8.322: Quantum Theory II

Problem Set #5 Solutions
March 19, 2007

1. **Variational principle versus perturbation theory**

   (a)

   $$\Delta H = \alpha(2a^2 + 2a^{\dagger 2} + a^{\dagger 2}a^2).$$

   Clearly the first order energy correction given by $\langle 0|\Delta H|0\rangle = 0$. We evaluate

   $$\langle 0|\Delta H|2\rangle = 2\alpha\sqrt{2}$$

   Thus

   $$\Delta E_0^{(2)} = -4\alpha^2$$

   (b) We evaluate

   $$\langle 2|\Delta H|2\rangle = 2\alpha$$

   We now have the matrix

   $$\begin{pmatrix} \frac{1}{2} & 2\sqrt{2}\alpha \\ 2\sqrt{2}\alpha & \frac{5}{2} + 2\alpha \end{pmatrix}$$

   which has eigenvalues

   $$\lambda_\pm = \frac{3}{2} + \alpha \pm \sqrt{1 + 2\alpha + 9\alpha^2}$$

   Thus the ground state energy is bounded by λ_-.

   (c) We compare $\frac{1}{2} - 4\alpha^2$ to λ_-. We find that in the region $-\frac{1}{2} < \alpha < 0$ the variational estimate is lower than the answer from perturbation theory.

2. **Variational principle for the anharmonic oscillator**

   (a) First we note

   $$I_0(\beta) = \int_{-\infty}^{\infty} dx x^{2n} e^{-\beta x^2} = \sqrt{\frac{\pi}{\beta}} = N(\beta)^{-2}$$

Then

$$I_n(\beta) = \left(-\frac{d}{d\beta}\right)^n I_0(\beta) = \left(-\frac{d}{d\beta}\right)^n \sqrt{\frac{\pi}{\beta}}$$
$$= \sqrt{\pi}\left(\frac{1}{2}\right)\left(\frac{3}{2}\right)\left(\frac{5}{2}\right)\cdots\left(\frac{2n-1}{2}\right)\beta^{-n-1/2}$$

Thus

$$\frac{I_n(\beta)}{I_0(\beta)} = \frac{(2n-1)!!}{(2\beta)^n}$$

(b) We find

$$\langle\psi_\beta|\frac{x^2}{2}|\psi_\beta\rangle = \frac{I_1(\beta)}{2I_0(\beta)} = \frac{1}{4\beta}$$

and

$$\langle\psi_\beta|\frac{p^2}{2}|\psi_\beta\rangle = \frac{1}{2I_0(\beta)}\int_{-\infty}^{\infty} dx\,\left(-\beta+\beta^2x^2\right)e^{-\beta x^2}$$
$$= \frac{-\beta I_0(\beta)+\beta^2 I_1(\beta)}{2I_0(\beta)} = \frac{\beta}{4}$$

Thus

$$\langle\psi_\beta|H_0|\psi_\beta\rangle = \frac{1}{4}\left(\beta+\frac{1}{\beta}\right)$$

Minimizing this expression gives $\beta = 1$ and $E_0 = \frac{1}{2}$ which are the correct values for the unperturbed oscillator.

(c) From (a) we know

$$\langle\psi_\beta|\lambda x^{2n}|\psi_\beta\rangle = \frac{\lambda(2n-1)!!}{(2\beta)^n}$$

We minimize w.r.t to β and call minimum function $\tilde{\beta}(n,\lambda)$

$$\frac{\partial}{\partial\beta}\langle\psi_\beta|H|\psi_\beta\rangle = \frac{1}{4}\left(1-\frac{1}{\tilde{\beta}^2}\right) - \frac{n\lambda(2n-1)!!}{2^n\tilde{\beta}^{n+1}} = 0$$

which gives

$$\frac{1}{4n}\left(\tilde{\beta}-\frac{1}{\tilde{\beta}}\right) = \frac{\lambda(2n-1)!!}{2^n\tilde{\beta}^n}$$

giving

$$E_0(n,\lambda) = \frac{1}{4}\left(\tilde{\beta}+\frac{1}{\tilde{\beta}}+\frac{1}{n}\left(\tilde{\beta}-\frac{1}{\tilde{\beta}}\right)\right)$$

