. Obviously, not a good approach, and it failed (reached only $N \sim 40$, when 10^6 was needed).

Error estimates

First of all, comparing to “highly accurate numerical integration programs found online” is **not** a valid approach!

General approach: calculate with number of points N, then with 2N, take the latter result and assume that the error is smaller than their difference.

Can we actually make that assumption? If the error is CN^{-a}, then the difference will be $C[N^{-a}-(2N)^{-a}]=C(2N)^{-a}[2^{a}-1]$. $2^{a}-1>1$ when $a>1$. So need to confirm what a is – need at least 3 values of N then, and if you do more, this will let you check that your N is large enough that you have reached the asymptotic regime. Generally, you can assume that a is the same throughout (check just in case for a few values of A), but **not C**!

Relying entirely on theory when making error estimates is dangerous – you need to be 100% confident that your theoretical considerations are correct, and you generally can't! On the other hand, do make sure that your “experimental” results make sense theoretically, i.e., that you understand your value of a – you may detect some errors this way.

When you see that the dependence is exponential, likewise need to estimate the parameters of that dependence.

Fitting for small A

Small!!! Use a very narrow range. Since your calculation is very accurate, you may use as few points as there are parameters. Some people included more terms in the expansion – this is OK, but, of course, you need to be confident what the powers are – are you sure there are no fractional powers?

Theory

$$T(A)=4\int_0^1 \frac{dz}{\sqrt{1-z^2}\sqrt{1+A^2(1+z^2)}}$$

For small A (first 2 terms):

$$T(A)\approx 4\int_0^1 \frac{dz}{\sqrt{1-z^2}}-2A^2\int_0^1 \frac{(1+z^2)\,dz}{\sqrt{1-z^2}}=4\arcsin 1-2A^2\int_0^1 \frac{(z^2-1+2)\,dz}{\sqrt{1-z^2}}$$

$$=2\pi-2\pi A^2+2A^2\int_0^1\sqrt{1-z^2}\,dz=2\pi-2\pi A^2+2A^2\int_0^1\sqrt{1-z^2}\,d(z^2)/2\sqrt{z^2}$$

$$=2\pi-2\pi A^2+A^2\,\Gamma(3/2)\,\Gamma(1/2)/\Gamma(2)=2\pi-(3/2)\pi A^2$$

Theory for large A

$$T(A)=4\int_0^1 \frac{dz}{\sqrt{1-z^2}\sqrt{1+A^2(1+z^2)}} \qquad A^2(1+z^2)\gg 1$$

$$T(A)=\frac{4}{A}\int_0^1 \frac{dz}{\sqrt{1-z^4}}=\frac{4}{A}\int_0^1 \frac{d(z^4)}{4(z^4)^{3/4}(1-z^4)^{1/2}}=\frac{1}{A}B(1/4,1/2)$$

$=5.244115/A.$ Next term is $O(1/A^3)$.

Fitting function for all A

For **all** A up to ∞ – means it has to have the correct large-A asymptotic dependence (±1-2% in the coefficient). It would be nice to make sure that T(0) is (nearly) correct and that there is no linear term at small A.

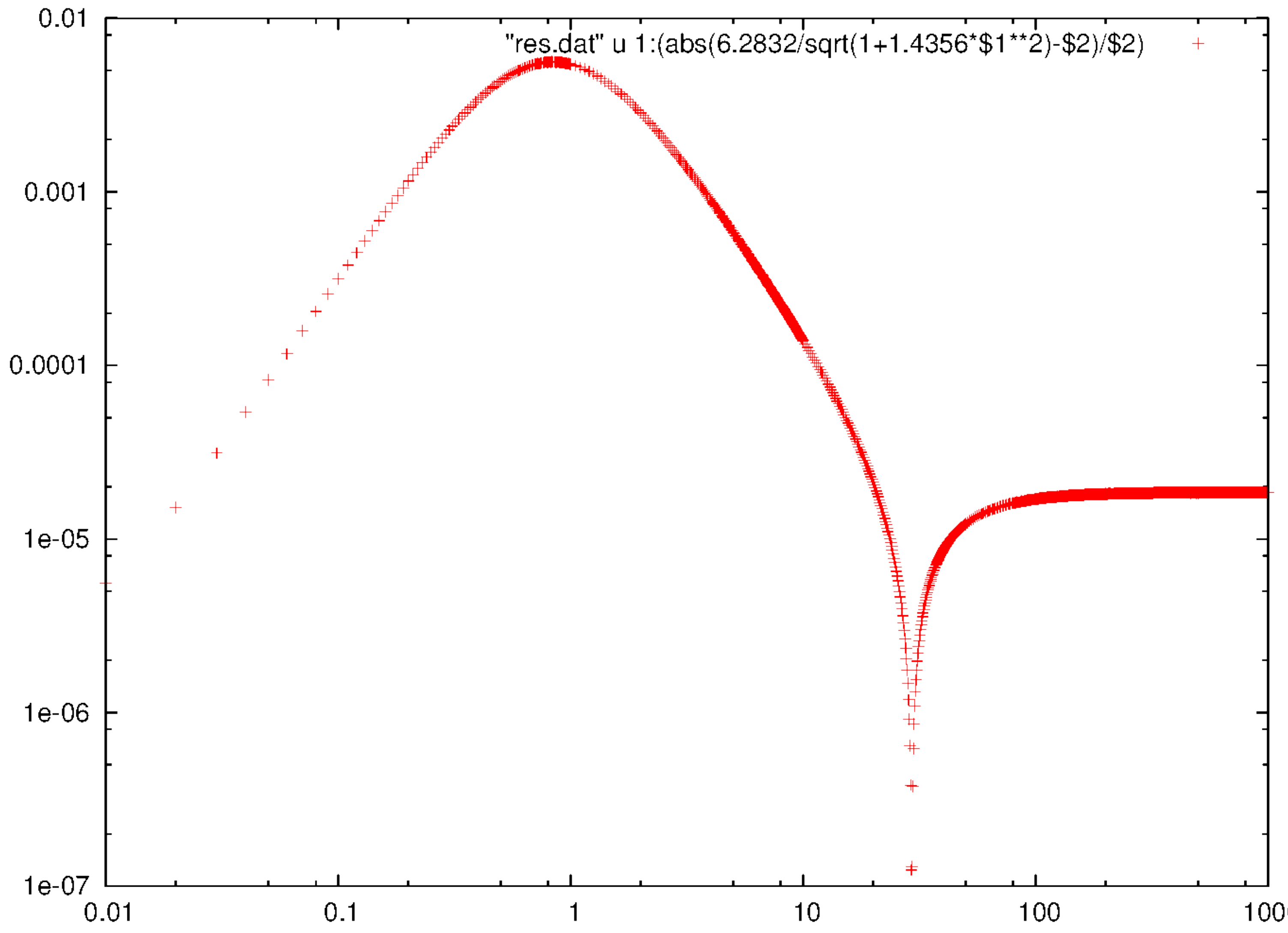
$$T(A)\approx\frac{B_1}{\sqrt{1+B_2A^2}}$$

