Problem 1. Central Limit Theorem and Random Walk

In a random walk, a collegiate drunkard starts at the origin and takes a step of size a, to the right with probability p and to the left with probability $1 - p$.

(a) Take $p = 1/2$, i.e. equal probability of right and left steps. Determine the probability of the drunkard having position X, i.e. $P(X)$, after three steps. Plot $P(X)$ where X can be one of $X = 0, \pm 1, \pm 2, \pm 3$. Note how your graph begins to approach a Gaussian after just three steps.

(b) Now keep p general. What is the mean and variance variance in the drunkard's position X after one step, and after two steps?

(c) After n steps (with $n \gg 1$) find his mean position $\langle X \rangle$, and the std. deviation in his position $\sigma_X = \sqrt{\langle \delta X^2 \rangle}$. Check your result by comparing with the figure below

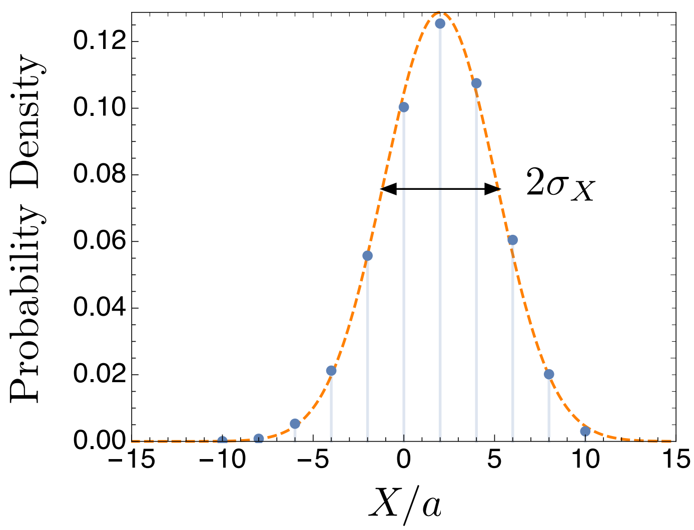


Figure 1: Probability of our drunkard having position X after $n = 10$ steps (the blue points). Of course after 10 steps the drunkard will be between $-10 \ldots 10$, and it is easy to show that he will be only at the even sites, i.e. $-10, -8, -6, \ldots 10$. For $p = 0.6$, I find $\langle X \rangle = 2.0$. Twice the std deviation, $2\sigma_X$, is shown in the figure and is about six in this case. The orange curve is a gaussian (a.k.a the "bell-shaped" curve) approximation discussed in class and approximately agrees with the points – this is the central limit theorem. Recall that the central limit theorm says that if the number of steps n is large, the probability of X (a sum of n independent events) is approximately $P(x)\, \mathrm{d}X \propto \exp(-(X - \langle X \rangle)^2/2\sigma_X^2)$. Evidently the gaussian approximation works well already for $n = 10$.

Hint: X is a sum N independent events x_i where $x_i = \pm a$. Use results from class on the probability distribution of a *sum* of independent events.

(d) (Optional. Don't turn in) If p is very nearly $\frac{1}{2}$, say $p = 0.5001$, determine how many steps it will take before the mean value $\langle X \rangle$ is definitely different from zero. By "definitely" I mean that $\langle X \rangle$ is "more than two sigma" away from zero, $\langle X \rangle > 2\sigma_X$. If $p = \frac{1}{2} + \epsilon$ (with ϵ tiny), you should find (approximately) that

$$N_{\text{steps}} \simeq \frac{1}{\epsilon^2} \tag{1}$$

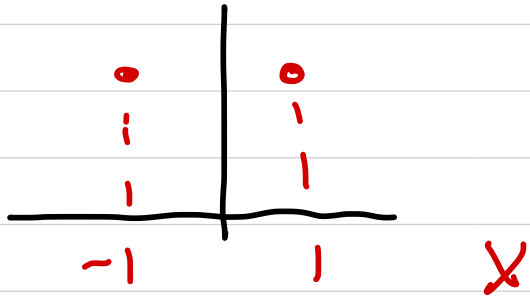
up to corrections of order ϵ. Here $p = \frac{1}{2} + \epsilon$ with $\epsilon = 0.0001$, how does the result scale with ϵ, e.g. if I where two half ϵ how would the number of required steps change?

