

```
> restart;
```

Marder, Chapter 1, problem 5(a). Work in units of  $\phi_0$ .

First, how many atoms do we have within the 1.5 cutoff?

Hexagonal lattice:

The second neighbor is square root of 3 times the nearest neighbor distance.

Now consider the square lattice. 2nd neighbor is square root of 2 times nearest neighbor distance.

If the lattice constant is bigger than 1.5, there is no interaction and the crystal energy is 0 per atom.

If the lattice is large enough that only nearest neighbors interact, we get

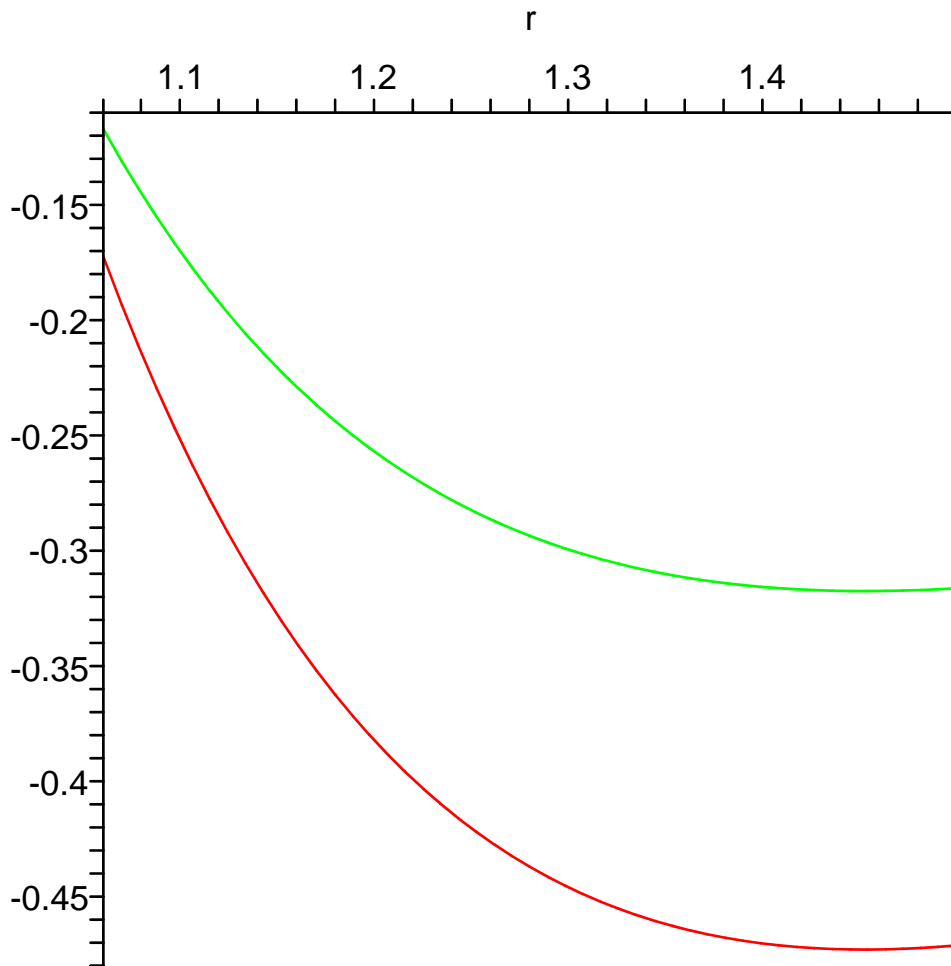
```
> E_square := (1/2) * 4 * exp(-r) * (1/r^3 - 1);
```

$$E_{\text{square}} := 2 e^{(-r)} \left( \frac{1}{r^3} - 1 \right)$$

```
> E_hex := (1/2) * 6 * exp(-r) * (1/r^3 - 1);
```

$$E_{\text{hex}} := 3 e^{(-r)} \left( \frac{1}{r^3} - 1 \right)$$

```
> plot({E_square, E_hex}, r=1.5/sqrt(2)..1.5);
```



>

Without second neighbor interactions, the hexagonal lattice is always more stable, because it has more neighbors.

