

```
(%i1) kill(all);
(%o0) done
```

1 Yukawa potential and force

```
(%i1) U_1: -g^2*sqrt(m(r))/r*(exp(-mu*r/sqrt(m(r))));
```

$$(U_1) \quad -\frac{g^2 e^{-\frac{\mu r}{\sqrt{m(r)}}}}{r \sqrt{m(r)}}$$

```
(%i2) F_1: -diff(U_1, r);
```

$$(F_1) \quad \frac{g^2 e^{-\frac{\mu r}{\sqrt{m(r)}}} \sqrt{m(r)} \left(\frac{\mu r \left(\frac{d}{dr} m(r) \right)}{2 m(r)^{3/2}} - \frac{\mu}{\sqrt{m(r)}} \right)}{r} + \frac{g^2 e^{-\frac{\mu r}{\sqrt{m(r)}}} \left(\frac{d}{dr} m(r) \right)}{2 r \sqrt{m(r)}} - \frac{g^2 e^{-\frac{\mu r}{\sqrt{m(r)}}} \sqrt{m(r)}}{r^2}$$

```
(%i3) ratsimp(%);
```

$$(\%o3) \quad \frac{e^{-\frac{\mu r}{\sqrt{m(r)}}} \left(\sqrt{m(r)} \left(g^2 \mu r^2 \left(\frac{d}{dr} m(r) \right) - 2 g^2 \mu r m(r) \right) + g^2 r m(r) \left(\frac{d}{dr} m(r) \right) - 2 g^2 m(r)^2 \right)}{2 r^2 m(r)^{3/2}}$$

```
(%i4) U_2: Z_1*Z_2*m(r)^(1/2)*e^2/(4*pi*epsilon_0*r);
```

$$(U_2) \quad \frac{Z_1 Z_2 e^2 \sqrt{m(r)}}{4 \pi \epsilon_0 r}$$

```
(%i5) F_2: -diff(U_2, r);
```

$$(F_2) \quad \frac{Z_1 Z_2 e^2 \sqrt{m(r)}}{4 \pi \epsilon_0 r^2} - \frac{Z_1 Z_2 e^2 \left(\frac{d}{dr} m(r) \right)}{8 \pi \epsilon_0 r \sqrt{m(r)}}$$

1.1 Graphics

```
(%i8) a[0]: 5.2917721092e-11;
      r[p]: 0.8751e-15/a[0];
      r[Ni]: 3.78e-15/a[0];
```

ARRSTORE: use_fast_arrays=false; allocate a new property hash table for \$A

```
(%o6) 5.2917721092 10-11
```

ARRSTORE: use_fast_arrays=false; allocate a new property hash table for \$R

```
(%o7) 1.653699331606885 10-5
```

```
(%o8) 7.143164750855933 10-5
```

```
(%i9) str: [g=1, mu=1, Z_1=1, Z_2=1, e=1, R=r[Ni]];
```

```
(str) [g=1, mu=1, Z_1=1, Z_2=1, e=1, R=7.143164750855933 10-5]
```

```
(%i11) U_2a: ratsubst(1, 4*pi*epsilon_0, U_2);
      F_2a: ratsubst(1, 4*pi*epsilon_0, F_2);
```

$$(U_2a) \quad \frac{Z_1 Z_2 e^2 \sqrt{m(r)}}{r}$$

$$(F_2a) \quad -\frac{Z_1 Z_2 e^2 r \left(\frac{d}{dr} m(r) \right) - 2 Z_1 Z_2 e^2 m(r)}{2 r^2 \sqrt{m(r)}}$$

```
(%i12) m(r):= (2.-exp(log(2.)*exp(-r/R))) ;
```

```
(%o12) m(r):=2-exp(log(2) exp(-r/R))
```

```
(%i16) U_11: ev(U_1, str);
F_11: ev(F_1, str, diff);
U_21: ev(U_2a, str);
F_21: ev(F_2a, str, diff);
```