(d) Set $\lambda = 1$

$$n=1 \longrightarrow \frac{1}{2\beta} = \frac{1}{4}\left(\beta - \frac{1}{\beta}\right) \longrightarrow \beta = \sqrt{3}$$

$$n=2 \longrightarrow \frac{3}{4\beta^2} = \frac{1}{8}\left(\beta - \frac{1}{\beta}\right) \longrightarrow \beta = 2$$

$$n=3 \longrightarrow \frac{15}{8\beta^3} = \frac{1}{12}\left(\beta - \frac{1}{\beta}\right) \longrightarrow \beta = \sqrt{\frac{1}{2} + \frac{\sqrt{91}}{2}} \approx 2.30$$

Which gives

$$E_0(1,1) = \frac{\sqrt{3}}{2}$$

$$E_0(2,1) = \frac{13}{16}$$

$$E_0(3,1) = \frac{1}{18}\sqrt{\frac{1}{5}\left(269 + 91\sqrt{91}\right)} \approx 0.838$$

Comparing to perturbation theory, $\beta = 1$, and $E_0^P = \frac{1}{4}\left(\beta + \frac{1}{\beta}\right) + \frac{(2n-1)!!}{(2\beta)^n}$,

$$E_0(1,1) = 1$$

$$E_0(2,1) = 1.25$$

$$E_0(3,1) = 2.375$$

3. **Phases**

(a) The potential is shown in Figure 1.

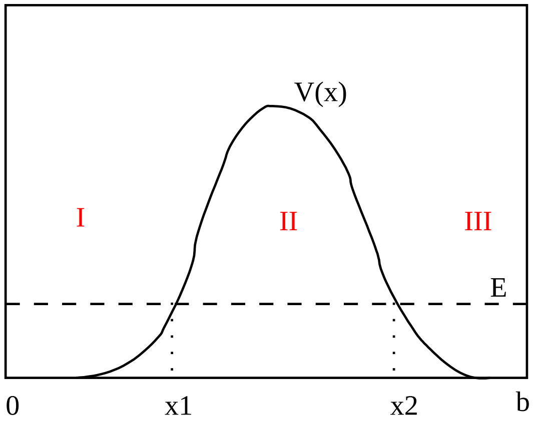

Figure 1: A high potential and a low energy state.

The WKB approximation gives the wavefunction in region II in the following form

$$\Psi_{II}(x) = \frac{c_+}{\sqrt{K(x)}}\ \exp[\frac{1}{\hbar}\int_{x_1}^{x} K(x')dx'] + \frac{c_-}{\sqrt{K(x)}}\ \exp[-\frac{1}{\hbar}\int_{x_1}^{x} K(x')dx']$$

where $K(x) = \sqrt{2m(V(x) - E)}$.

For special values of E, we have $c_+ = 0$, i. e. the wavefuntion is exponentially decaying in the classically forbidden region. Hence, by means of the connection formula, we obtain for region I

$$\Psi_I(x) = \frac{2c_-}{\sqrt{p(x)}}\ \cos\left[\frac{1}{\hbar}\int_{x}^{x_1} p(x')dx' - \frac{\pi}{4}\right]$$

Moreover, in order to respect the boundary condition $\Psi_I(0) = 0$, we must have

$$\frac{1}{\hbar}\int_0^{x_1} p(x')dx' - \frac{\pi}{4} = \frac{(2n+1)\pi}{2}$$

Hence, the special values of E are those which satisfy

$$\int_0^{x_1(E)} \sqrt{2m(E - V(x'))}dx' = \left(n + \frac{3}{4}\right)\pi\hbar$$

(b) For a generic choice of energy, we expect a decaying exponential in region II as we go from x_2 to x_1

$$\Psi_{II}(x) \propto \frac{1}{\sqrt{K(x)}}\ \exp\left[\frac{1}{\hbar}\int_{x_1}^{x} K(x')dx'\right] \propto \frac{1}{\sqrt{K(x)}}\ \exp\left[-\frac{1}{\hbar}\int_{x}^{x_2} K(x')dx'\right]$$