However, the square lattice jumps in energy when the second neighbors get within a distance of 1.5 of each atom. So the above expression is only valid down to  $r = 1.5/\sqrt{2}$ . The minimum energy of the hexagonal lattice over

this range is where

```
> fsolve(diff(E_hex,r)=0,r=1..2);
```

>

1.452626879

```
> eval(E_hex,r=1.5);
```

-0.4710525603

Now consider the range where the square lattice has second neighbors within 1.5 of each atom, but the hex lattice does not. Here the distance to second neighbors is

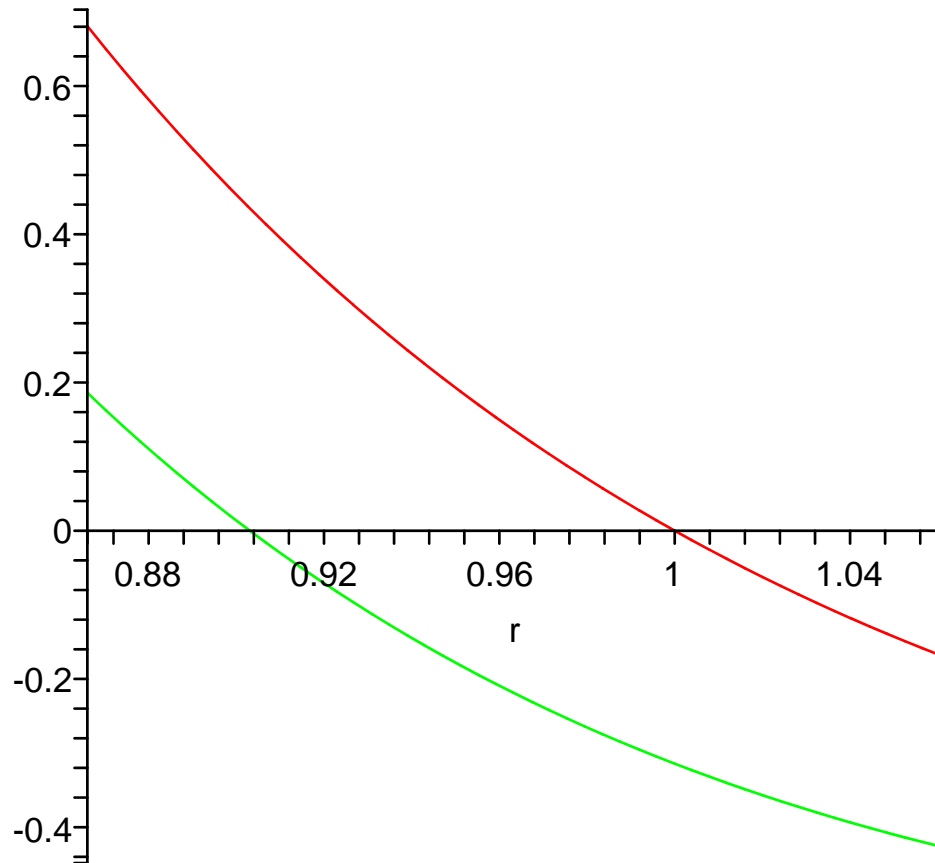
```
> r2square:=sqrt(2)*r;
```

$$r2square := \sqrt{2} r$$

```
> E_square:=(1/2)*(4*exp(-r)*(1/r^3-1)+4*exp(-r2square)*(1/r2square^3-1));
```

$$E\_square := 2 e^{(-r)} \left( \frac{1}{r^3} - 1 \right) + 2 e^{(-\sqrt{2} r)} \left( \frac{\sqrt{2}}{4 r^3} - 1 \right)$$

```
> plot({E_square,E_hex},r=1.5/sqrt(3)..1.5/sqrt(2))
```



```
> ;
```

In the above range, the square lattice is lower in energy than the hexagonal lattice. The square lattice reaches a minimum at the upper end of this range before its second lattices kick in.

```
>
```

```
> subs(r=1.5/sqrt(2),E_square);
```

$$2 e^{(-0.7500000000 \sqrt{2})} (0.5925925925 \sqrt{2} - 1) - 1.407407408 e^{(-1.5000000000)}$$

```
> evalf(%);
```

```
-0.4261763011
```

```
>
```

This is not as low as at  $r=0.779$ , so this is a less stable structure.

