2)

Prob 6.30

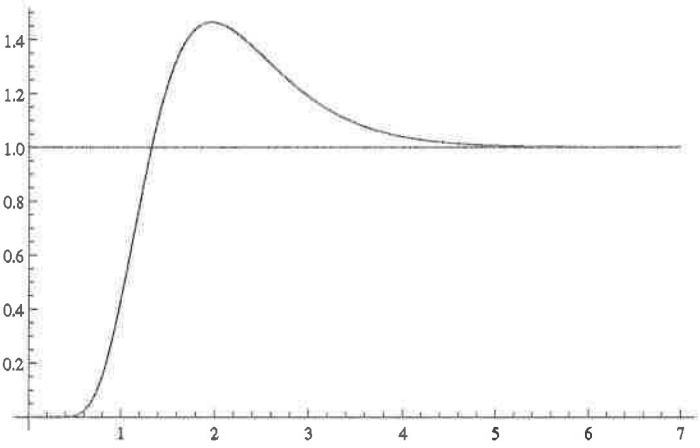
a) parahydrogen

```
In[61]:= z[β_] = Sum[(2 j + 1) Exp[-j (j + 1) β ϵ], {j, 0, 10, 2}]
```

$$\text{Out[61]= } 1 + 21\, e^{-110\,\beta\epsilon} + 17\, e^{-72\,\beta\epsilon} + 13\, e^{-42\,\beta\epsilon} + 9\, e^{-20\,\beta\epsilon} + 5\, e^{-6\,\beta\epsilon}$$

```
In[62]:= e[β_] = -D[Log[z[β]], β];

In[63]:= e[1 / (k T)];

In[64]:= cp[T_] = D[e[1 / (k T)], T] // Simplify;

In[65]:= ccp[x_] = cp[T] / k /. {T → x ϵ / k};

In[66]:= p2 = Plot[{ccp[x], 1}, {x, 0, 7}, PlotRange → All]
```

Out[66]=



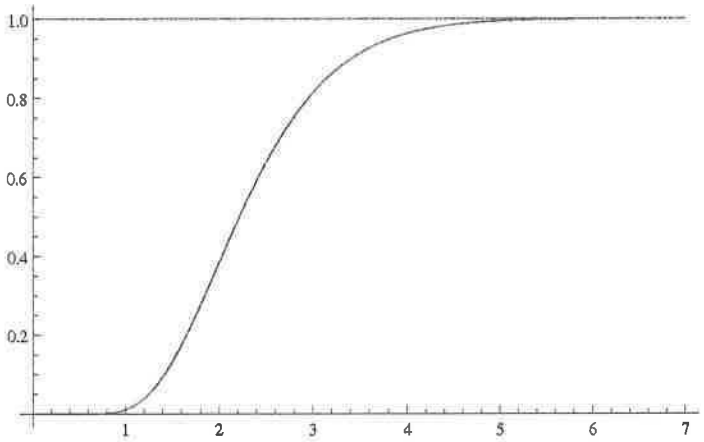
b) orthohydrogen

```
In[92]:= z[β_] = Sum[(2 j + 1) Exp[-j (j + 1) β ϵ], {j, 1, 10, 2}]
```

$$\text{Out[92]= } 19\,e^{-90\beta\epsilon} + 15\,e^{-56\beta\epsilon} + 11\,e^{-30\beta\epsilon} + 7\,e^{-12\beta\epsilon} + 3\,e^{-2\beta\epsilon}$$

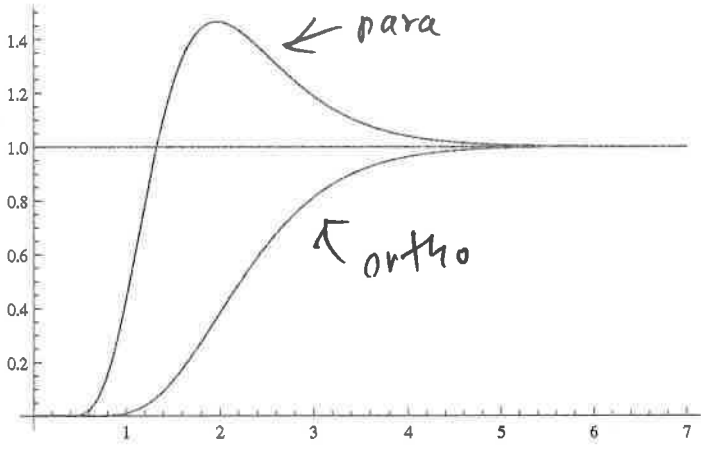
```
In[93]:= e[β_] = -D[Log[z[β]], β];

In[94]:= e[1 / (k T)];

In[95]:= co[T_] = D[e[1 / (k T)], T] // Simplify;

In[96]:= cco[x_] = co[T] / k /. {T → x ϵ / k};

In[97]:= p3 = Plot[{cco[x], 1}, {x, 0, 7}, PlotRange → All]
```