Hence,

$$\Psi_{III}(x) = \frac{2}{\sqrt{p(x)}}\ \cos\left[\frac{1}{\hbar}\int_{x_2}^{x} p(x')dx' - \frac{\pi}{4}\right] = \frac{2}{\sqrt{p(x)}}\ \cos\left[\frac{1}{\hbar}\int_{x_2}^{b} p(x')dx' + \underbrace{\frac{1}{\hbar}\int_{b}^{x} p(x')dx'}_{kx-kb} - \frac{\pi}{4}\right]$$

$$\Psi_{III}(x) \propto \sin(kx + \delta(k)), \qquad \text{for } x \gg b$$

Thus,

$$\delta(k) = 2\pi n + \frac{1}{\hbar}\int_{x_2}^{b} p(x')dx' - kb + \frac{\pi}{4} \qquad (n \in \mathbb{Z})$$

We note that taking the limit $b \to \infty$ is well defined for this expression and that thus for large enough b, δ is independent of b. $\delta(k)$ is still only determined up to a factor of $2\pi n$; however, this factor will be irrelevant for many purposes. For example, the scattering cross-section in three dimensions depends only on $\sin\delta$.

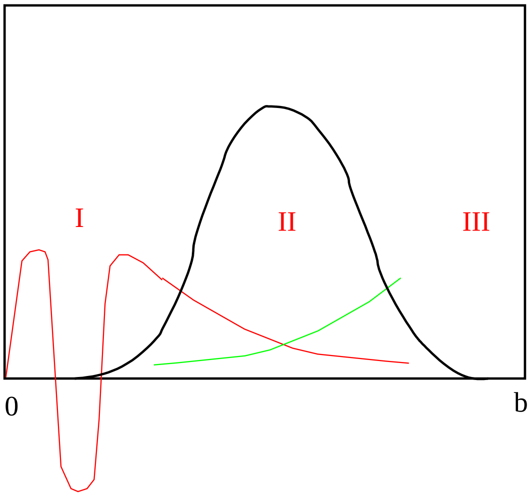

Figure 2: An exponentially small contribution (green) rises exponentially.

(c) For the above special values of the energy, the approximation fails to provide an estimate on $\delta(k)$. Since the WKB is not exact, it is possible that we missed an exponentially small, exponentially growing term at the turning point x_1. However this correction can become significant at x_2 and thus would effect the phase shift δ with terms of order unity.

4. **WKB Sum Rules** (a) The quantization condition reads

$$(n + \frac{1}{2})\pi\hbar = \int_{x_1(\kappa)}^{x_2(\kappa)} dx\ p(\kappa, x)$$

The highest bound state has zero binding energy, and thus $\kappa \approx 0$ for this state. Also, $x_1(0) = -\infty$ and $x_2(0) = \infty$. Hence,

$$(N + \frac{1}{2})\pi\hbar = \int_{-\infty}^{\infty} dx\ \sqrt{2mU(x)}$$

Since $N \gg 1$, we have

$$N\pi\hbar \approx \int_{-\infty}^{\infty} dx\ \sqrt{2mU(x)}$$

(b)

$$\rho(\kappa) = \left|\frac{dn}{d\kappa}\right| = \frac{1}{\pi\hbar}\int_{x_1(\kappa)}^{x_2(\kappa)} dx \left|\frac{dp}{d\kappa}\right|$$

$$\sum_{j=1}^{N} B_j = \int d\kappa \rho(\kappa)\frac{\hbar^2\kappa^2}{2m} = -\int d\kappa \frac{1}{\pi\hbar}\int_{x_1(\kappa)}^{x_2(\kappa)} dx \frac{dp}{d\kappa}\frac{\hbar^2\kappa^2}{2m}$$

Changing the order of integration

$$\sum_{j=1}^{N} B_j = -\int_{-\infty}^{\infty} dx \int_0^{\sqrt{2mU(x)}/\hbar} \frac{\hbar\kappa^2}{2\pi m}\frac{dp}{d\kappa}$$

and applying partial integration

$$\sum_{j=1}^{N} B_j = -\int_{-\infty}^{\infty} dx \left[\frac{\hbar\kappa^2}{2\pi m}p(\kappa, x)\right]_{\kappa=0}^{\sqrt{2mU(x)}/\hbar} + \int_{-\infty}^{\infty} dx \int_0^{\sqrt{2mU(x)}/\hbar} d\kappa \frac{\hbar\kappa}{\pi m}p(\kappa, x)$$

Since $p(\kappa = \sqrt{2mU(x)}/\hbar) = 0$, the boundary term vanishes, leaving

$$\sum_{j=1}^{N} B_j = \int_{-\infty}^{\infty} dx \int_0^{\sqrt{2mU(x)}/\hbar} d\kappa \frac{\hbar\kappa}{\pi m}\sqrt{2mU - \hbar^2\kappa^2} = \frac{2}{3\pi\hbar}\sqrt{2m}\int_{-\infty}^{\infty} dx\ U(x)^{3/2}.$$

