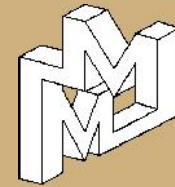


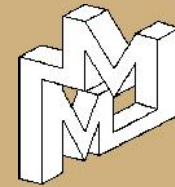
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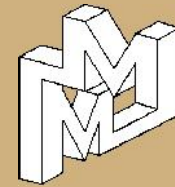
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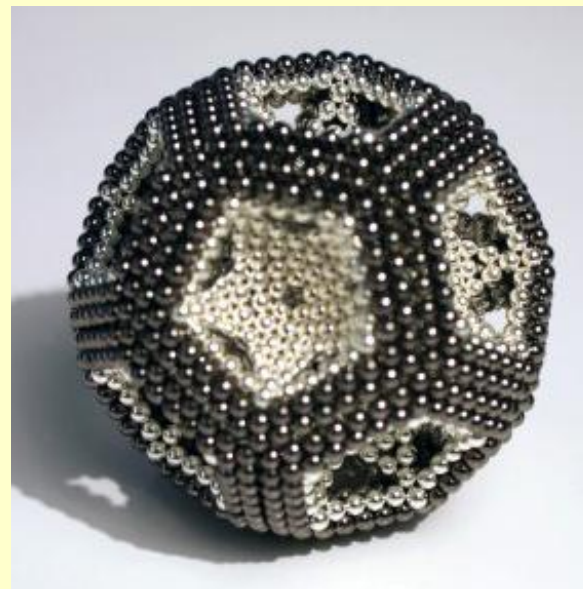
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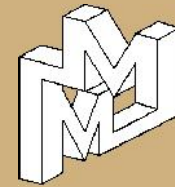
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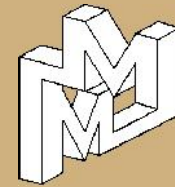
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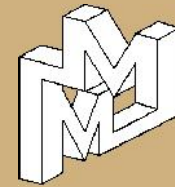
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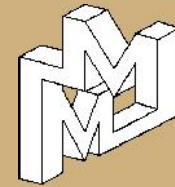
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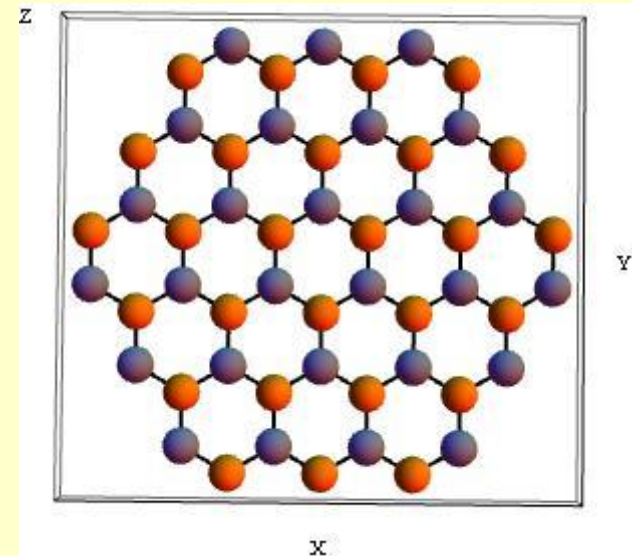
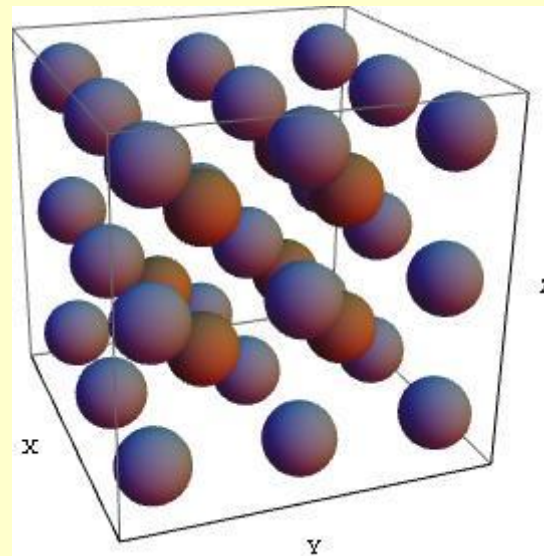
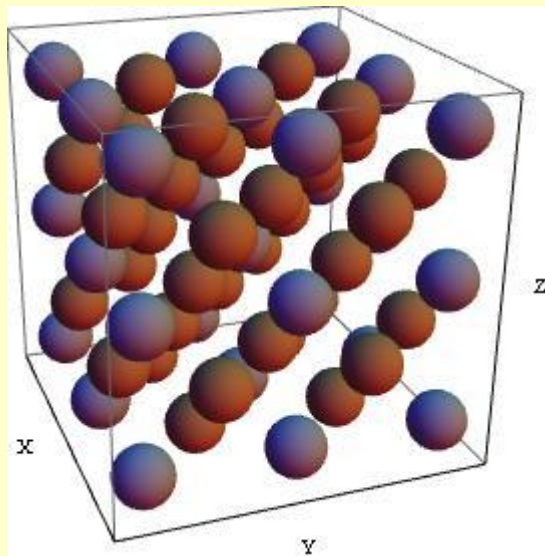


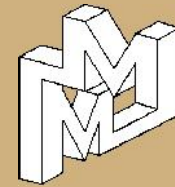
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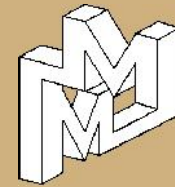
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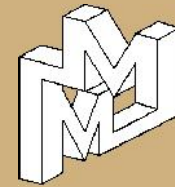
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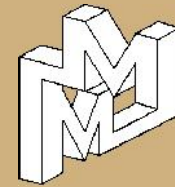
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$$\Delta l = kF, \quad k = \frac{l}{ES} \Rightarrow \frac{F}{S} = E \frac{\Delta l}{l}$$

