Mecánica estadística

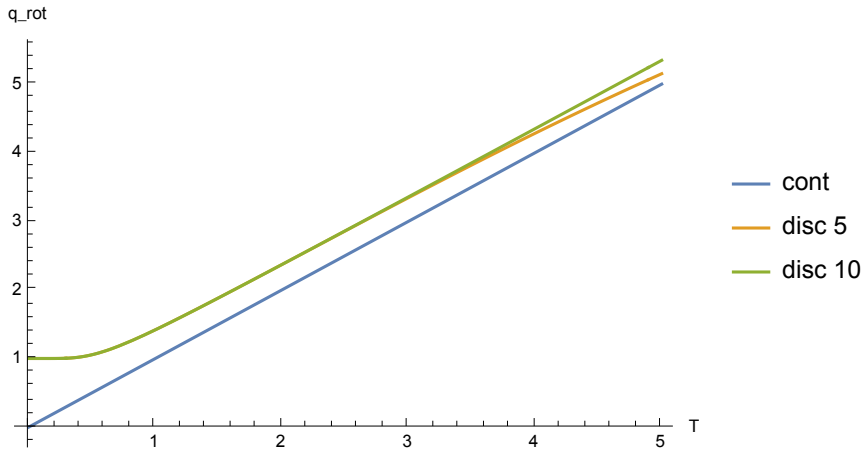
Taller de ejercicios

Definiciones

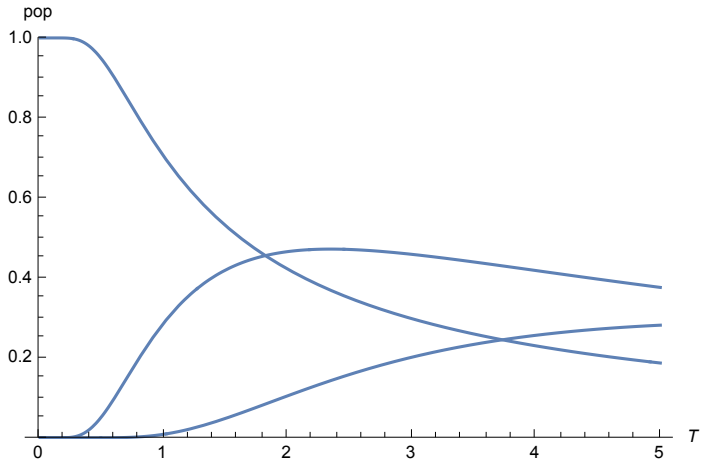
Gráficas de las funciones de partición

- Parte rotacional

```
Plot[{qrotlin[T, 1, 1], qrotdis[T, 1, 3, 1], qrotdis[T, 1, 10, 1]}, {T, 0, 5},
 AxesLabel → {"T", "q_rot"}, PlotLegends → {"cont", "disc 3", "disc 10"}]
```

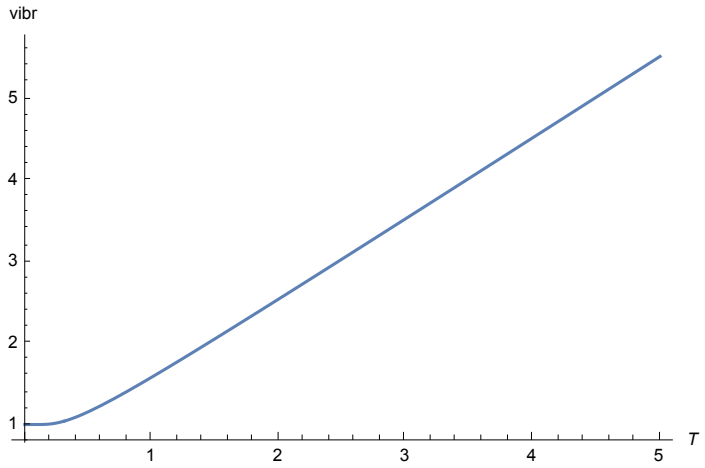



```
Plot[Table[(2 * i + 1) * Exp[-i * (i + 1) / T] / qrotdis[T, 1, 10, 1], {i, 0, 2}],
 {T, 0, 5}, AxesLabel → {"T", "pop"}, PlotRange → {0, 1}]
```