(c) The derivation is essentially the same.

$$\sum_{j=1}^{N} B_j^l = -\frac{1}{\pi\hbar}\int_{-\infty}^{\infty} dx \int_0^{\sqrt{2mU(x)}/\hbar} \frac{dp}{d\kappa}\left(\frac{\hbar^2\kappa^2}{2m}\right)^l$$

Now applying partial integration l times results in

$$\sum_{j=1}^{N} B_j^l = \frac{(2l)!!}{(2l+1)!!}\frac{\sqrt{2m}}{\pi\hbar}\int_{-\infty}^{\infty} dx\ U(x)^{(2l+1)/2}$$

where $(2l)!! \equiv (2)\cdot(4)\cdots(2l-2)\cdot(2l)$.

(d) The sum rules obtained in (a)–(c) are

$$N \approx \frac{1}{\pi}\int_{-\infty}^{\infty} dx\ U(x)^{1/2}$$

$$\sum_{j=1}^{N} B_j^l = \frac{(2l)!!}{(2l+1)!!}\frac{1}{\pi}\int_{-\infty}^{\infty} dx\ U(x)^{(2l+1)/2}$$

Now we evaluate these sum rules for the Pöschl–Teller potential

$$U(x) = A\ \mathrm{sech}^2(x)$$

Let us define the following quantity

$$\mathcal{J}_l := \int_{-\infty}^{\infty} dx\ (\mathrm{sech}\ x)^{2l+1}$$

This obeys the following equation

$$\mathcal{J}_l = \left(\frac{2l-1}{2l}\right)\mathcal{J}_{l-1}$$

and, as it can be easily derived,

$$\mathcal{J}_0 = \pi.$$

Hence,

$$\mathcal{J}_l = \frac{(2l-1)!!}{(2l)!!}\pi$$

therefore we obtain

$$N \approx A^{1/2} = \sqrt{p(p+1)}$$

and

$$\sum_{j=1}^{N} B_j^l = \frac{(2l)!!}{(2l+1)!!}\frac{(2l-1)!!}{(2l)!!}A^{(2l+1)/2} = \frac{A^{(2l+1)/2}}{2l+1}.$$

These are the WKB approximations.

If $A = p(p+1)$, then the exact values are

$$N = p$$

$$B_j = -j^2 \qquad (p = 1\ldots p)$$

The following table shows the values for $l = 1$

N	$\sum_{j=1}^{N} B_j$	**WKB**
1	1	0.9428
2	5	4.899
3	14	13.856
4	30	29.814
5	55	54.772
6	91	90.73
7	140	139.689
8	204	203.647

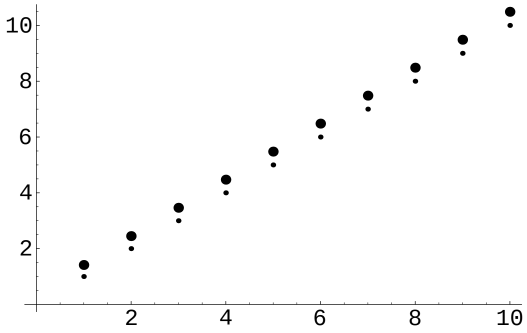

Figure 3: N as a function of p. (Small dots are the exact values, the big ones are the WKB approximation.) The difference is constant 1/2.

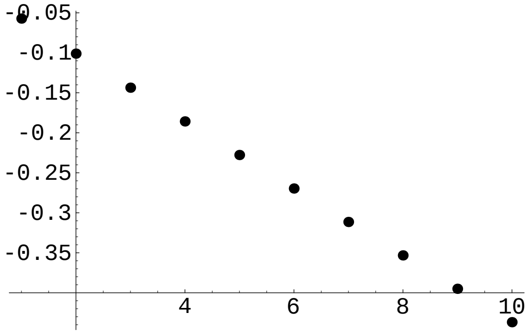

Figure 4: Difference of the exact values of $\sum B_j$ and the WKB approximation as a function of p. The error linearly grows with p.