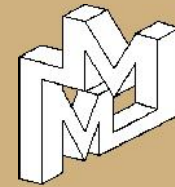
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(1635-1703)



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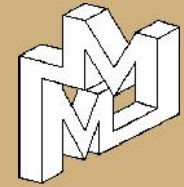
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— $\Delta l = kF$

— $\Delta l_x = k_x F, \Delta l_y = k_y F, \Delta l_z = k_z F$

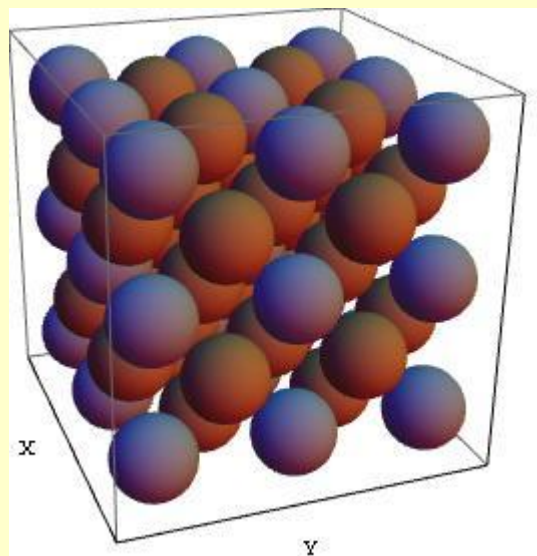
$\Delta \gamma_x = q_x T, \Delta \gamma_y = q_y T, \Delta \gamma_z = q_z T$

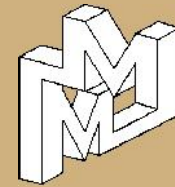
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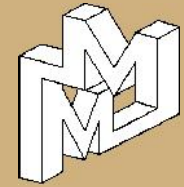
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$$\varphi(r) = \beta \left(\left(\frac{\alpha}{r} \right)^{12} - 2 \left(\frac{\alpha}{r} \right)^6 \right),$$

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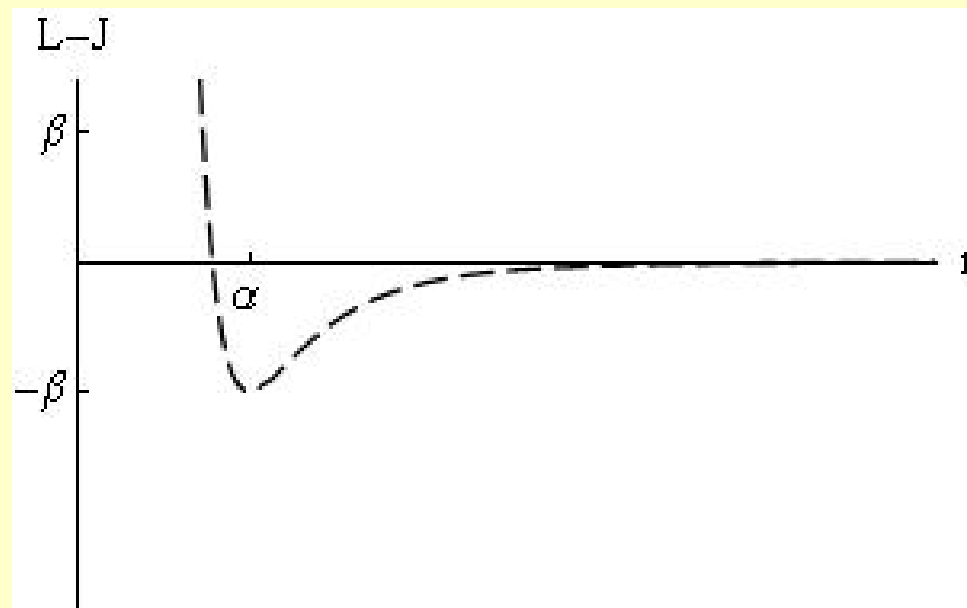
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$$\varphi(r) = \beta \left(\left(\frac{\alpha}{r} \right)^{12} - 2 \left(\frac{\alpha}{r} \right)^6 \right)$$

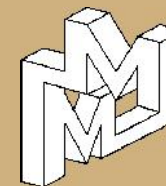
- :

$$f(r) \equiv -\frac{d\varphi(r)}{dr} = 12\beta \left(\frac{\alpha^{12}}{r^{13}} - \frac{\alpha^6}{r^7} \right)$$

• - :



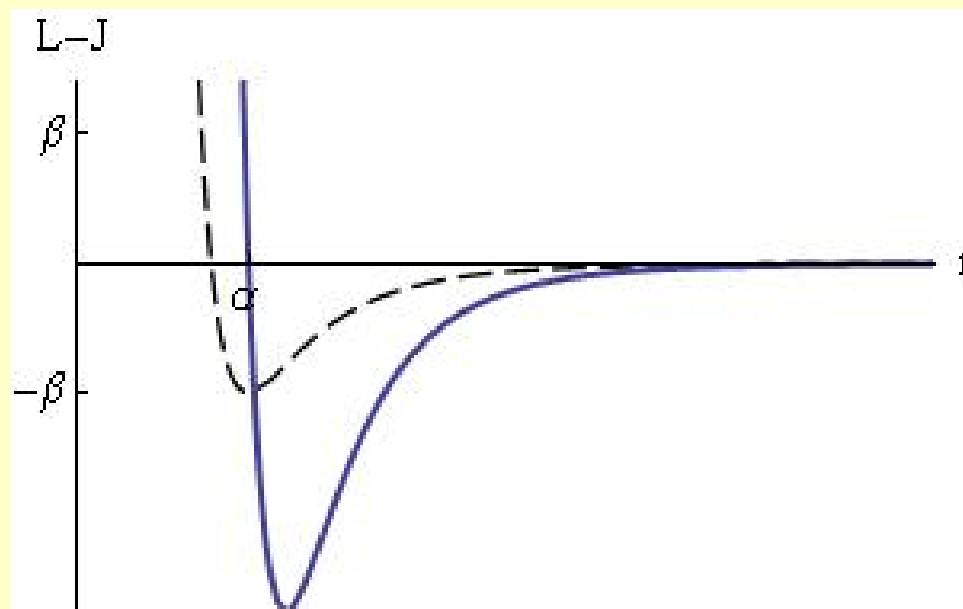
$a \approx \alpha$



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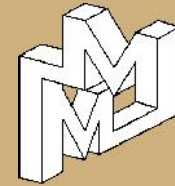
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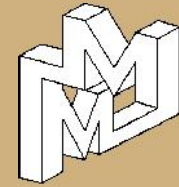
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$$f(r) = 12\beta \left(\frac{\alpha^{12}}{r^{13}} - \frac{\alpha^6}{r^7} \right)$$