Random Walk

After 1 step:

$$P_1 = 1/2$$

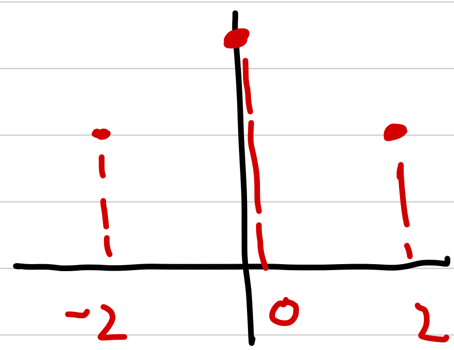
$$P_{-1} = 1/2$$



After 2 steps

$$P_2 = \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4}$$

$$P_0 = \frac{1}{2} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{2}$$



$$P_{-2} = \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4}$$

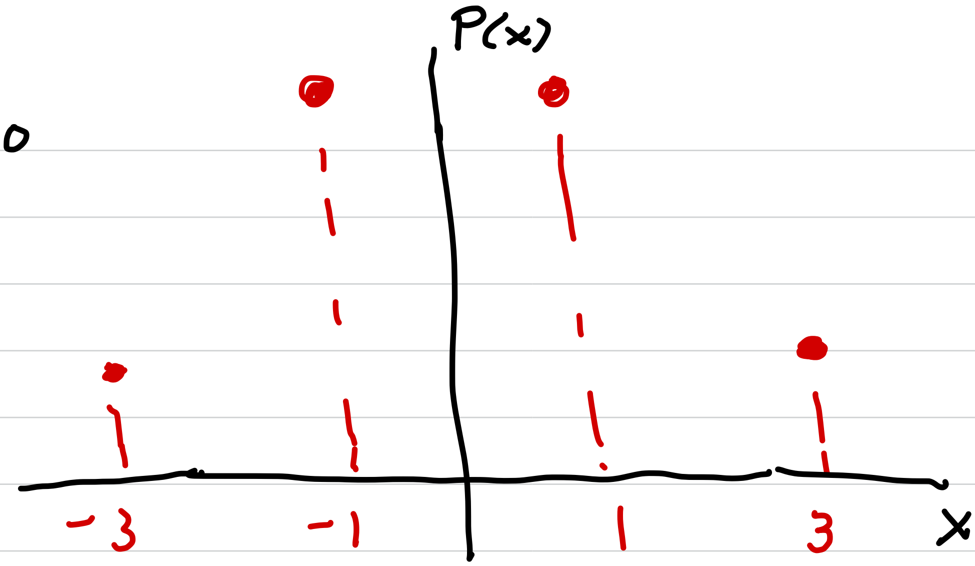
After 3 steps

$$P_3 = \frac{1}{4} \cdot \frac{1}{2} = \frac{1}{8}$$

$$P_1 = \frac{1}{4} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} = \frac{3}{8}$$

$$P_{-1} = \frac{3}{8}$$

$P_{-3} = \frac{1}{8}$, So



b) The mean and variance for one step are:

$$\overline{x} = a p - (1-p) a = a(2p-1) = \overline{x}_1$$

$$\overline{x^2} = a^2 p + (1-p) a^2 = a^2 = \delta x^2$$

$$\langle \delta x^2 \rangle = \overline{x}^2 - \overline{x}^2 = a^2 - a^2 (2p-1)^2$$