5. **Transmission and reflection from a Gaussian barrier**

(a) In the WKB approximation, the transition probability is

$$|T|^2 = e^{-\frac{2}{\hbar}\int_{x_1}^{x_2} dx\sqrt{2m(V(x)-E)}}.$$

We solve for the turning points and find that

$$x_{1,2} = \pm a\sqrt{2\ln\left(\frac{V_0}{E}\right)}.$$

Using $V(x) = V_0 e^{-\frac{1}{2}x^2/a^2}$, we now proceed to evaluate the integrals.

$$\begin{aligned}\ln\left(|T|^2\right) &= -\frac{2}{\hbar}\int_{x_1}^{x_2} dx\sqrt{2m\left(V(x)-E\right)} \\ &= -\frac{2}{\hbar}\int_{x_1}^{x_2} dx\sqrt{2mV_0}\sqrt{e^{-\frac{x^2}{2a^2}} - \frac{E}{V_0}} \\ &= -4\Delta\int_0^{\sqrt{-2\ln z}} dx\sqrt{e^{-\frac{x^2}{2}} - z}\end{aligned}$$

This integral cannot be done exactly but we want to find its form for small z.

$$\begin{aligned}\ln\left(|T|^2\right) &\approx -4\Delta\int_0^{\sqrt{-2\ln z}} dx e^{-\frac{x^2}{4}} \\ &\approx -4\Delta\sqrt{\pi}\mathrm{Erf}\left(\frac{x}{2}\right) \\ &\approx -4\Delta\sqrt{\pi} + \cdots\end{aligned}$$

Note that if you approximate the potential with a parabola, you obtain the same functional dependence on the height and width but a different numerical prefactor. In this case the $4\sqrt{\pi}$ becomes $\pi\sqrt{2}$.

(b) From PS4 problem 6, we know that

$$\begin{aligned}\delta(E) &= \frac{1}{2\hbar}\int_{-\infty}^{\infty} dx\left(p(x) - k\right) \\ &= \frac{1}{2\hbar}\int_{-\infty}^{\infty} dx\left[\sqrt{2mE}\sqrt{1 - \frac{V_0}{E}e^{-\frac{x^2}{2a^2}}} - k\right] \\ &= -\frac{V_0}{\hbar}\sqrt{\frac{m}{2E}}\int_{-\infty}^{\infty} dx e^{-\frac{x^2}{2a^2}} \\ &= -\frac{aV_0}{2\hbar}\sqrt{\frac{m\pi}{E}}\end{aligned}$$

(c) From the notes, we have that

$$|R(E)|^2 = \exp\left(-\frac{2}{\hbar}\int_{-p_0(E)}^{p_0(E)} dp\ \mathrm{Im}\left[V^{-1}(E-\frac{p^2}{2m})\right]\right).$$

Here

$$\mathrm{Im}\left[V^{-1}(E-\frac{p^2}{2m})\right] = \sqrt{2a^2\ln\left(\frac{E-\frac{p^2}{2m}}{V_0}\right)}$$

Thus

$$\begin{aligned}|R(E)|^2 &= \exp\left(-\frac{4}{\hbar}\int_0^{p_0(E)} dp\ \sqrt{2a^2\ln\left(\frac{E-\frac{p^2}{2m}}{V_0}\right)}\right)\\ &= -4\sqrt{2}\Delta\int_0^{\sqrt{z-1}} dp\ \sqrt{\ln\left(z-p^2\right)}\end{aligned}$$

Again we expand and we find that

$$|R|^2 = -4\sqrt{2}\Delta\left(\sqrt{(z-1)\ln z} - \frac{(z-1)^{3/2}}{6z} + \cdots\right)$$

(d) We take $\Delta = 10$ and evaluate $|T|^2$ and $|R|^2$, using the two integrals in (a) and (c) that we could not evaluate exactly. Note that $4\sqrt{\pi}\Delta \approx 70.9$.

For T^2 the approximation is only valid when $z \ll 1$.

For R^2 the approximation is only valid when $z \gg 1$.