Out[97]=




```
In[98]:= Show[p2, p3]
```

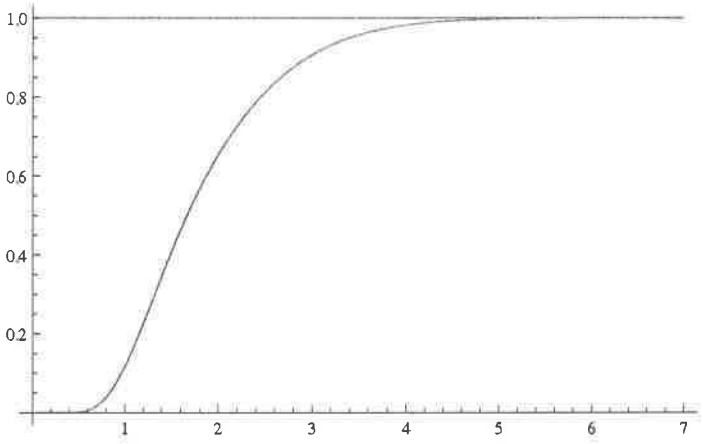
Out[98]=



c) normal hydrogen

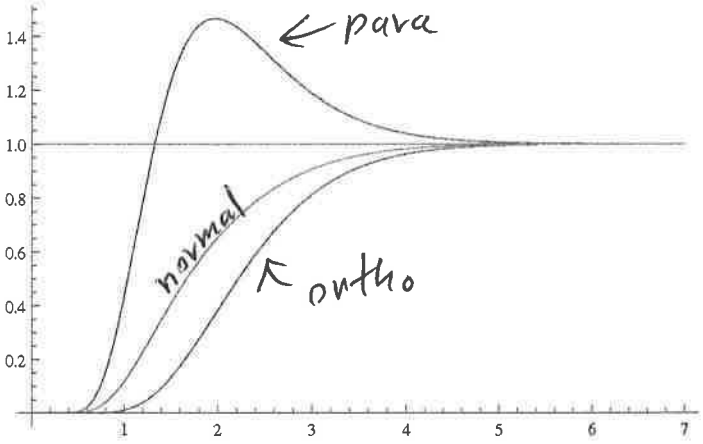
```
In[99]:= ccn[x_] = 1 / 4 ccp[x] + 3 / 4 cco[x];

In[100]:= p4 = Plot[{ccn[x], 1}, {x, 0, 7}, PlotRange → All, PlotStyle → RGBColor[1, 0, 0]]
```

Out[100]=




```
In[101]:= Show[p2, p3, p4]
```

Out[101]=



- **d) catalyzed cooled hydrogen**

nuclear spin degeneracy

In[103]:=
```
z[β_] =
 Sum[(2 j + 1) Exp[-j (j + 1) β ϵ], {j, 0, 10, 2}] + Sum[3 (2 j + 1) Exp[-j (j + 1) β ϵ], {j, 1, 10, 2}]
```

Out[103]= $1 + 21\, e^{-110\beta\epsilon} + 57\, e^{-90\beta\epsilon} + 17\, e^{-72\beta\epsilon} + 45\, e^{-56\beta\epsilon} + 13\, e^{-42\beta\epsilon} + 33\, e^{-30\beta\epsilon} + 9\, e^{-20\beta\epsilon} + 21\, e^{-12\beta\epsilon} + 5\, e^{-6\beta\epsilon} + 9\, e^{-2\beta\epsilon}$