$$= a^2 (1 - ((2p)^2 - 2(2p) + 1) = 4a^2 p(1-p)$$

Now the mean and variance add

$$\left.\begin{aligned} \overline{X}_2 &= 2\overline{x} = 2a(2p-1) \\ \langle \delta X_2^2 \rangle &= 2\langle \delta x^2 \rangle = 8a^2 p(1-p) \end{aligned}\right\}$$

two steps are twice one step

c) Now for part (c)

$$\bar{X}_N = N a (2p-1)$$

For $N=10$ $p=0.6$ $\bar{X}_N = 10\,(2\ 0.6-1) = 2$

This clearly agrees with the figure wich is centered at $X/a = 2$

Similarly we compute the variance

$$\langle \delta x_N^2 \rangle = 4N\, a^2\, p(1-p) \quad \text{for } N=10 \quad p=0.6$$

we find $\langle \delta x_N^2 \rangle \simeq 9.6$ so $\sigma \equiv \sqrt{\langle \delta x^2 \rangle} \simeq 3.1$

Comparison with the graph gives $2\sigma \simeq 6.2$ which seems about right.

d) The mean is $Na(1-2p) = \langle x \rangle$. The standard deviation is $\sigma_x = \sqrt{N}\, 2a\, (p(1-p))^{1/2}$. Requiring that $\langle x \rangle > 2\sigma_x$ gives

$$N(1-2p) > 2\sqrt{N}\,(4p(1-p))^{1/2}$$

Solving for N we have

$$N > \frac{16\, p(1-p)}{(1-2p)^2}$$

So for $p = 1/2 + \varepsilon$, we have

$$N > \frac{16\, \tfrac{1}{2}(1-\tfrac{1}{2})}{(2\varepsilon)} \simeq \frac{1}{\varepsilon^2}$$

Problem 2. Counting

Consider 400 atoms laid out in a row. Each atom can be in one of two states a ground state with energy 0 and an excited state with energy Δ. Assume that 100 of the atoms are excited, so the total energy is $U = 100\,\Delta$.

(a) Show that there are e^{225} configurations, called microstates, for this energy U. One microstate is shown below.

(b) Suppose that we make a partition of the energy so that the first 200 atoms have an energy of $80\,\Delta$, and the next 200 atoms have an energy of $20\,\Delta$ (see below). The terminology here is that we have specified the "macrostate" (i.e. the 80/20 split), leaving the microstates (exactly which atoms are up are down) to be further specified. How many microstates are there with this macrostate? One microstate for this 80/20 split macrostate is shown below[1]