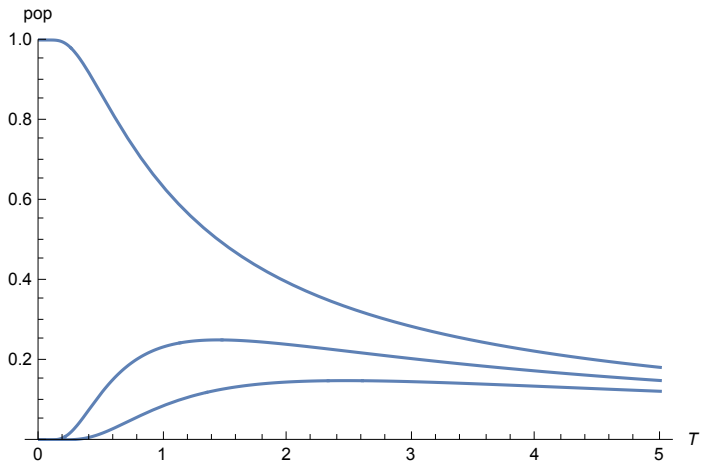


Parte vibracional

```
Plot[qvibr[T, {1}], {T, 0, 5}, AxesLabel → {"T", "q_vibr"}]
```



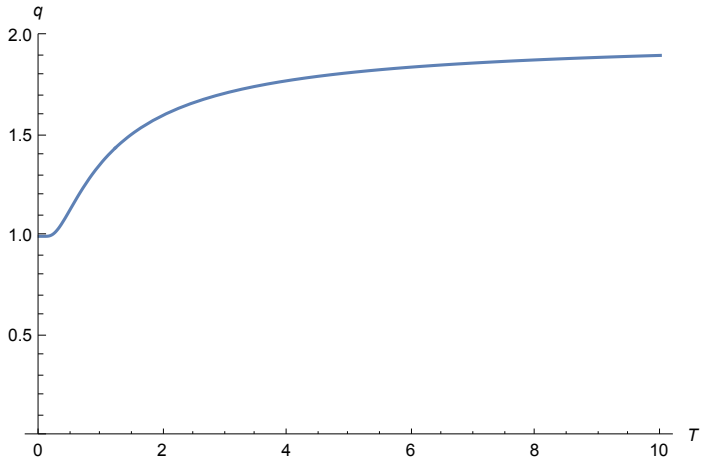

```
Plot[Table[Exp[-i / T] / qvibr[T, {1}], {i, 0, 2}],
 {T, 0, 5}, AxesLabel → {"T", "pop"}, PlotRange → {0, 1}]
```



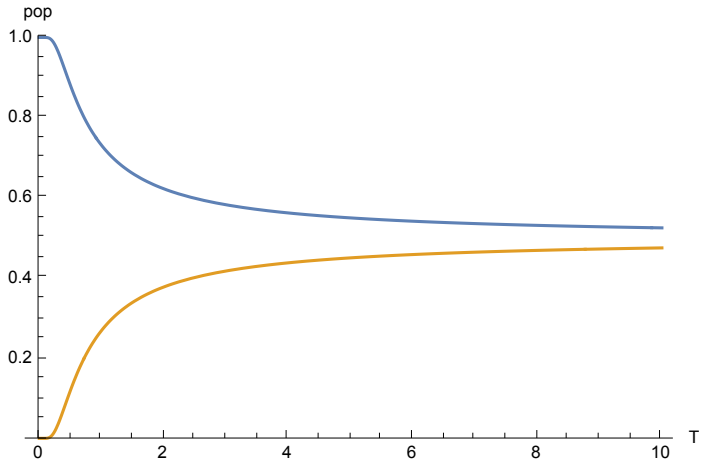
Parte electrónica

Ejemplo: sistema con dos estados

```
Plot[qele[T, {0, 1}, {1, 1}], {T, 0, 10}, AxesLabel → {"T", "q"}, PlotRange → {0, 2}]
```