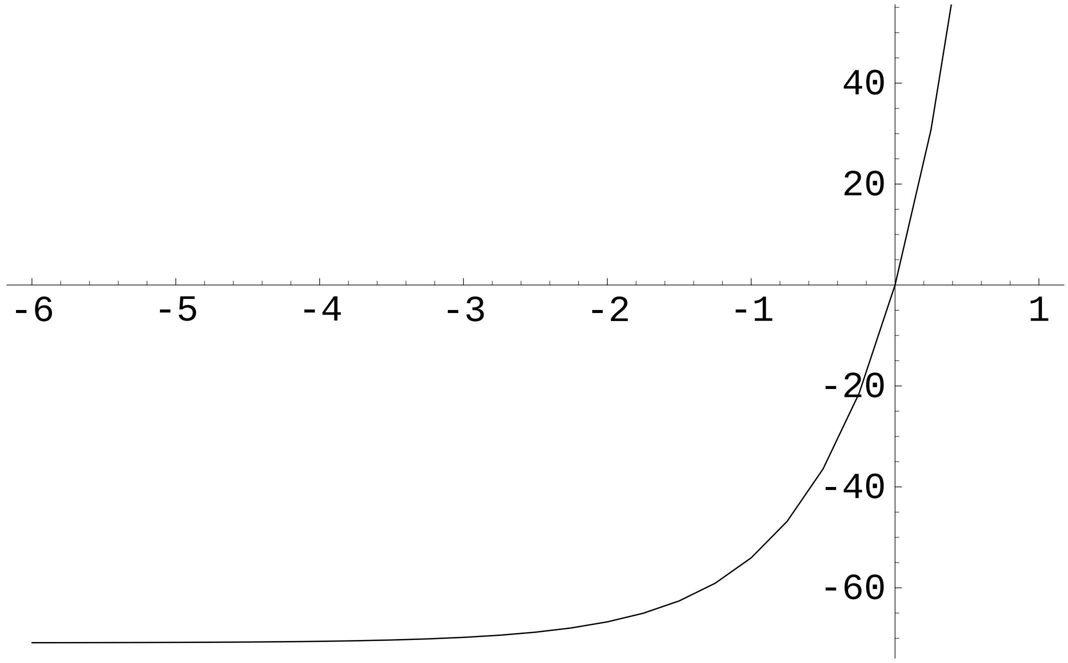

Figure 5: $\ln|T|^2$ as a function of $\log_{10}z$.

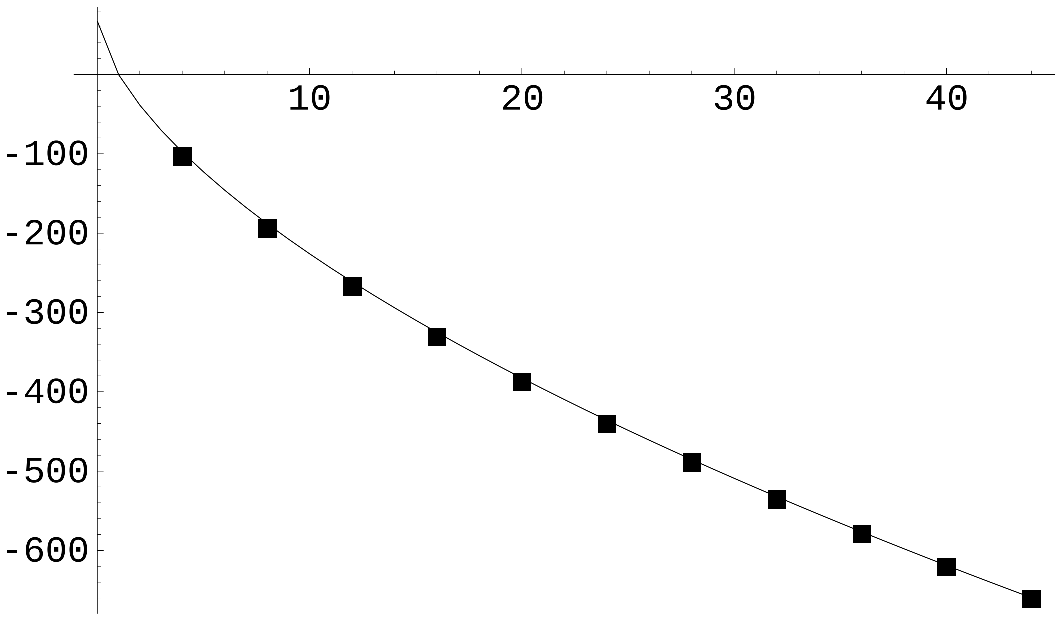

Figure 6: $\ln|R|^2$ as a function of z. The solid line is the numerical integration and the squares are points from the formula derived in (c).