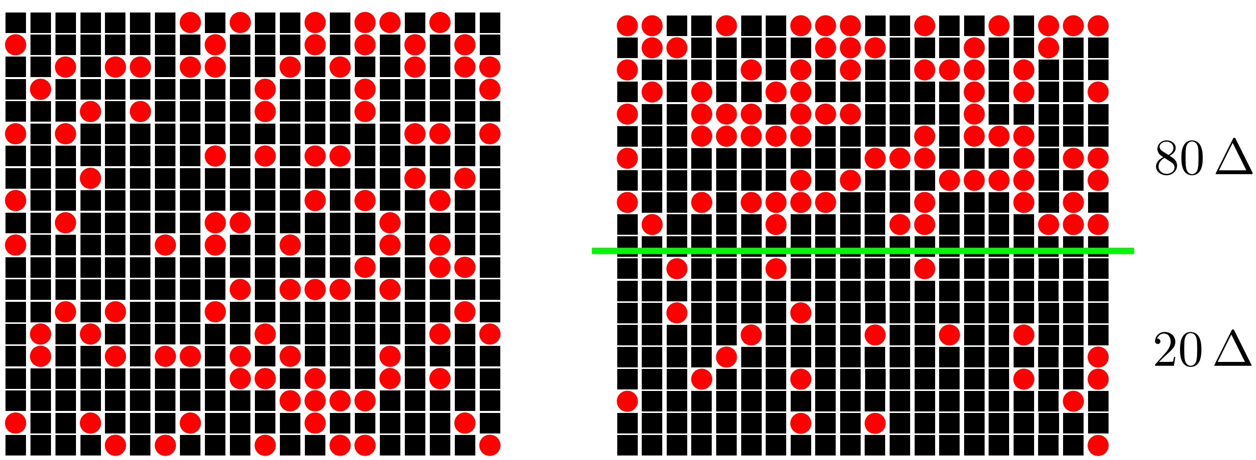


Figure 2: (a) A microstate where the energy is not partitioned. (b) a microstate where the energy is partitioned – 80% on the top and 20% on the bottom.

[1] Answer: e^{200}.

Solution:

(a) We are making a selection of $N_1 \simeq 100$ atoms out of $N = 400$ to be excited, with $N_2 = 300$ not excited:

$$\begin{aligned} \ln \Omega =& \ln \frac{N!}{N_1!N_2!} \simeq -N_1 \ln(N_1/N) - N_2 \ln(N_2/N) && (2) \\ =& 400 \left[-\frac{1}{4} \ln(\frac{1}{4}) - \frac{3}{4} \ln(\frac{3}{4}) \right] && (3) \\ \simeq& 225; && (4) \end{aligned}$$

Thus there e^{225} microstates.

(b) The reasoning is similar for top half, we are selecting 80 out of 200. So for the first half

$$\begin{aligned} \ln \Omega_1 =& \ln \frac{N!}{N_1!N_2!} \simeq -N_1 \ln(N_1/N) - N_2 \ln(N_2/N) && (5) \\ =& 200 \left[-\frac{80}{200} \ln(\frac{80}{200}) - \frac{120}{200} \ln(\frac{120}{200}) \right] && (6) \\ \simeq& 135.; && (7) \end{aligned}$$

While the bottom half we are selecting 20 out of 200

$$\begin{aligned} \ln \Omega_1 =& \ln \frac{N!}{N_1!N_2!} \simeq -N_1 \ln(N_1/N) - N_2 \ln(N_2/N) && (8) \\ =& 200 \left[-\frac{20}{200} \ln(\frac{20}{200}) - \frac{180}{200} \ln(\frac{180}{200}) \right] && (9) \\ \simeq& 65.; && (10) \end{aligned}$$

So the total number of configurations is a product

$$\ln(\Omega_1 \Omega_2) = \ln(\Omega_1) + \ln(\Omega_2) \simeq 200. \qquad (11)$$

Problem 3. The Gamma function

The $\Gamma(x)$ function can be defined as[2]

$$\boxed{\Gamma(x) \equiv \int_0^\infty \mathrm{d}u e^{-u} u^{x-1} = \int_0^\infty \frac{\mathrm{d}u}{u}\, e^{-u} u^x} \tag{12}$$

A plot of $\Gamma(x)$ is shown below. $\Gamma(n)$ provides a unique generalization of $(n-1)!$ when n is not an integer and even negative or complex. It will come up a number of times in this course and is good to know.