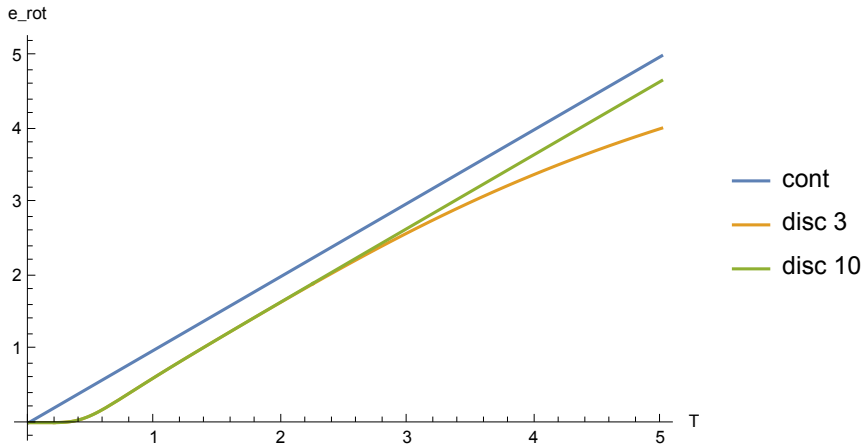



```
Plot[{1 / qele[T, {0, 1}, {1, 1}], Exp[-1 / T] / qele[T, {0, 1}, {1, 1}]},
 {T, 0, 10}, PlotRange → {0, 1}, AxesLabel → {"T", "pop"}]
```

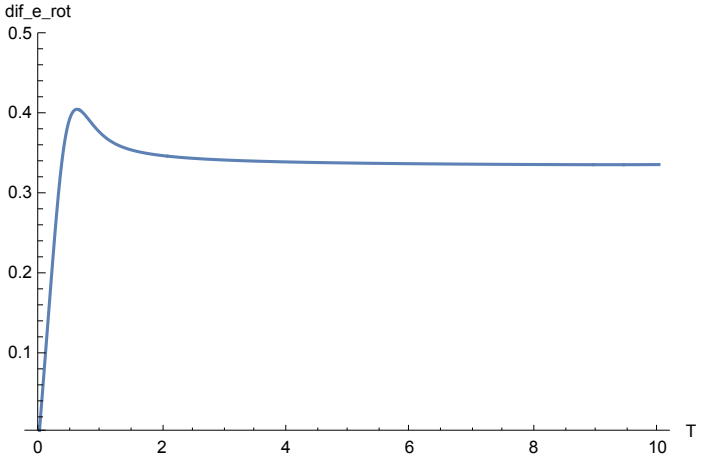


Gráficas de la energía

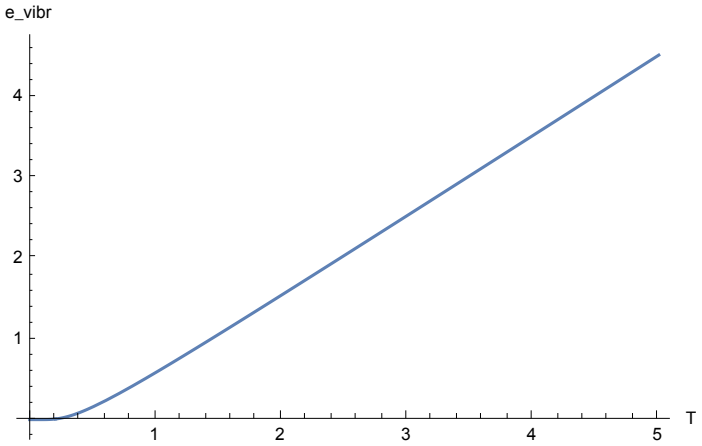
```
Plot[{erotlin[T] / (Na * k), erotdis[T, 1, 3] / (Na * k), erotdis[T, 1, 10] / (Na * k)},
 {T, 0, 5}, AxesLabel → {"T", "e_rot"},
 PlotLegends → {"cont", "disc 3", "disc 10"}]
```