$$f(a) + f(\sqrt{2}a) + f(\sqrt{3}a) + f(2a) =$$

$$= \beta \frac{(17918091 + 139968\sqrt{2} + 8192\sqrt{3})\alpha^6 - 1728(10449 + 648\sqrt{2} + 128\sqrt{3})a^6}{a^{13}} \alpha^6 =$$

$$= \beta \frac{12.144 \alpha^6 - 13.411 a^6}{a^{13}} = \beta \frac{C_1 \alpha^6 - C_2 a^6}{a^{13}}$$



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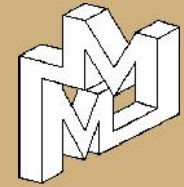
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$$\varphi(r) = \frac{\beta}{m-n} \left(n \left(\frac{\alpha}{r} \right)^m - m \left(\frac{\alpha}{r} \right)^n \right), \quad m > n$$

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$$f(r) \equiv -\frac{d\varphi(r)}{dr} = \frac{mn\beta}{m-n} \left(\frac{\alpha^m}{r^{m+1}} - \frac{\alpha^n}{r^{n+1}} \right)$$

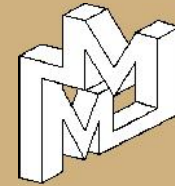


- ():

$$\varphi(r) = \frac{\beta}{m n} \left(n \left(\frac{\alpha}{r} \right)^m - m \left(\frac{\alpha}{r} \right)^n \right), \quad m > n$$

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$$f(r) \equiv -\frac{d\varphi(r)}{dr} = \beta \left(\frac{\alpha^m}{r^{m+1}} - \frac{\alpha^n}{r^{n+1}} \right)$$



$$\left\{ \begin{array}{l} m\mathbf{a}_i = \sum_k \frac{\mathbf{x}_k - \mathbf{x}_i}{|\mathbf{x}_k - \mathbf{x}_i|} f(|\mathbf{x}_k - \mathbf{x}_i|), \\ \mathbf{a}_i = \frac{d^2 \mathbf{x}_i}{dt^2} \end{array} \right.$$

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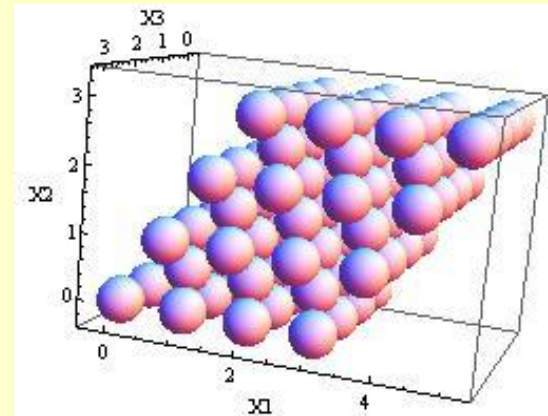
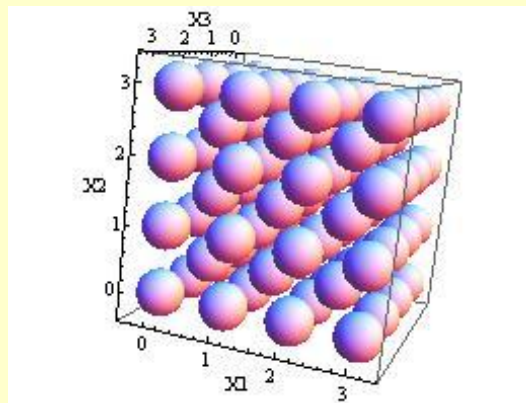
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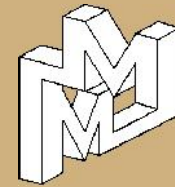
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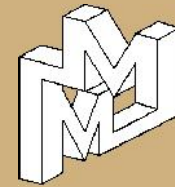
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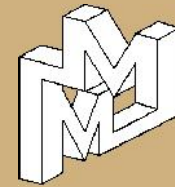
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(1789-1857)

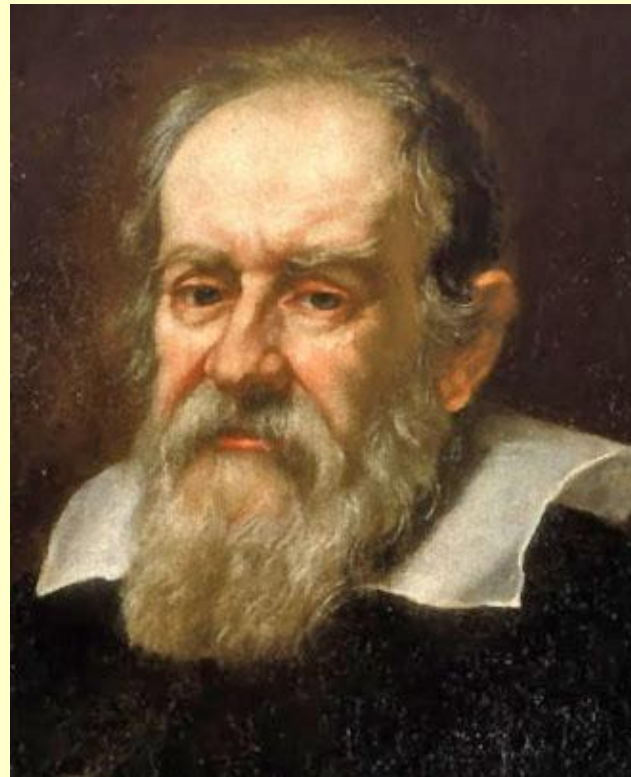


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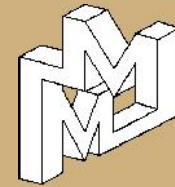
$$S \equiv n \Delta S$$