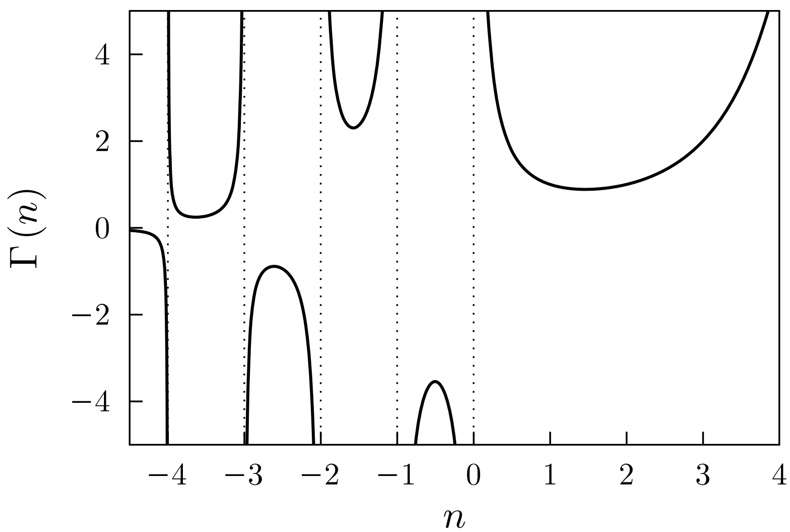


Fig. C.1 The gamma function $\Gamma(n)$ showing the singularities for integer values of $n \le 0$. For positive, integer n, $\Gamma(n) = (n-1)!$.

Figure 3: Appendix C.2 of our book

(a) Using notions of generating functions, briefly explain why $\Gamma(n) = (n-1)!$ for n integer.

(b) Prove that $\Gamma(\frac{1}{2}) = \sqrt{\pi}$. *Hint:* try a substitution $y = \sqrt{u}$.

The following identity is needed below.

$$\boxed{\Gamma(x+1) = x\Gamma(x)\,,} \tag{13}$$

or

$$x! = x \cdot (x-1)!\,, \tag{14}$$

but now x is a real number, and $x!$ is defined by $\Gamma(x+1)$.

(c) (Optional. Dont turn in) Use integration by parts to prove the identity in Eq. (12).

[2] I like to write $\Gamma(x) = \int_0^\infty \frac{du}{u}\, e^{-u} u^x$, which makes the x is more explicit. Also the measure du/u is invariant under a homogeneous rescaling, e.g. under change of variables $u \to u' = \lambda u$ we have $du'/u' = du/u$.

(d) Use the results of this problem to show that $\Gamma(\frac{7}{2}) = 15\sqrt{\pi}/8$. What is the result numerically? $7/2$ is between two integers. Show that $\Gamma(7/2)$ is between the appropriate factorials related to those two integers?

(e) The "area" (i.e. circumference) of a "sphere" in two dimensions (i.e. the circle) is $2\pi r$. The area of a sphere in three dimensions is $4\pi r^2$. A general formula for the area of the sphere in d dimensions is derived in the book is (the proof is simple, using what we know)

$$A_d(r) = \frac{2\pi^{d/2}}{(\frac{d}{2}-1)!} r^{d-1} = \frac{2\pi^{d/2}}{\Gamma(d/2)} r^{d-1} \tag{15}$$

Show that this formula gives the familiar result for $d = 2$ and $d = 3$.

Gamma Fcn

(a) According to the previous problem

$$n! = \int_0^\infty dx\; e^{-x}\, x^n$$

$$= \underbrace{\int_0^\infty \frac{dx}{x}\; e^{-x}\, x^{n+1}}_{\text{definition of } \Gamma(n+1)} = \Gamma(n+1)$$

(b) So

$$\Gamma(1/2) = \int_0^\infty \frac{dx}{x}\; e^{-x}\, x^{1/2}$$

- writing $y = \sqrt{x}$, $dy = \frac{1}{2}\frac{dx}{\sqrt{x}}$, or

$$2\frac{dy}{y} = \frac{dx}{x}$$

- So we find

$$\Gamma(1/2) = 2\int_0^\infty \frac{dy}{\cancel{y}}\; e^{-y^2}\, \cancel{y} = \int_{-\infty}^{\infty} dy\, e^{-y^2}$$

- This is a gaussian integral, $\int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}\frac{x^2}{\sigma^2}} = \sqrt{2\pi\sigma^2}$,

with $\sigma^2 = 1/2$, so $\boxed{\Gamma(1/2) = \sqrt{\pi}}$

- Then (this is optional):