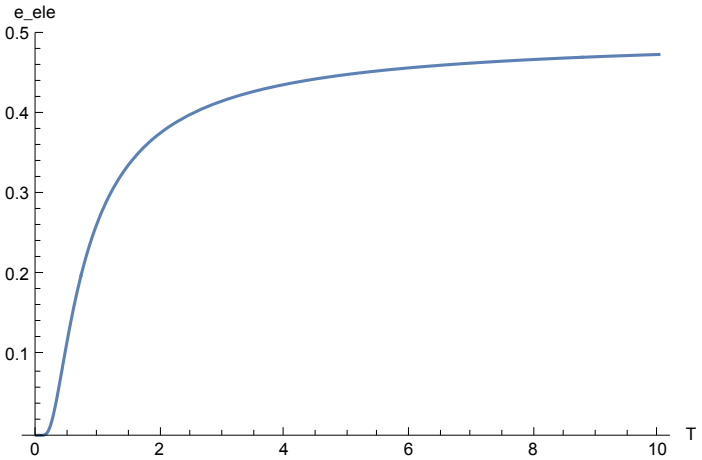
```
Plot[(erotlin[T] - erotdis[T, 1, 10]) / (Na * k),
 {T, 0, 10}, AxesLabel → {"T", "dif_e_rot"}, PlotRange → {0, .5}]
```




```
Plot[evibr[T, {1}] / (Na * k), {T, 0, 5}, AxesLabel → {"T", "e_vibr"}]
```

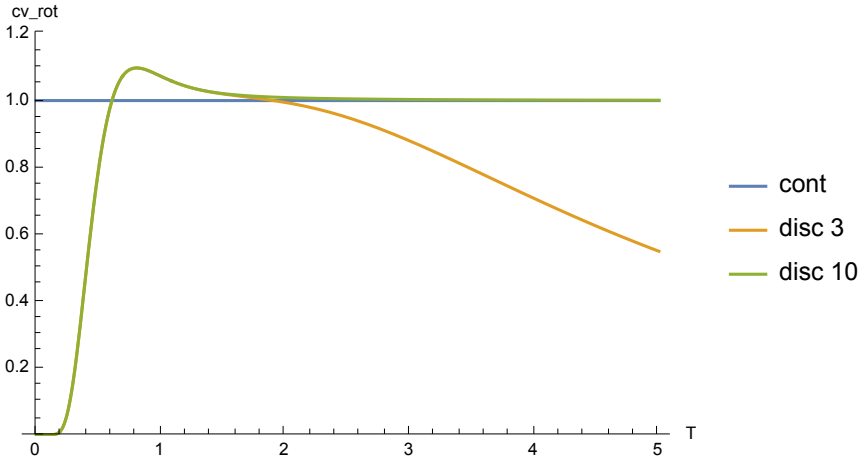



```
Plot[eele[T, {0, 1}, {1, 1}] / (Na * k), {T, 0, 10},
 AxesLabel → {"T", "e_ele"}, PlotRange → {0, 0.5}]
```

