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1. (a) We begin, when integrating using Gauss-Laguerre quadrature, by transforming the integrals in question,

$$I = \frac{\int_0^\infty (x^4+1)xe^{-\sqrt{4x^2+1}}dx}{\int_0^\infty xe^{-\sqrt{4x^2+1}}dx} \tag{1}$$

into ones of the form

$$\int_0^\infty f(x)e^{-x}. \tag{2}$$

We begin with the numerator, which we will call I_N. Choosing the substitution $w = \sqrt{4x^2+1}$, we get

$$x = \sqrt{\frac{w^2-1}{4}}, \quad x^4+1 = \left(\frac{w^2-1}{4}\right)^2 + 1, \quad dx = \frac{w}{2\sqrt{w^2-1}}dw$$

Then we find

$$\begin{aligned} I_N &= \int_1^\infty \frac{w}{2\sqrt{w^2-1}} \left(\left(\frac{w^2-1}{4}\right)^2+1\right)\sqrt{\frac{w^2-1}{4}}e^{-w}dw \\ &= \int_0^\infty \frac{w}{4}\left(\left(\frac{w^2-1}{4}\right)^2+1\right)e^{-w}dw \end{aligned}$$

Using another substitution, $x = w-1$, we can see

$$I_N = \int_0^\infty \frac{x+1}{4}\left(\left(\frac{x^2+2x}{4}\right)^2+1\right)e^{-x-1} \tag{3}$$

where we easily identify

$$f_N(x) = \frac{x+1}{4e}\left(\left(\frac{x^2+2x}{4}\right)^2+1\right). \tag{4}$$

For the denominator, we use the same two substitutions, finding

$$\begin{aligned} I_D &= \int_0^\infty xe^{-\sqrt{4x^2+1}}dx \\ &= \int_1^\infty \frac{w}{4}e^{-w}dw \\ &= \int_0^\infty \frac{x+1}{4e}e^{-x}dx \end{aligned} \tag{5}$$

$$\implies f_D(x) = \frac{x+1}{4e}. \tag{6}$$

We can then use Gauss-Laguerre quadrature to find these integrals:

$$I_N \approx \sum_{i=1}^n f_N(x_i)w_i \tag{7}$$

$$I_D \approx \sum_{i=1}^n f_D(x_i)w_i \tag{8}$$

where the x_i are the roots of the n-th order Laguerre polynomial, and w_i are the respective weights. These can be found using `np.polynomial.laguerre.laggauss(n)`.
Using a 16-th order Laguerre polynomial, we found $I \approx 10.250000000000082$, which is pretty bang on 10.25.

(b) For a Monte Carlo integration method, we choose the Metropolis method, as the integral in equation (1) is of the form

$$I = \frac{\int p(x)f(x)dx}{\int p(x)dx}. \tag{9}$$

We can identify $f(x) = x^4 + 1$, and thus we need to sample according to

$$p(x) = xe^{-\sqrt{4x^2+1}}. \tag{10}$$

Using the Metropolis method allows us to not have to normalise this $p(x)$, which is nice as the integral of it is a bit ugly.
To begin with, we generate $N_0 = 500\,000$ points x_i, according to $p(x)$ using the Metropolis random walk/Markov chain method, with $\Delta = 2$ for an acceptance rate of about 45%.
In order to avoid correlation between points we compute the autocorrelation function

$$C(j) = \frac{\langle x_{i+j}x_i\rangle - \langle x_i\rangle^2}{\langle x_i^2\rangle - \langle x_i\rangle^2} \tag{11}$$

for a range of j values, and find the first j for which $C(j) \leq 0.01$. Figure 1 shows the results.

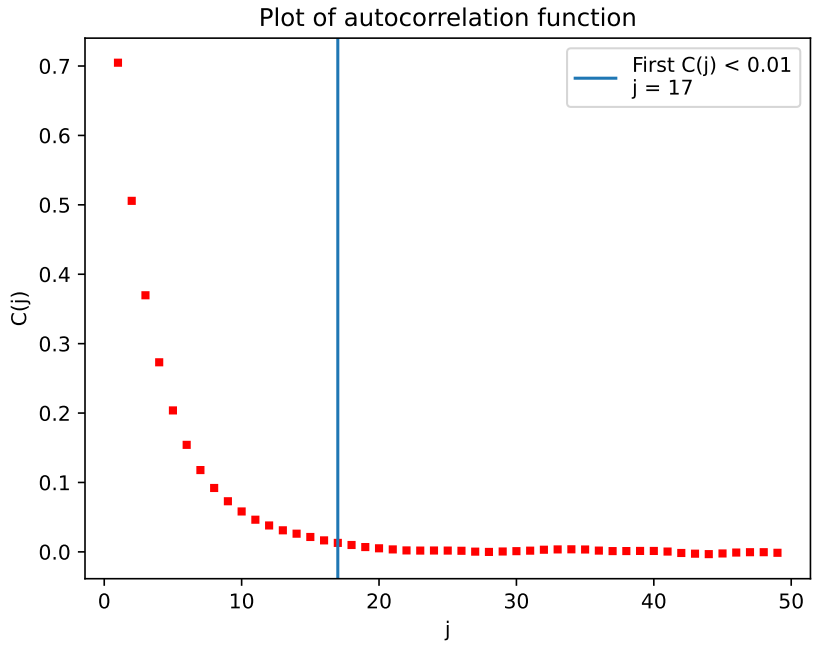

Figure 1: Plot of the autocorrelation function for the N_0 generated values, giving us $C(j = 17)$ as the first value ≤ 0.01.