$\boxed{c)}$ $$\Gamma(x) = \int_0^\infty \frac{du}{u}\, e^{-u}\, u^{x+1}$$

$$\Gamma(x+1) = \int_0^\infty du\, e^{-u}\, u^x$$

$$= \int_0^\infty -de^{-u}\, u^x$$

$$= e^{-u} u^x \Big|_0^\infty + \int_0^\infty e^{-u}\, x\, u^{x-1}$$

$$= 0 + x \int_0^\infty e^{-u}\, u^{x-1}$$

$$= x\,\Gamma(x)$$

$\boxed{d)}$ So if $\Gamma(7/2) = \frac{5}{2}\Gamma\left(\frac{5}{2}\right) = \frac{5}{2}\cdot\frac{3}{2}\,\Gamma\left(\frac{3}{2}\right)$

$$= \frac{5}{2}\cdot\frac{3}{2}\cdot\frac{1}{2}\,\Gamma\left(\frac{1}{2}\right)$$

$$= \frac{15}{8}\sqrt{\pi} \simeq 3.3$$

Now $3 < \frac{7}{2} < 4$ so we expect (and find)

$$2! < \frac{15\sqrt{\pi}}{8} < 3! \quad \text{or} \quad 2 < 3.3 < 6$$

e) $$A_2 = \frac{2\pi^{2/2}}{\Gamma(1)} r = 2\pi r$$

$$A_3 = \frac{2\pi^{d/2}}{\Gamma(\frac{3}{2})} r^2 = \frac{2\pi^{3/2}}{\frac{1}{2}\Gamma(1/2)} r^2$$

using $\Gamma(1/2) = \sqrt{\pi}$ we have:

$$A_3 = 4\pi r^2$$

Problem 4. Two State System

Consider an array of N atoms forming a medium at temperature T, with each atom possessing two energy states: a ground state with energy 0 and an excited state with energy Δ.

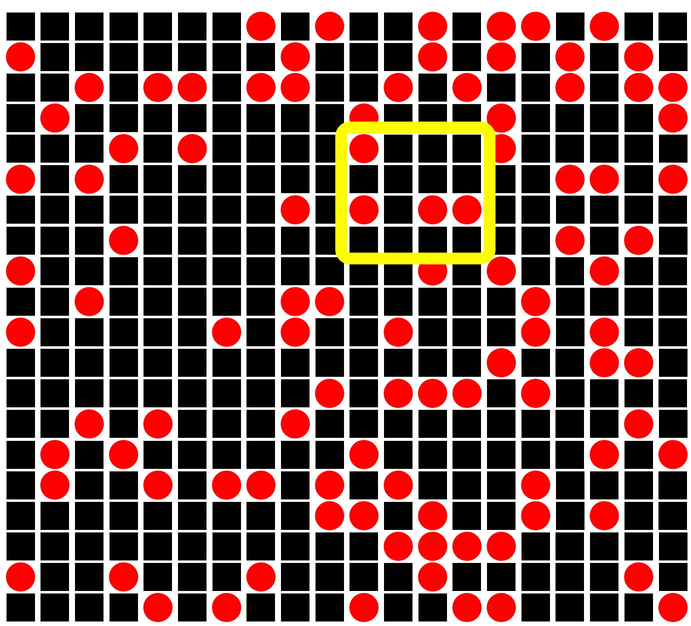
(a) Determine the temperature at which the number of excited atoms reaches $N/4$. You should find $kT = \Delta/\ln 3$.

(b) Calculate both the mean energy $\langle \epsilon \rangle$ and the variance of energy $\langle (\delta\epsilon)^2 \rangle$ for an individual atom. Your results should take the following form:

$$\left\langle (\delta\epsilon)^2 \right\rangle = \frac{\Delta^2 e^{-\beta\Delta}}{(1 + e^{-\beta\Delta})^2}$$

Additionally, create a graph depicting $\frac{\langle (\delta\epsilon)^2 \rangle}{(kT)^2}$ as a function of $\frac{\Delta}{kT}$.

