```
> restart;
```

**Marder problem 2.7.**

Let us calculate crystal energy per atom as a function of the nearest neighbor distance r.

First define a function for the two-body interaction energy given in the problem.

(The first three lines of the procedure definition are needed to get plot to work.

Plotting of procedures in Maple is not straightforward, but the trick below makes

it work.)

```
> f:=proc(r)
  if not (r::numeric) then
      return 'procname'(args)
  end if;
  if(r<1.5) then exp(-r)*((1/r^3)-1) else 0 end if;
  end proc;
>
>
```

$$f := \mathbf{proc}(r)$$
$$\quad \mathbf{if\ not}\ r::numeric\ \mathbf{then\ return}\ 'procname'(args)\ \mathbf{end\ if};$$
$$\quad \mathbf{if}\ r < 1.5\ \mathbf{then}\ \exp(-r)*((1)/(r\text{^}3) - 1)\ \mathbf{else}\ 0\ \mathbf{end\ if};$$
$$\mathbf{end\ proc};$$

```
> plot(f(r),r=0.8..1.6);
```
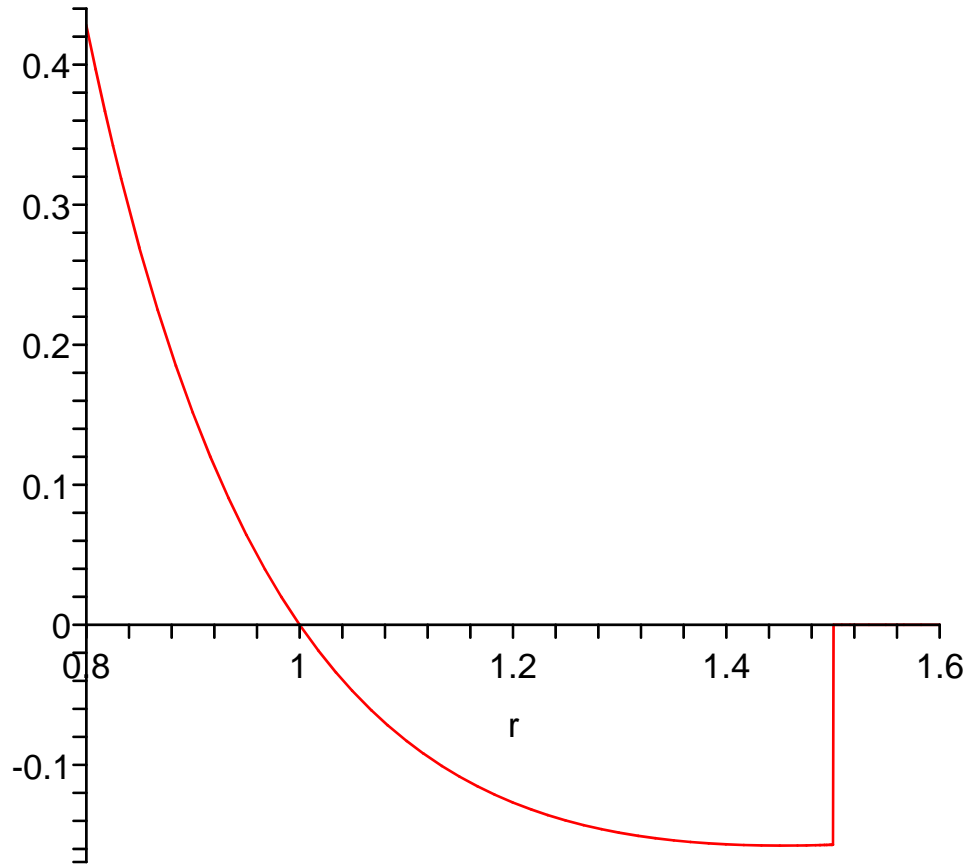