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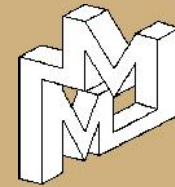
$$t = \Delta f / \Delta S$$



(1564-1642)



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S ≡ nΔS
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t = F / ΔS
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$$t_n = F / \Delta S$$

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$$\mathbf{n} \cdot \mathbf{F} = t_n$$

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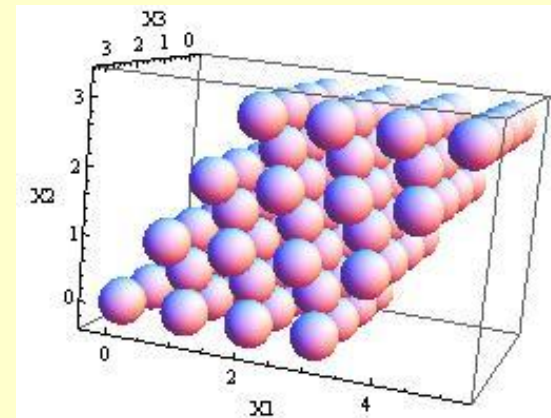
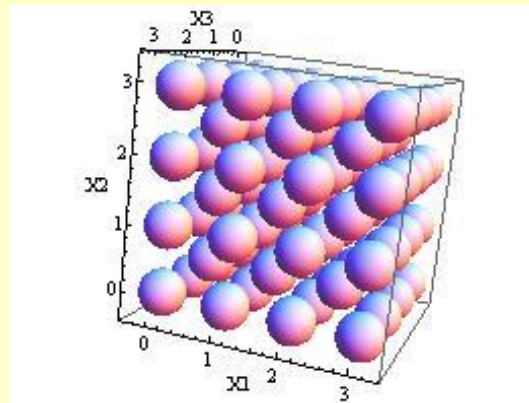
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$$: N^2 a^2,$$

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$$: N^2 a^2 \sqrt{1 + \gamma^2}$$



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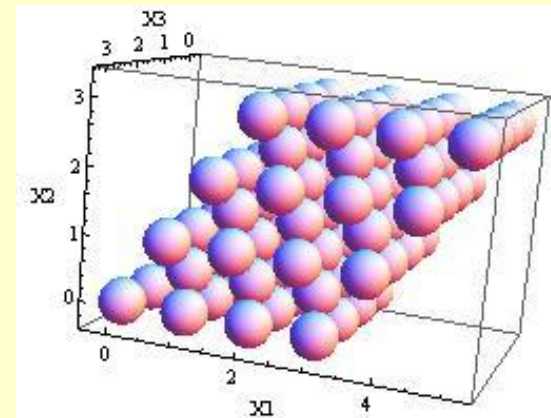
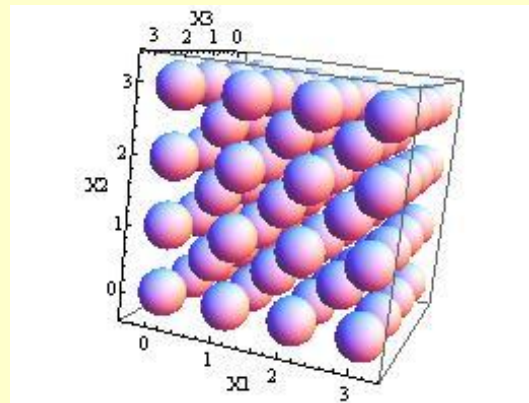
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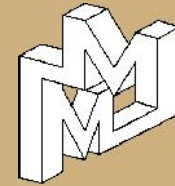
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$$: \mathbf{N}_R = \{1, 0, 0\},$$

$$: \hat{\mathbf{n}}_R = \left\{ \frac{1}{\sqrt{1+\gamma^2}}, -\frac{\gamma}{\sqrt{1+\gamma^2}}, 0 \right\}$$





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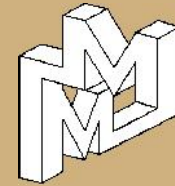
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$$\sigma_{11}(\gamma) = \gamma(t_{Up})_1 + \sqrt{1 + \gamma^2} (t_R)_1, \quad \sigma_{22}(\gamma) = (t_{Up})_2,$$

$$\sigma_{12}(\gamma) = \gamma(t_{Up})_2 + \sqrt{1 + \gamma^2} (t_R)_2, \quad \sigma_{21}(\gamma) = (t_{Up})_1,$$

$$\sigma_{13} = (t_{Up})_3 + \sqrt{1 + \gamma^2} (t_R)_3, \quad \sigma_{23} = (t_{Up})_3$$