(c) Suppose you have a collection of 16 such atoms (shown below). Calculate the average values of $\langle E \rangle$, $\langle (\delta E)^2 \rangle$ and $\langle E^2 \rangle$, where E represents the total energy of all 16 atoms. What approximately is the probability distribution for the energy E?



Solution

(a) The probability of being excited is (see lecture):

$$P_1 = \frac{e^{-\beta\Delta}}{Z} = \frac{e^{-\beta\Delta}}{1+e^{-\beta\Delta}} = \frac{1}{e^{\beta\Delta}+1}.$$

We want to find T (or $\beta = 1/kT$) when $P_1 = \frac{1}{4}$. Simple algebra yields:

$$e^{\beta\Delta} + 1 = 4 \quad \Rightarrow \quad kT = \frac{\Delta}{\ln(3)}.$$

(b) The mean energy is:

$$\langle \epsilon \rangle = P_0 \cdot 0 + P_1 \cdot \Delta = P_1 \Delta = \frac{\Delta}{e^{\beta\Delta}+1}.$$

The mean energy squared is:

$$\left\langle \epsilon^2 \right\rangle = P_0 \cdot 0^2 + P_1 \cdot \Delta^2 = P_1 \Delta^2 = \frac{\Delta^2}{e^{\beta\Delta}+1}.$$

Thus, the variance is given by:

$$\begin{aligned}
\left\langle (\delta\epsilon)^2 \right\rangle &= \left\langle \epsilon^2 \right\rangle - \langle \epsilon \rangle^2 && (16)\\
&= \frac{\Delta^2}{e^{\beta\Delta}+1}\left(1 - \frac{1}{(e^{\beta\Delta}+1)^2}\right) && (17)\\
&= \frac{\Delta^2 e^{\beta\Delta}}{(e^{\beta\Delta}+1)^2}, && (18)
\end{aligned}$$

which matches the problem statement after simplification.

(c) The energy is a sum:

$$E = \epsilon_1 + \ldots \epsilon_{16}.$$

The total energy behaves like a random walk, with each atom having $\epsilon = 0$ or $\epsilon = \Delta$. Since the atoms are identical:

$$\langle E \rangle = 16 \langle \epsilon \rangle .$$

Similarly, for a sum of statistically independent terms. The variance of a sum is the sum of the variances:

$$\left\langle (\delta E)^2 \right\rangle = 16 \left\langle (\delta\epsilon)^2 \right\rangle .$$

Utilizing the identical nature of the atoms, we find:

$$\begin{aligned}
\left\langle E^2 \right\rangle &= \langle E \rangle^2 + \left\langle (\delta E)^2 \right\rangle && (19)\\
&= 16^2 \langle \epsilon \rangle^2 \left(1 + \frac{1}{16}\frac{\left\langle (\delta\epsilon)^2 \right\rangle}{\langle \epsilon \rangle^2}\right), && (20)\\
&= 16^2 \langle \epsilon \rangle^2 \left(1 + \frac{e^{\beta\Delta}}{16}\right) . && (21)
\end{aligned}$$

In the limit that 16 is very large the second term can often be neglected.

Since E is a *sum* of many (i.e. 16) *independent and identical* objects, we have that its probability distribution will tend to a Gaussian. This is the Central Limit Theorem. The probability of having energy between E and $E + \mathrm{d}E$ is

$$\mathrm{d}\mathscr{P} = \frac{1}{\sqrt{2\pi \langle \delta E^2 \rangle}} e^{-(E-\langle E \rangle)^2/2\left\langle \delta E^2 \right\rangle} \mathrm{d}E \tag{22}$$

where $\langle \delta E^2 \rangle$ and $\langle E \rangle$ were given above. In the notation we have adopted, the probability density is

$$\frac{\mathrm{d}\mathscr{P}}{\mathrm{d}E} = P(E) = \frac{1}{\sqrt{2\pi \langle \delta E^2 \rangle}} e^{-(E-\langle E \rangle)^2/2\left\langle \delta E^2 \right\rangle} \tag{23}$$