This tells us how many numbers in the Markov chain to skip each time we choose one to be part of our final distribution. We also need to consider the starting values, as the method goes through a transient phase before equilibrating. To find how many numbers to chop off the start, we can find the moving average of the N_0 generated values, and see when it begins to level level off. Figure 2 shows the results.

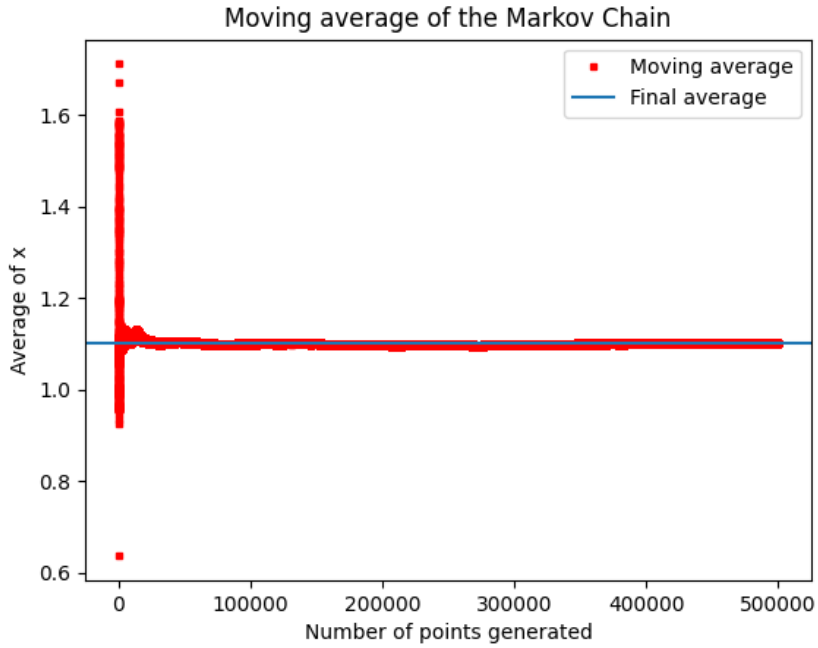

Figure 2: Plot of the moving average of the N_0 points in the generated Markov chain, along with the final average, to see when the moving average begins to level off.

By inspection, we can see it levels off at around 20 000 points, so we choose to cut off the first 20 000 points. Doing this and skipping every 17 points leaves us with around 28 000 points in our distribution. Figure 3 shows the results.
With these randomly generated numbers x_i, we can finally compute I in equation (1) using

$$I \approx \frac{1}{N}\sum_{i=1}^{N} f(x_i) \tag{12}$$

where $N \sim 28\,000$. We find $I \approx 10.48 \pm 0.29$. This uncertainty is calculated using

$$u(I) = \frac{\sigma}{\sqrt{N}} = \frac{\sqrt{\langle f^2\rangle - \langle f\rangle^2}}{\sqrt{N}}. \tag{13}$$

(c) Performing the integral I in equation (1) in Mathematica, we find the exact result to be $\frac{41}{4} = 10.25$. We see that Gauss-Laguerre worked very well, producing the result to an accuracy that could likely be waved away with computer precision. We also see that the Monte Carlo method result agrees with the exact and Gauss-Laguerre results.

2. We aim to solve the boundary value problem

$$\frac{d^2V}{dr^2} + \frac{2}{r}\frac{dV}{dr} = 0 \tag{14}$$

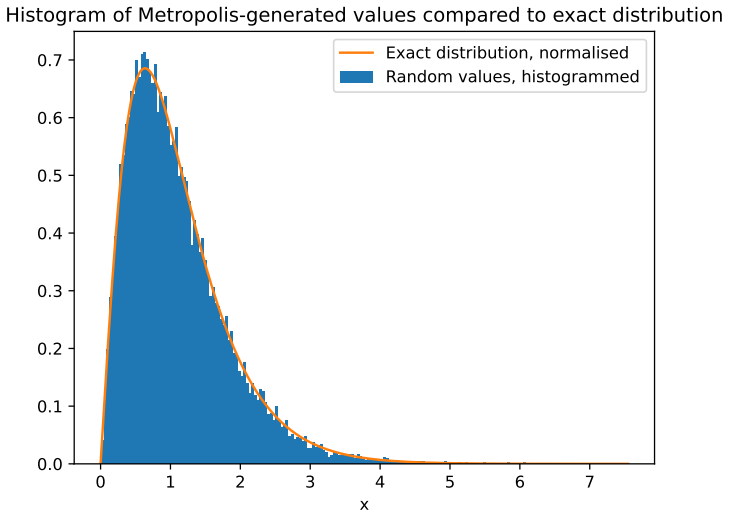

Figure 3: Histogram of the x-values calculated using the Metropolis method, distributed according to equation (10), along with the exact distribution. Note that the histogram is normalised to 1 over the interval shown, while $p(x)$ is normalised over the semi-infinite interval, so there may be some discrepancies.

