Problem 6.23

Problem 6.23. For a CO molecule, the constant ϵ is approximately 0.00024 eV. (This number is measured using microwave spectroscopy, that is, by measuring the microwave frequencies needed to excite the molecules into higher rotational states.) Calculate the rotational partition function for a CO molecule at room temperature (300 K), first using the exact formula 6.30 and then using the approximate formula 6.31.

In[1]:=
```
ϵ = Quantity[0.00024, "Electronvolts"];
```

In[2]:=
```
k = Quantity[1, "BoltzmannConstant"];
T = Quantity[300, "Kelvins"];
```

Let 'x' = the dimensionless quantity $\frac{\epsilon}{k\,T}$. In this problem, it is quite small.

In[4]:=
```
x = ϵ / (k T)
```

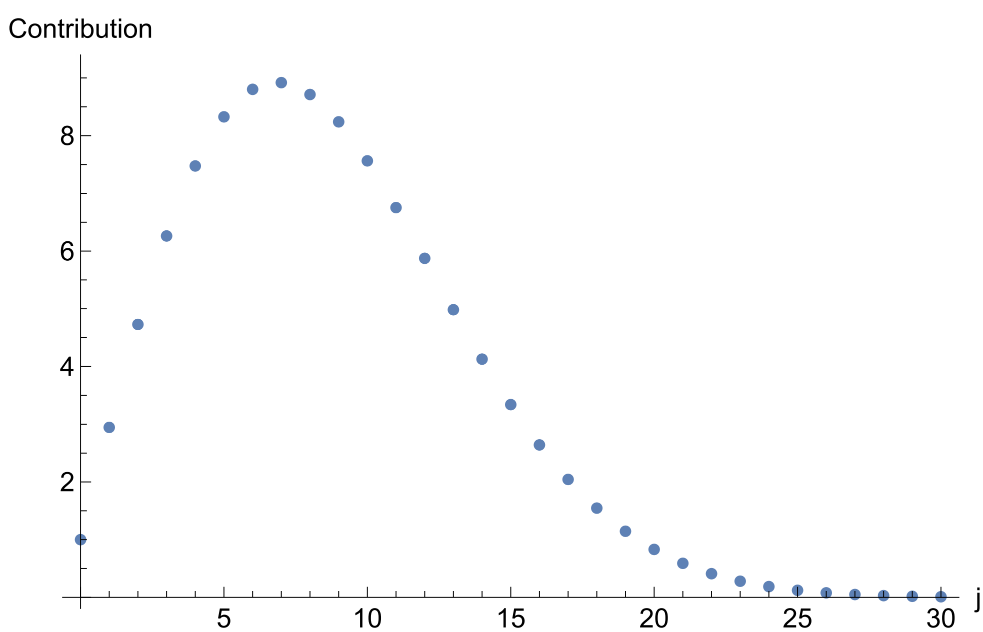
Out[4]=
```
0.00928361
```

In[7]:=
```
(* Unnormalized probability
 function:  Include the degeneracy -- there are 2j + 1 states for each energy.*)
Pu[x_, j_] := (2 j + 1) * Exp[-j (j + 1) * x]
```

Look at each of the first 30 terms in the partition function sum. The first 25 or so are important, but after that they are negligible.

In[9]:=
```
ListPlot[Table[{j, Pu[x, j]}, {j, 0, 30}] ,
 AxesLabel → {"j", "Contribution"}, LabelStyle → Larger, ImageSize → Scaled[0.8]]
```

Out[9]=

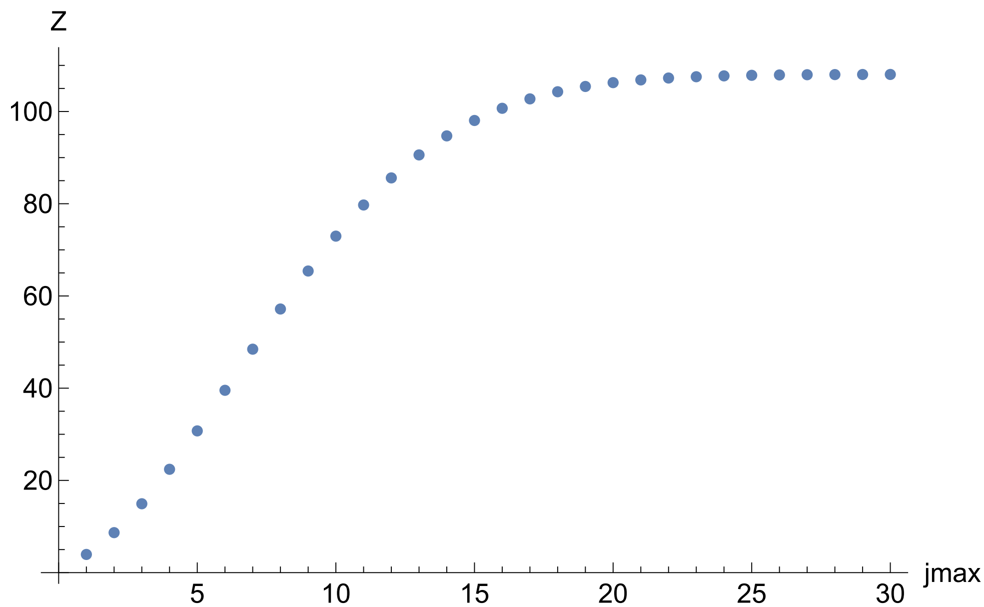


Write a function to numerically approximate the partition function up to 'jmax' terms.

In[10]:=
```
Z[x_, jmax_] := Sum[Pu[x, j], {j, 0, jmax}]
```

In[11]:=
```
ListPlot[Table[{jmax, Z[x, jmax]}, {jmax, 1, 30}],
 AxesLabel → {"jmax", "Z"}, LabelStyle → Larger, ImageSize → Scaled[0.8]]
```

Out[11]=



The sum converges fairly well after about 25 terms. Compare the actual sum to the approximate value $1/x = \frac{kT}{\epsilon}$.

In[19]:=
```
TableForm[Table[{jmax, Z[x, jmax]}, {jmax, 20, 30, 1}] ,
 TableHeadings → {None, {"jmax", "Z"}}]
```

Out[19]//TableForm=

jmax	Z
20	106.261
21	106.851
22	107.261
23	107.54
24	107.727
25	107.849
26	107.928
27	107.977
28	108.007
29	108.026
30	108.036

In[20]:=
```
1 / x (* Approximate high-temperature formula (x << 1)*)
```

Out[20]=

107.717