Finally let's look at  $r$  close enough that we are getting second neighbors in the hex lattice, too.

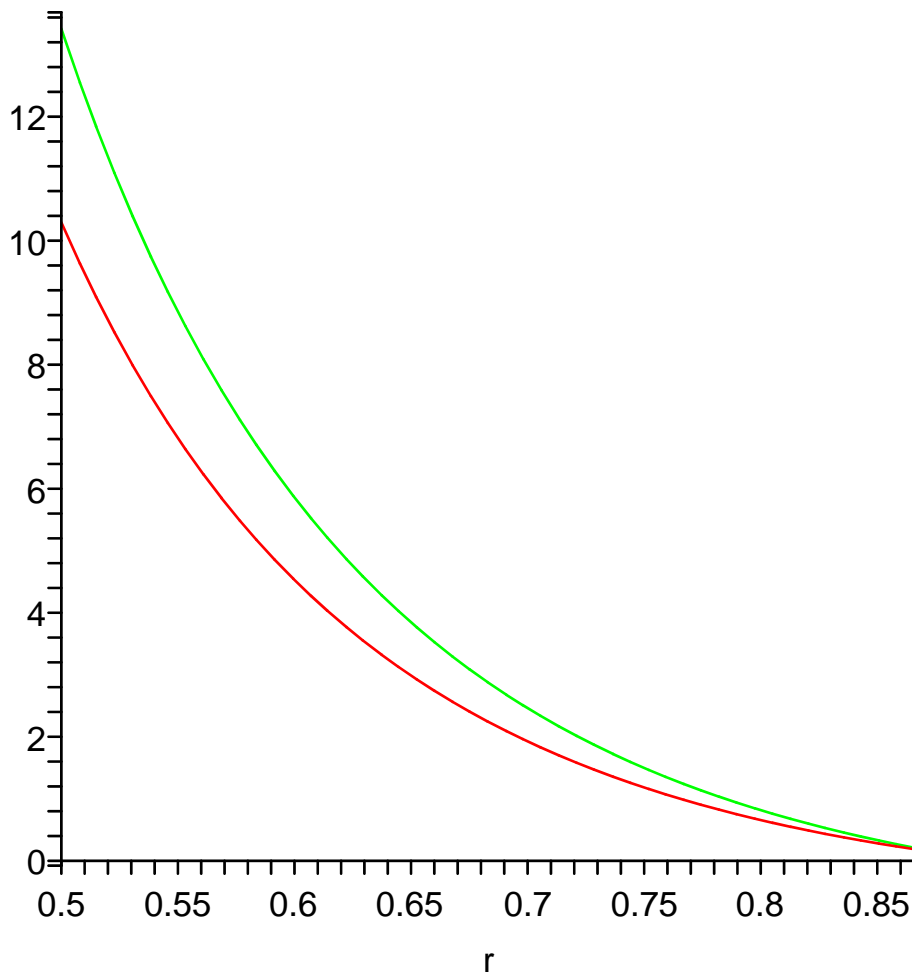
```
> r2hex:=sqrt(3)*r;
```

```
r2hex :=  $\sqrt{3} r$ 
```

```
> E_hex:=(1/2)*((6*exp(-r)*(1/r^3-1)+6*exp(-r2hex)*(1/r2hex^3-1)));
```

$$E_{hex} := 3 e^{(-r)} \left( \frac{1}{r^3} - 1 \right) + 3 e^{(-\sqrt{3} r)} \left( \frac{\sqrt{3}}{9 r^3} - 1 \right)$$

```
> plot({E_square,E_hex},r=0.5..1.5/sqrt(3));
```



In this region the repulsive part of the potential is dominant.

The most stable crystal is a hexagonal lattice with a lattice constant of 1.47.