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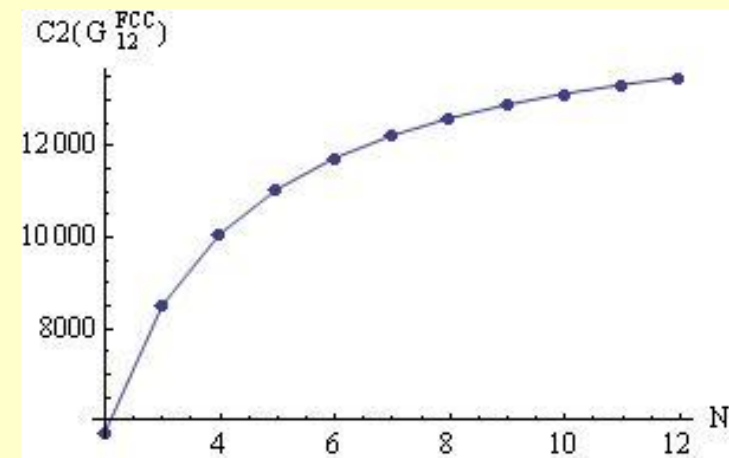
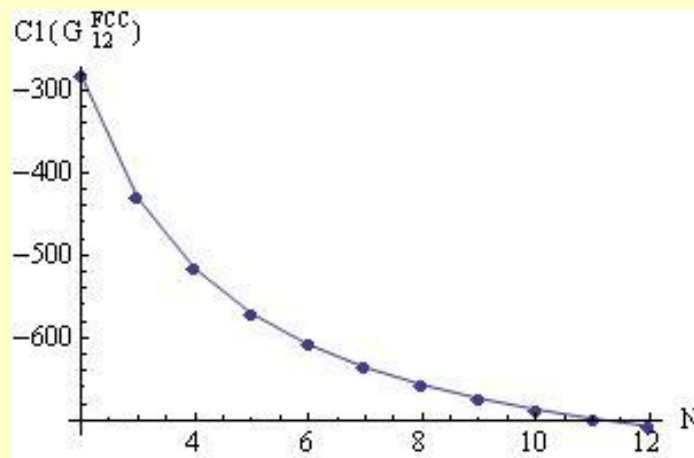
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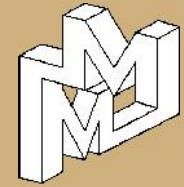
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∴

$$\begin{cases} \sigma_{12} = C_{1212}\gamma, \\ \sigma_{21} = C_{1221}\gamma, \\ \sigma_{11} = \sigma_{13} = \sigma_{22} = \sigma_{23} = \sigma_{31} = \sigma_{32} = \sigma_{33} = 0. \end{cases}$$

- $$G_{ij} = \frac{\alpha^6 (C1_{ij} a^6 + C2_{ij} \alpha^6) \beta}{a^{15}}$$





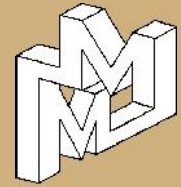
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$$f(x) = a(x - x_0)^k + b$$

$$G_{12 \ N}^{FCC} = \frac{\alpha^6 \left((1343.13(N + 0.47)^{-1.01} - 811.86)a^6 + (-23608.90(N + 0.41)^{-1.008} + 15367.82)\alpha^6 \right) \beta}{a^{15}}$$

$$G_{12 \ \infty}^{FCC} = \frac{\alpha^6 (-811.86a^6 + 15367.82\alpha^6) \beta}{a^{15}}$$

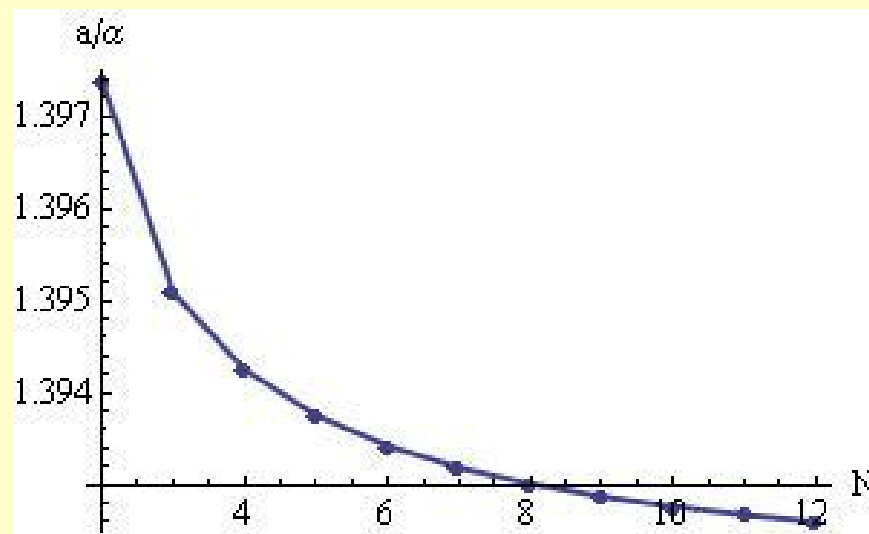


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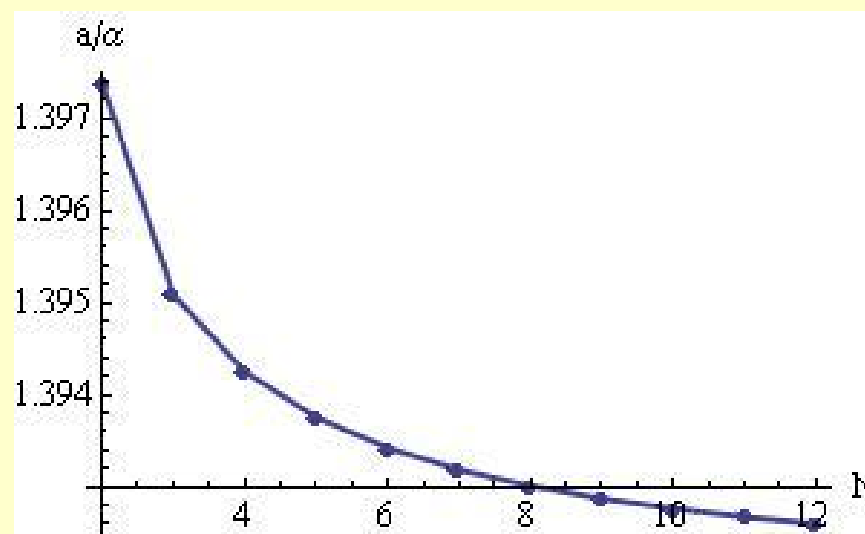
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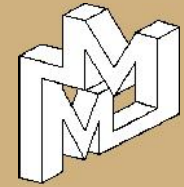