Can get B_1 and B_2 without numerical results, just from theory.

$$B_1=2\pi\approx 6.2832;\ B_1/\sqrt{B_2}\approx 5.2441 \ \Rightarrow\ B_2\approx 1.4356.$$

$$T(A) \approx \frac{6.2832}{\sqrt{1+1.4356\,A^2}} \qquad \frac{3}{2}\pi \approx 4.7124$$

For small A, $T(A) \approx 6.2832\left(1-(1.4356/2)\,A^2\right) \approx 6.2832 - 4.5101\mathrm{A}^2$



Proof that S(E) ~ ∫T(E')dE'.

Equivalent to proving that $\frac{dS(E)}{dE}=C\,T(E),$ plus S(0) = 0 (obvious).

$$S(E)=2\int_{-A(E)}^{A(E)}|p(x,E)|\,dx=2\sqrt{2m}\int_{-A(E)}^{A(E)}\sqrt{E-U(x)}\,dx$$

General rule:

$$\frac{d}{dy}\int_{a(y)}^{b(y)}f(x,y)\,dx=\int_{a(y)}^{b(y)}\frac{\partial f(x,y)}{\partial y}\,dx+\frac{db(y)}{dy}f(b(y),y)-\frac{da(y)}{dy}f(a(y),y)$$

Note that U(±A)=0, so the last 2 terms are zero.

$$\frac{dS(E)}{dE}=\sqrt{2m}\int_{-A(E)}^{A(E)}\frac{dx}{\sqrt{E-U(x)}}=T(E)$$

Most people integrated T(E) instead, but you need to be careful with the integration limits!

$$\int_0^E T(E')dE' = \sqrt{2m}\int_0^E dE' \int_{-A(E')}^{A(E')} \frac{dx}{\sqrt{E'-U(x)}} = \sqrt{2m}\int_{-A(E)}^{A(E)} dx \int_{U(x)}^{E} \frac{dE'}{\sqrt{E'-U(x)}}$$

$$= \sqrt{2m}\int_{-A(E)}^{A(E)} 2[\sqrt{E-U(x)} - \sqrt{U(x)-U(x)}]\,dx = S(E)$$

2.2. Calculating S(E).

$$S(E)=\int_0^E T(E')dE'$$

The simplest thing: trapezoidal integration. But keep in mind: what you have calculated in Problem 1 is T(A), not T(E)!!! Some people calculated instead

$$\int_0^A T(A')dA'$$

$$S(E(A_n))\approx\frac{1}{2}\sum_{j=1}^{n}[T(A_j)+T(A_{j-1})][E(A_j)-E(A_{j-1})]$$

What some did instead is

$$\sum_{j=1}^{n}\frac{1}{2}[T(A_j)+T(A_{j-1})][A_j-A_{j-1}]$$

No need to re-calculate the sum from scratch for each new A_n – just add 1 term!

$$S(E(A_n)) \approx \frac{1}{2}\sum_{j=1}^{n}[T(A_j)+T(A_{j-1})][E(A_j)-E(A_{j-1})]$$

Error estimate: compare

$$S(E(A_{2n})) \approx \frac{1}{2}\sum_{j=1}^{2n}[T(A_j)+T(A_{j-1})][E(A_j)-E(A_{j-1})]$$

and

$$S^{(2)}(E(A_{2n})) \approx \frac{1}{2}\sum_{j=1}^{n}[T(A_{2j})+T(A_{2j-2})][E(A_{2j})-E(A_{2j-2})]$$

For reliability, you can also calculate $S^{(3)}$ with the step of 3, etc., to see the trend. For the trapezoidal rule, expect the quadratic dependence on the step – no singularities, no surprises – the error of $S^{(2)}$ should be 4 times the error of S, etc.

Energy levels. Do linear interpolation. $O(h^2)$ error matches that of the trapezoidal calculation of S(E), so no need to use higher-degree polynomials.

The error, of course, consists of many contributions. Too hard to take them into account one by one. Much better: simply use S(E) and then use $S^{(2)}(E)$ and compare. This neglects the error of T(E).

Graphical representation.

Direct calculation of energy levels

For integration, use another Gauss-Chebyshev scheme for

$$\int_{-1}^{1} \sqrt{1-x^2}\, f(x)\, dx$$

Just go through the code.

Relative difference between the indirect and direct calculation