```
be = 0.066725;
ga = 0.031091;
fi  = 2^(-1/3);
n[r_] := 1/Pi * Exp[-2 * r];
ec[r_] := -2 * 0.015545 * (1 + 0.20548 * ((3/4)^(1/3) * Exp[2 * r/3])) *
    (Log[1 + 1/(2 * 0.015545 * (14.1189 * (((3/4)^(1/3) * Exp[2 * r/3])^0.5) + 6.1977 *
            ((3/4)^(1/3) * Exp[2 * r/3]) + 3.3662 * (((3/4)^(1/3) * Exp[2 * r/3])^
                1.5) + 0.62517 * (((3/4)^(1/3) * Exp[2 * r/3])^(1 + 1))))]);
A[r_] := be/ga * 1/(Exp[- ec[r]/(ga * fi^3)] - 1);
t[r_] := 1/fi * 1/(Sqrt[4/Pi * (3 * Pi^2 * n[r])^(1/3)]);
H[r_] := ga * (fi)^3 * Log[1 + be/ga * (t[r])^2
        ((1 + A[r] * (t[r])^2)/(1 + A[r] * (t[r])^2 + (A[r])^2 * (t[r])^4))];
NIntegrate[H[r] * 4 * Pi * r^2 * n[r], {r, 0, Infinity}]


0.0162081

n[r_] := 2/Pi * Exp[-2 * r];
ex[r_] := - (3/(4 * Pi)) * (3 * Pi^2 * (n[r]))^(1/3);
s[r_] := Norm[Grad[n[r], {r}]]/(2 * (3 * Pi^2)^(1/3) * n[r]^(4/3));
k = 0.804;
mu = 0.21951;
Fx[r_] := 1 + k - k/(1 + mu * (s[r])^2/k)
NIntegrate[0.5 * ex[r] * n[r] * 4 * Pi * r^2 * Fx[r], {r, 0, Infinity}]

-0.30594


(*He+1s *)
n[r_] := 8/Pi * Exp[-4 r]
rs[r_] := (3/(4 * Pi * n[r]))^(1/3)
ec[r_] := -2 * 0.015545 * (1 + 0.20548 * (rs[r])) *
   (Log[1 + 1/(2 * 0.015545 * (14.1189 * ((rs[r])^0.5) + 6.1977 * (rs[r]) +
           3.3662 * ((rs[r])^1.5) + 0.62517 * ((rs[r])^(1 + 1))))])
be = 0.066725;
ga = 0.031091;
fi  = 2^(-1/3);
A[r_] := be/ga * 1/(Exp[- ec[r]/(ga * fi^3)] - 1);
t[r_] := 1/fi * 1/(Sqrt[4/Pi * (3 * Pi^2 * n[r])^(1/3)]);
H[r_] := ga * (fi)^3 * Log[1 + be/ga * (t[r])^2
        ((1 + A[r] * (t[r])^2)/(1 + A[r] * (t[r])^2 + (A[r])^2 * (t[r])^4))];
NIntegrate[H[r] * 4 * Pi * r^2 * n[r], {r, 0, Infinity}]



0.0138161
```

```
n[r_] := 16 / Pi * Exp[-4 r]
s[r_] := - (64 e^-4 r) / π / (2 * (3 * Pi^2) ^ (1 / 3) * n[r] ^ (4 / 3));
ex[r_] := - (3 / (4 * Pi)) * (3 * Pi^2 * (n[r])) ^ (1 / 3);
k = 0.804;
mu = 0.21951;
Fx[r_] := 1 + k - k / (1 + mu * (s[r]) ^2 / k)
 NIntegrate[0.5 * ex[r] * n[r] * 4 * Pi * r^2 * Fx[r], {r, 0, Infinity}]
```

```
- 0.61188
```

```
(* (He+2p) *)
n[r_, θ_] := 1 / Pi * r^2 * Exp[-2 r] * (Cos[θ]) ^2
rs[r_, θ_] := (3 / (4 * Pi * n[r, θ])) ^ (1 / 3)
ec[r_, θ_] := -2 * 0.015545 * (1 + 0.20548 * (rs[r, θ])) *
   (Log[1 + 1 / (2 * 0.015545 * (14.1189 * ((rs[r, θ]) ^0.5) + 6.1977 * (rs[r, θ]) +
           3.3662 * ((rs[r, θ]) ^1.5) + 0.62517 * ((rs[r, θ]) ^ (1 + 1))))])
be = 0.066725;
ga = 0.031091;
fi = 2 ^ (-1 / 3);
A[r_, θ_] := be / ga * 1 / (Exp[- ec[r, θ] / (ga * fi^3)] - 1);
t[r_, θ_] := 1 / fi * 1 / (Sqrt[4 / Pi * (3 * Pi^2 * n[r, θ]) ^ (1 / 3)]);
H[r_, θ_] := ga * (fi) ^3 * Log[1 + be / ga * (t[r, θ]) ^2 ((1 + A[r, θ] * (t[r, θ]) ^2) /
         (1 + A[r, θ] * (t[r, θ]) ^2 + (A[r, θ]) ^2 * (t[r, θ]) ^4))];
NIntegrate[H[r, θ] * 2 * Pi * r^2 * n[r, θ] * Sin[θ], {r, 0, Infinity}, {θ, 0, Pi}]
```

```
0.016235
```

```
In[2154]:= n[r_, θ_] := (Cos[θ]) ^2 * 2 / Pi * r^2 * Exp[-2 r]
s[r_, θ_] :=
   Norm[Grad[n[r, θ], {r, θ, ϕ}, "Spherical"]] / (2 * (3 * Pi^2) ^ (1 / 3) * n[r, θ] ^ (4 / 3));
ex[r_, θ_] := - (3 / (4 * Pi)) * (3 * Pi^2 * (n[r, θ])) ^ (1 / 3);
k = 0.804;
mu = 0.21951;
Fx[r_, θ_] := 1 + k - k / (1 + mu * (s[r, θ]) ^2 / k)
Assuming[Element[{r, θ}, Reals],
 NIntegrate[0.5 * ex[r, θ] * n[r, θ] * 2 * Pi * r^2 * Fx[r, θ] * Sin[θ],
   {θ, 0, Pi}, {r, 0, Infinity}, WorkingPrecision → 13]]

Out[2160]= - 0.2148643596687
```