In[104]:=
```
e[β_] = -D[Log[z[β]], β];
```

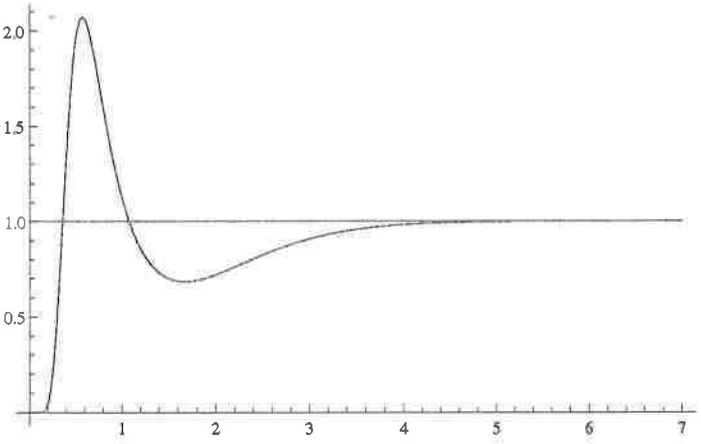
In[105]:=
```
e[1 / (k T)];
```

In[106]:=
```
cch[T_] = D[e[1 / (k T)], T] // Simplify;
```

In[107]:=
```
ccch[x_] = cch[T] / k /. {T → x ϵ / k};
```

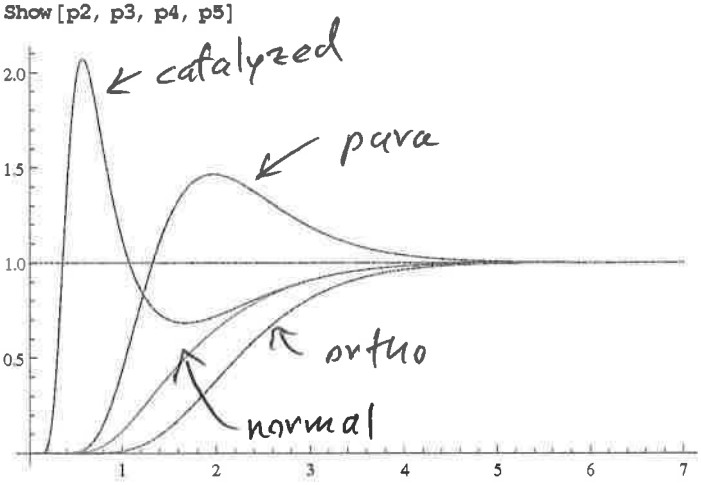
In[108]:=
```
p5 = Plot[{ccch[x], 1}, {x, 0, 7}, PlotRange → All]
```

Out[108]=



In[109]:=
```
Show[p2, p3, p4, p5]
```

Out[109]=



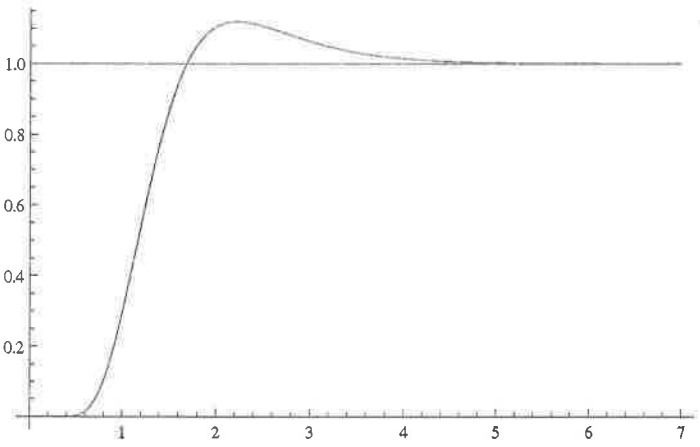
e) deuterium

ortho D_2 even

odd para D_2

```
In[124]:= ccd[x_] = 2 / 3 ccp[x] + 1 / 3 cco[x];

In[125]:= p6 = Plot[{ccd[x], 1}, {x, 0, 7}, PlotRange → All, PlotStyle → RGBColor[1, 0, 0]]
```

Out[125]=




```
In[133]:= Show[p4, p6]
```

normal D_2

normal H_2

Out[133]=