BCC: eight nearest neighbors at r, six next-nearest-neighbors at 2r/sqrt(3).
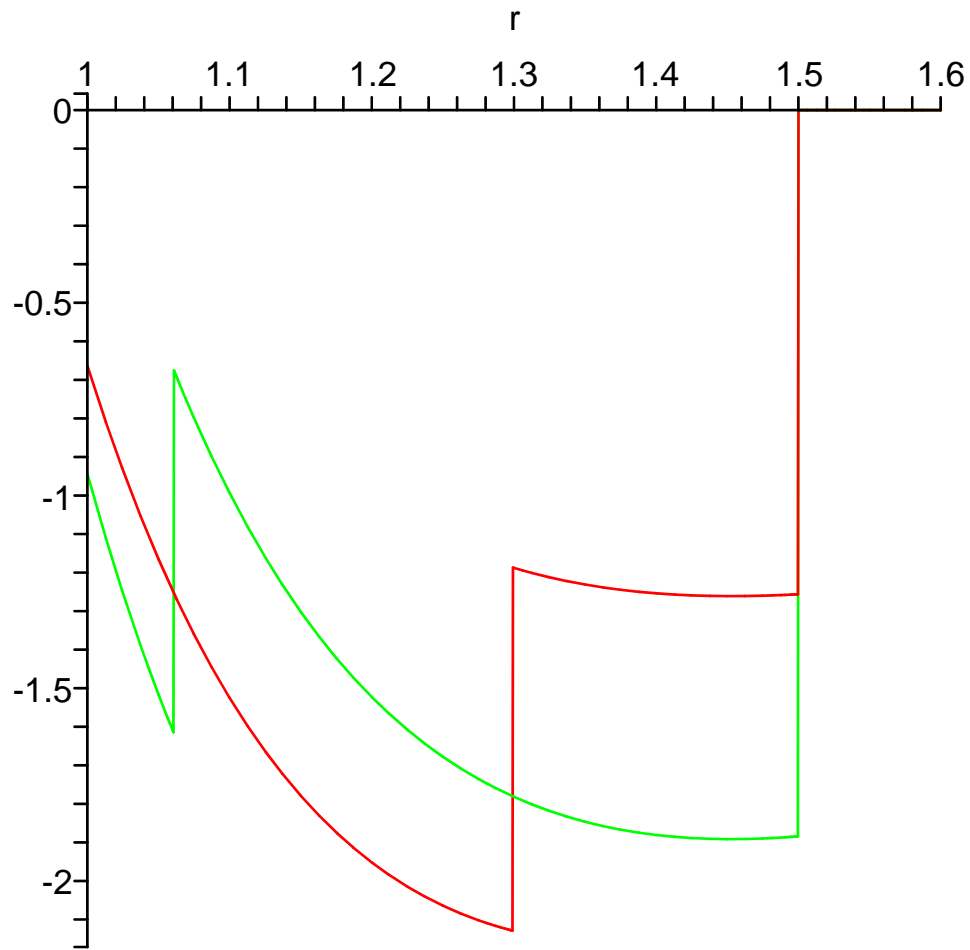FCC: 12 nn at r, six nnn at r*sqrt(2).

HCP:  Same nn and nnn as FCC.  (Third neighbors are different in the two structures, but let's ignore those, which

 means that the hcp and fcc energies are equal.)

```
> E_bcc:=8*f(r)+6*f(2*r/1.732);
```
$$E\_bcc := 8\,f(r) + 6\,f(1.154734411\,r)$$

```
> E_fcc:=12*f(r)+6*f(r*1.414);
```
$$E\_fcc := 12\,f(r) + 6\,f(1.414\,r)$$

```
> plot({8*f(r)+6*f(2*r/1.732),12*f(r)+6*f(r*1.414)},r=1..1.6);
```

r

1    1.1    1.2    1.3    1.4    1.5    1.6

0

-0.5

-1

-1.5

-2

The lowest energy is the BCC structure (red curve), when the nnn distance is just less than 1.5. This occurs at nearest neighbor distance r=

```
> evalf(1.5*sqrt(3)/2);
```
                                    1.299038106

```
>
```