with BCs $V(r = 1\,\mathrm{m}) = 20\,\mathrm{V}$ and $V(r = 3\,\mathrm{m}) = 55\,\mathrm{V}$. Since this is a linear, second order ODE, we can simply use the linear finite difference scheme to solve it. To do this, we first approximate the derivatives as finite differences. Using the notation $V_i = V(r_i)$, and constructing a grid with spacing Δr, we have

$$\begin{aligned} 0 &= \frac{V_{i-1} - 2V_i + v_{i+1}}{\Delta r^2} + \frac{2}{r_i}\frac{V_{i+1} - V_{i-1}}{2\Delta r} \\ &= V_{i-1}\underbrace{\left(1 - \frac{\Delta r}{r_i}\right)}_{\alpha} - 2V_i + V_{i+1}\underbrace{\left(1 + \frac{\Delta r}{r_i}\right)}_{\beta} \\ &= \alpha V_{i-1} - 2V_i + \beta V_{i+1} \end{aligned}$$

We can now consider this problem to be a matrix equation $A\mathbf{V} = \mathbf{w}$ where A is a band matrix, $\mathbf{V}$ is the V_i's that make up the solution to equation (14), and $\mathbf{w}$ is effectively the RHS of the ODE.
If we split our interval into $N + 2$ points, going from $i = 0$ to $i = N + 1$, we can construct our matrix equation:

$$\begin{pmatrix} -2 & \beta & 0 & \cdots & 0 \\ \alpha & -2 & \beta & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \cdots & \alpha & -2 & \beta \\ 0 & \cdots & \cdots & \alpha & -2 \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \\ \vdots \\ V_{N-1} \\ V_N \end{pmatrix} = \begin{pmatrix} -\alpha V_0 \\ 0 \\ \vdots \\ 0 \\ -\beta V_{N+1} \end{pmatrix} \tag{15}$$

What is important to note here is the appearance of our BCs in $\mathbf{w}$, on the RHS. This is due to a quirk in how the matrix gets constructed, but allows us to solve this system exactly,

in one step, as we know all of A and $\mathbf{w}$ explicitly, so we can just invert A. Doing this with `np.linalg.solve` and tacking on the two BCs, as this method does not return them in $\mathbf{V}$, we find the plot in figure 4.

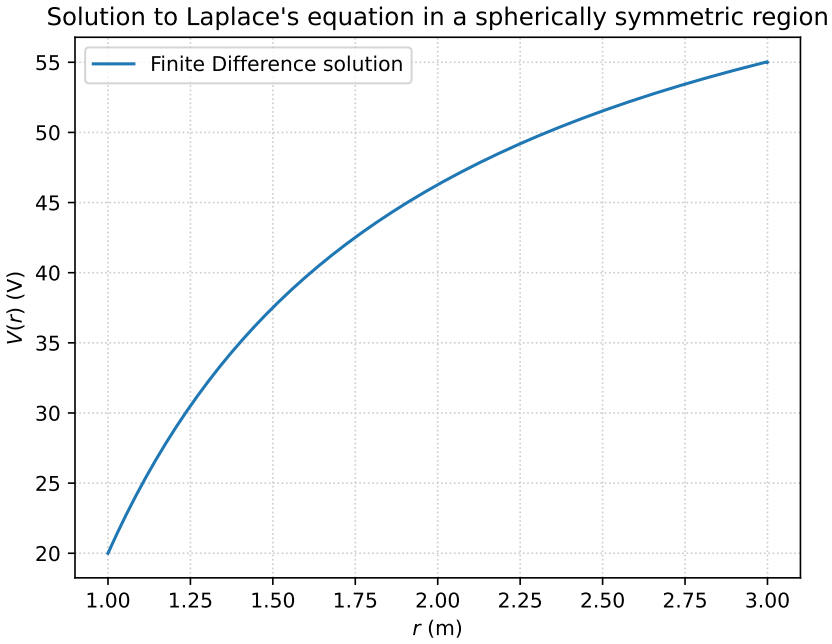

Figure 4: Plot of the solution to equation (14) using the linear finite difference method, with $V(r = 1\,\mathrm{m}) = 20\,\mathrm{V}$ and $V(r = 3\,\mathrm{m}) = 55\,\mathrm{V}$. A step of $\Delta r = 0.001$ was used.