In[3006]:=
```
(*H 2p*)
n[r_, θ_] := 1 / (32 * Pi) * r^2 * Exp[-r] * (Cos[θ])^2
rs[r_, θ_] := (3 / (4 * Pi * n[r, θ])) ^ (1 / 3)
ec[r_, θ_] := -2 * 0.015545 * (1 + 0.20548 * (rs[r, θ])) *
    (Log[1 + 1 / (2 * 0.015545 * (14.1189 * ((rs[r, θ])^0.5) + 6.1977 * (rs[r, θ]) +
            3.3662 * ((rs[r, θ])^1.5) + 0.62517 * ((rs[r, θ]) ^ (1 + 1))))])
be = 0.066725;
ga = 0.031091;
fi = 2^(-1 / 3);
A[r_, θ_] := be / ga * 1 / (Exp[- ec[r, θ] / (ga * fi^3)] - 1);
t[r_, θ_] := 1 / fi * 1 / (Sqrt[4 / Pi * (3 * Pi^2 * n[r, θ]) ^ (1 / 3)]);
H[r_, θ_] := ga * (fi)^3 * Log[1 + be / ga * t[r, θ]^2 ((1 + A[r, θ] * (t[r, θ])^2) /
            (1 + A[r, θ] * (t[r, θ])^2 + (A[r, θ])^2 * (t[r, θ])^4))];
NIntegrate[H[r, θ] * 2 * Pi * r^2 * n[r, θ] * Sin[θ], {θ, 0, Pi},
 {r, 0, Infinity}, WorkingPrecision → 12]
```

Out[3015]= 0.0128925496000

In[2929]:=
```
n[r_, θ_] := 2 / (32 * Pi) * r^2 * Exp[-r] * (Cos[θ])^2
(*s[r_,θ_]:=
  Norm[Grad[n[r,θ],{r,θ,ϕ},"Spherical"]]/(2*(3*Pi^2)^(1/3)*n[r,θ]^(4/3));*)
u[r_, θ_] := r^2 * Exp[-2 * r] / (256 * Pi^2) *
    ((Cos[θ])^4 * (2 - r)^2 + 4 * (Sin[θ])^2 * (Cos[θ])^2) /
     ((2 * (3 * Pi^2) ^ (1 / 3))^2 * (n[r, θ]) ^ (8 / 3));
(*Evaluate[Norm[Grad[n[r,θ],{r,θ,ϕ},"Spherical"]]]*)
ex[r_, θ_] := - (3 / (4 * Pi)) * (3 * Pi^2 * n[r, θ]) ^ (1 / 3);
k = 0.804;
mu = 0.21951;
Fx[r_, θ_] := 1 + k - k / (1 + mu * (u[r, θ]) / k)
NIntegrate[0.5 * ex[r, θ] * n[r, θ] * 2 * Pi * r^2 * Fx[r, θ] * Sin[θ],
 {θ, 0, Pi}, {r, 0, Infinity}]
```

Out[2935]= -0.107432

```
Evaluate[-0.804 / (1 + 0.21951 / 0.804 *
```