$$\begin{aligned}
 (U_{11}) \quad & - \frac{\sqrt{2 - \%e^{\log(2) \%e^{-13999.39711428572 r}} \%e^{\frac{r}{\sqrt{2 - \%e^{\log(2) \%e^{-13999.39711428572 r}}}}}}}{r} \\
 (F_{11}) \quad & \frac{6999.698557142859 \log(2) \%e^{\frac{r}{\sqrt{2 - \%e^{\log(2) \%e^{-13999.39711428572 r}}}}}}{\sqrt{2 - \%e^{\log(2) \%e^{-13999.39711428572 r}}}} - \frac{\log(2) \%e^{-13999.39711428572 r} - 13999.39711428572 r}{r \sqrt{2 - \%e^{\log(2) \%e^{-13999.39711428572 r}}}} + \left(\frac{\sqrt{2 - \%e^{\log(2) \%e^{-13999.39711428572 r}}}}{6999.698557142859 \log(2) r \%e^{\log(2) \%e^{-13999.39711428572 r} - 13999.39711428572 r}} - \frac{1}{\sqrt{2 - \%e^{\log(2) \%e^{-13999.39711428572 r}}}} \right) \\
 & - \frac{r}{\sqrt{2 - \%e^{\log(2) \%e^{-13999.39711428572 r}}}} \Big/ r - \frac{\sqrt{2 - \%e^{\log(2) \%e^{-13999.39711428572 r}}}}{r^2} - \frac{r}{\sqrt{2 - \%e^{\log(2) \%e^{-13999.39711428572 r}}}} \\
 (U_{21}) \quad & \frac{\sqrt{2 - \%e^{\log(2) \%e^{-13999.39711428572 r}}}}{r} \\
 (F_{21}) \quad & - \frac{13999.39711428572 \log(2) r \%e^{\log(2) \%e^{-13999.39711428572 r} - 13999.39711428572 r} - 2 (2 - \%e^{\log(2) \%e^{-13999.39711428572 r}})}{2 r^2 \sqrt{2 - \%e^{\log(2) \%e^{-13999.39711428572 r}}}}
 \end{aligned}$$

```
(%i17) Gp: [[r[Ni], -1e5], [r[Ni], 1e5]];
```

```
(Gp) [[7.143164750855933 10-5, -100000.0], [7.143164750855933 10-5, 100000.0]]
```

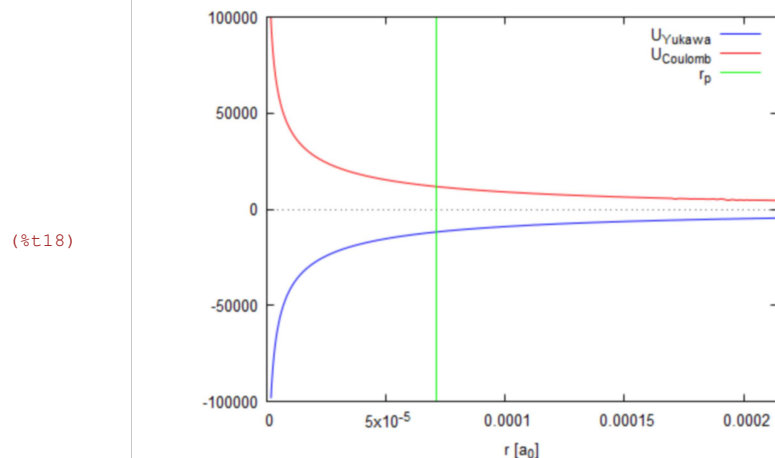
```
(%i18) wxplot2d([U_11, U_21, [discrete, Gp]], [r, 0, 3*r[Ni]], [y, -1e5, 1e5],
[xlabel, "r [a_0]"],
[legend, "U_{Yukawa}", "U_{Coulomb}", "r_p"])
```

plot2d: expression evaluates to non-numeric value somewhere in plotting range.

plot2d: some values were clipped.

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plot2d: some values were clipped.



```
(%i19) Gp: [[r[Ni], -1e10], [r[Ni], 1e10]];
```

```
(Gp) [[7.143164750855933 10-5, -1.0 1010], [7.143164750855933 10-5, 1.0 1010]]
```

```
(%i20) wxplot2d([F_11,F_21,[discrete,Gp]], [r,0,3*r[Ni]], [y,-1e10,1e10],
[xlabel, "r [a_0]"],
[legend, "F_{Yukawa}", "F_{Coulomb}", "r_p"])$
```

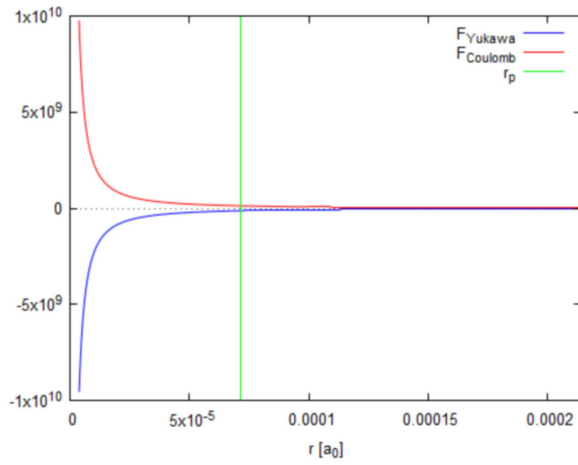
plot2d: expression evaluates to non-numeric value somewhere in plotting range.

plot2d: some values were clipped.

plot2d: expression evaluates to non-numeric value somewhere in plotting range.

plot2d: some values were clipped.

(%t20)



2 Yukawa force in coordinates r_1

```
(%i21) U_Y: -g^2/r_1*exp(-alpha*m*r_1);
```

$$(U_Y) \quad -\frac{g^2 e^{-\alpha m r_1}}{r_1}$$

```
(%i22) F_Y: -diff(U_Y, r_1);
```

$$(F_Y) \quad -\frac{\alpha g^2 m e^{-\alpha m r_1}}{r_1} - \frac{g^2 e^{-\alpha m r_1}}{r_1^2}$$