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a:

$$\frac{a}{\alpha} = 0.0104(N + 0.0834)^{-1.03} + 1.3918$$





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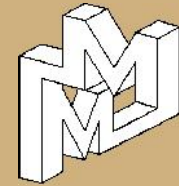
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$$a_* = 1.3918\alpha$$

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$$\alpha = \frac{a_*}{1.3918}$$

$$\beta = \frac{G_* \alpha^3}{66.4548} = 0.0150 G_* \alpha^3 = 0.05581 G_* a_*^3$$

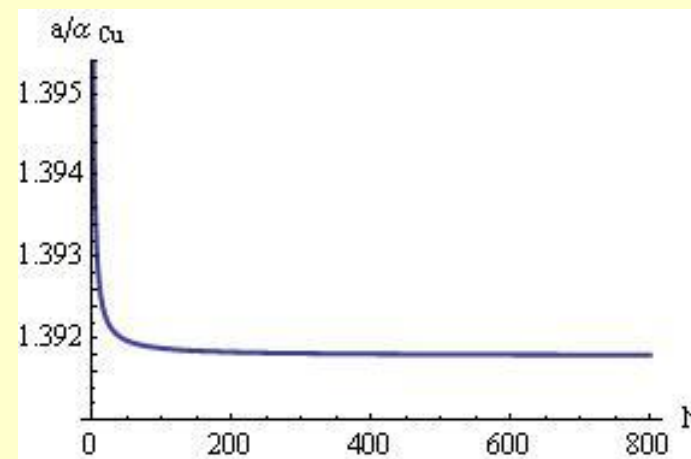
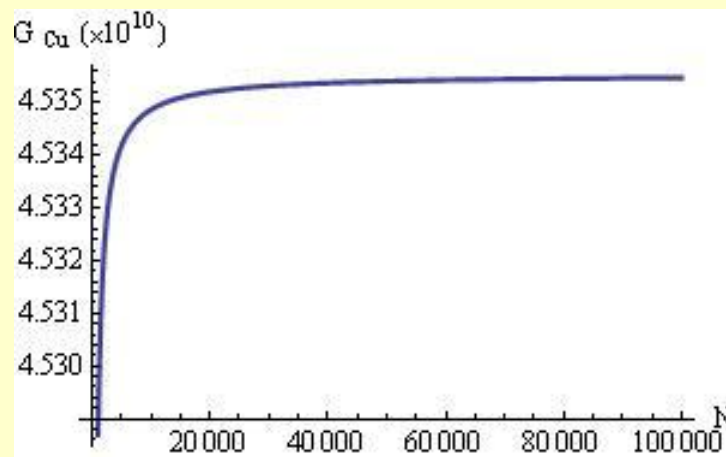


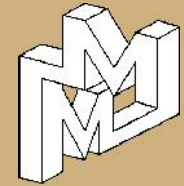
- : $a = 0.3615 \times 10^{-9}$ (), $G = 4.55 \times 10^{10}$ (/ 2)

- - :

$\alpha = 2.5974 \times 10^{-10}$ (), $\beta = 1.1959 \times 10^{-20}$ ()

- :





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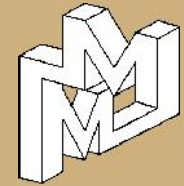
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– 1 : $G = 4.54 \times 10^{10} (/ ^2)$

– 1 — $G = 4.53 \times 10^{10} (/ ^2)$

– 100 — $G = 4.51 \times 10^{10} (/ ^2)$

– 10 — $G = 4.28 \times 10^{10} (/ ^2)$



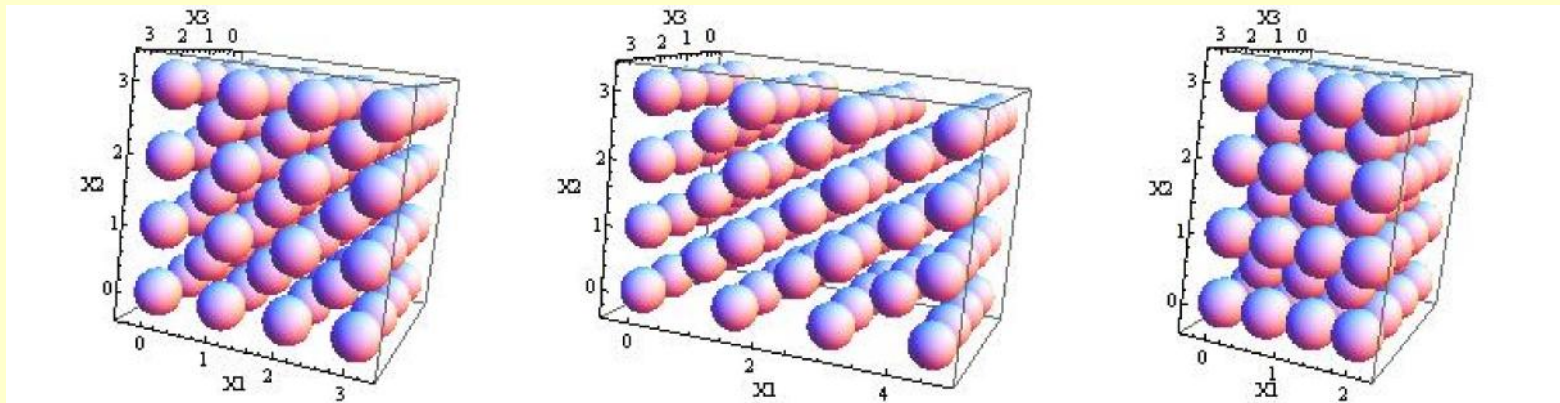
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$$: N^2 a^2,$$