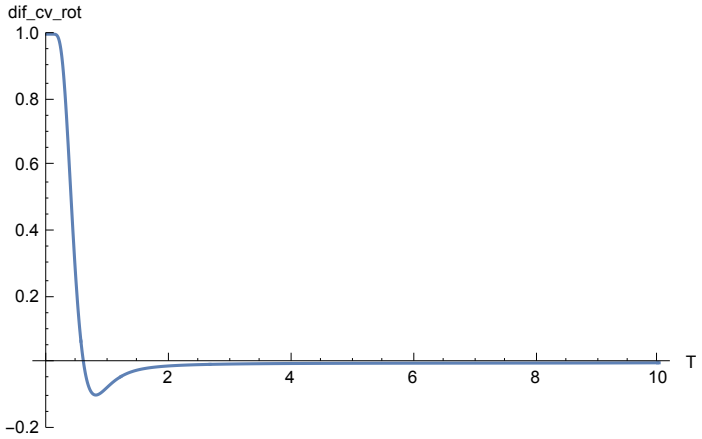


Gráficas de la capacidad calorífica

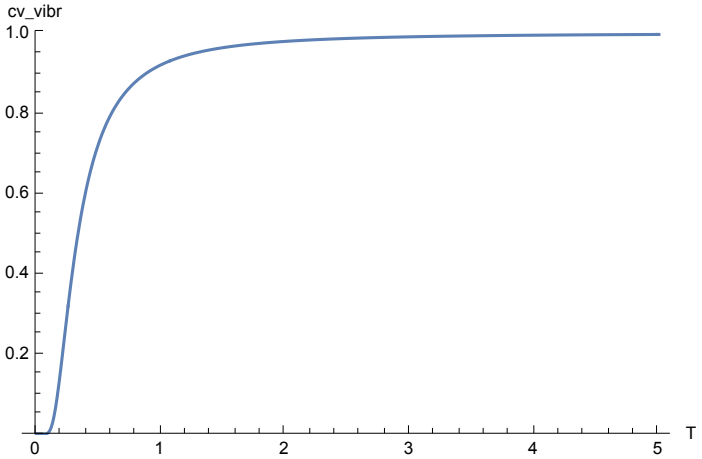
```
Plot[{cvrotlin[T] / (Na * k), cvrotdis[T, 1, 3] / (Na * k),
   cvrotdis[T, 1, 10] / (Na * k)}, {T, 0, 5}, AxesLabel → {"T", "cv_rot"},
 PlotLegends → {"cont", "disc 3", "disc 10"}, PlotRange → {0, 1.2}]
```



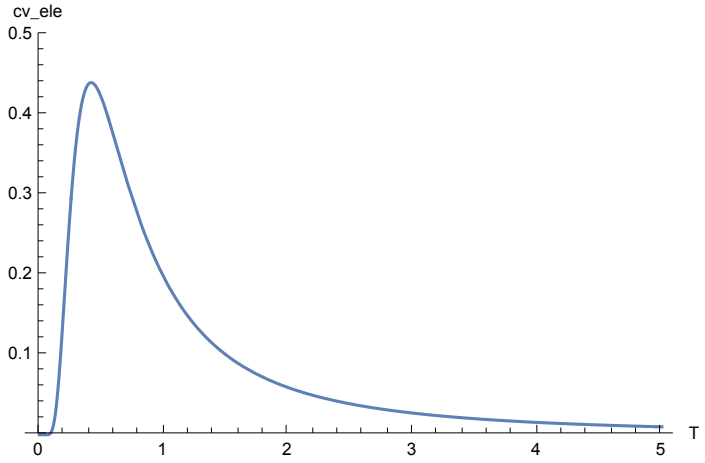

```
Plot[(cvrotlin[T] - cvrotdis[T, 1, 10]) / (Na * k), {T, 0, 10},
 AxesLabel → {"T", "dif_cv_rot"}, PlotRange → {-0.2, 1}]
```




```
Plot[cvvibr[T, {1}] / (Na * k), {T, 0, 5},
 AxesLabel → {"T", "cv_vibr"}, PlotRange → {0, 1}]
```



```
Plot[cvele[T, {0, 1}, {1, 1}] / (Na * k), {T, 0, 5},
 AxesLabel → {"T", "cv_ele"}, PlotRange → {0, 0.5}]
```



Ejemplos de las funciones de partición