$$: \lambda N^2 a^2$$



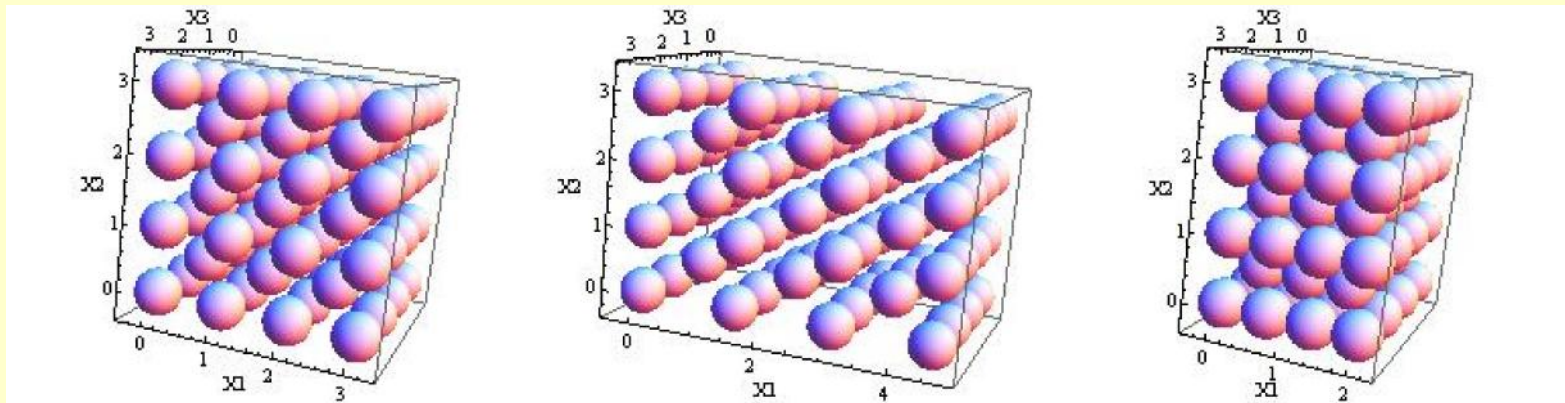
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$$: \mathbf{N}_R = \{1, 0, 0\},$$

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$$: \hat{\mathbf{n}}_R = \{1, 0, 0\}$$



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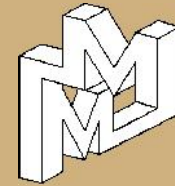
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$$\sigma_{11}(\lambda) = (t_R)_1, \quad \sigma_{22}(\lambda) = (t_{Up})_2,$$

$$\sigma_{12}(\lambda) = (t_R)_2, \quad \sigma_{21}(\lambda) = (t_{Up})_1,$$

$$\sigma_{13}(\lambda) = (t_R)_3, \quad \sigma_{23}(\lambda) = (t_{Up})_3$$



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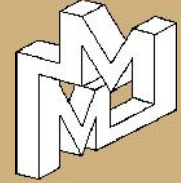
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$$\begin{cases} \sigma_{11} = C_{1111}(\lambda - 1), \\ \sigma_{22} = \sigma_{33} = C_{1122}(\lambda - 1), \\ \sigma_{12} = \sigma_{21} = \sigma_{13} = \sigma_{31} = \sigma_{23} = \sigma_{32} = 0. \end{cases}$$



$$E_{11}^{\text{FCC}}_{\infty} = \alpha^6 (-2626.65 a_*^6 + 37232.60 \alpha^6) \beta / a_*^{15}$$

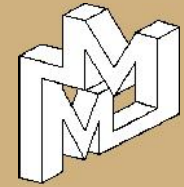
$$E_{22}^{\text{FCC}}_{\infty} = E_{33}^{\text{FCC}}_{\infty} = \alpha^6 (-2512.43 a_*^6 + 27729.90 \alpha^6) \beta / a_*^{15}$$

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$$E_{11}^{\text{FCC}} = 127.36 \beta^{\text{FCC}} / (\alpha^{\text{FCC}})^3$$

$$E_{22}^{\text{FCC}} = E_{33}^{\text{FCC}} = 66.47 \beta^{\text{FCC}} / (\alpha^{\text{FCC}})^3$$



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$$\sigma_{11/22} \alpha^3 / \beta$$

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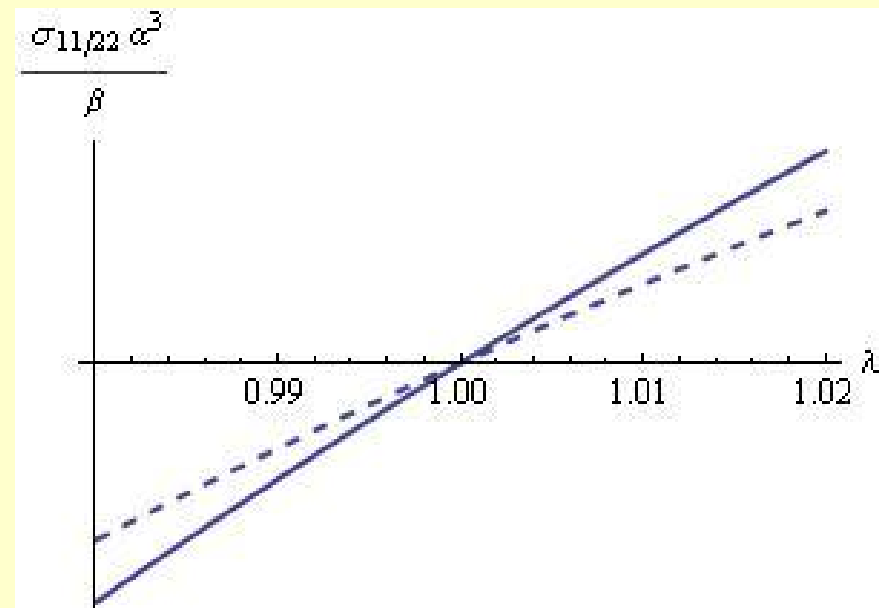
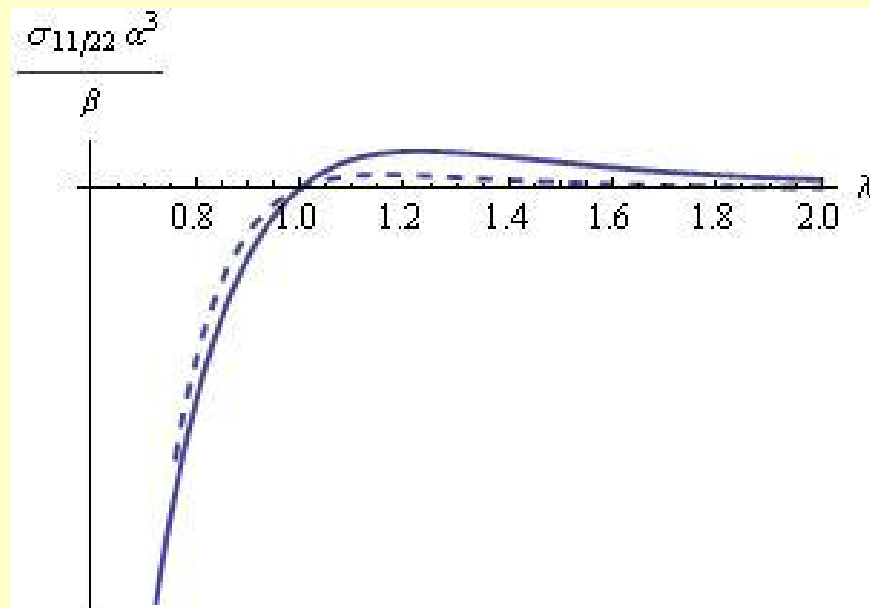
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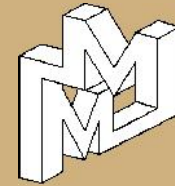
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$$E_{11}^{\text{Cu}} = 8.719 \times 10^{10} \text{ ()},$$

$$E_{22}^{\text{Cu}} = E_{33}^{\text{Cu}} = 4.551 \times 10^{10} \text{ ()}$$

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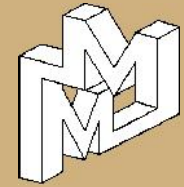
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$$E_{11}^{\text{Cu}} = 8.4 \times 10^{10} \text{ ()},$$

$$E_{11}^{\text{Cu}} = 11.0 \times 10^{10} \text{ ()}.$$

-

3.5%!



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:

$$v = 0.343$$

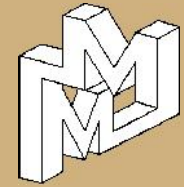
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:

$$v^{\text{Cu}} = 0.35, v^{\text{Al}} = 0.34$$

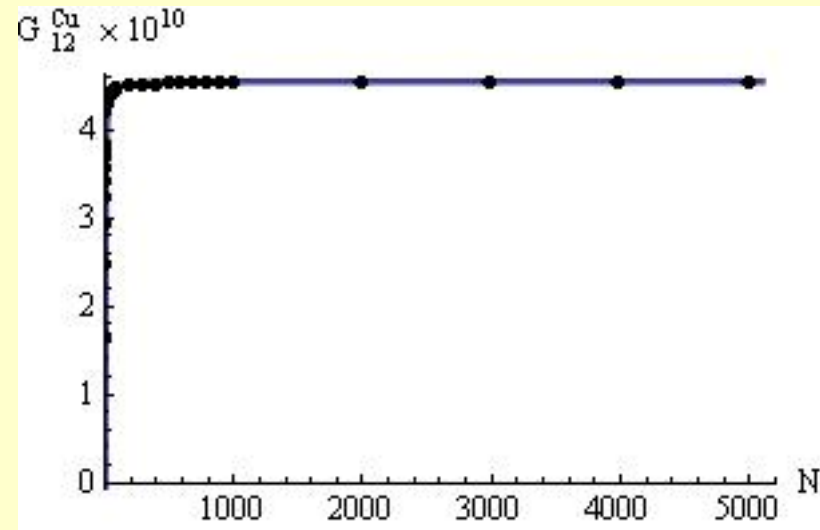
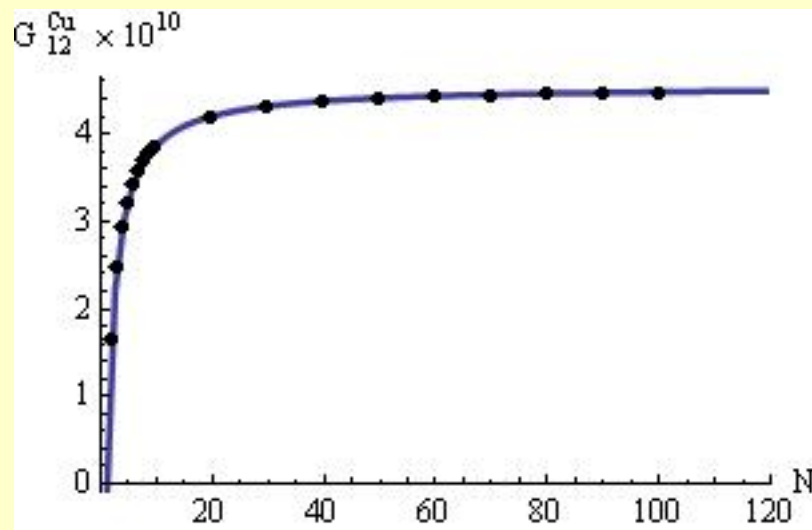
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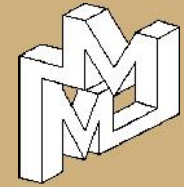
2%!



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- , 8 , 8 (Open MP)





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N 5000!

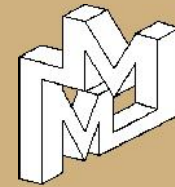
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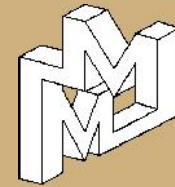
$$(N^2 + 3(N - 1)^2)N$$

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5000: 499850015000



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