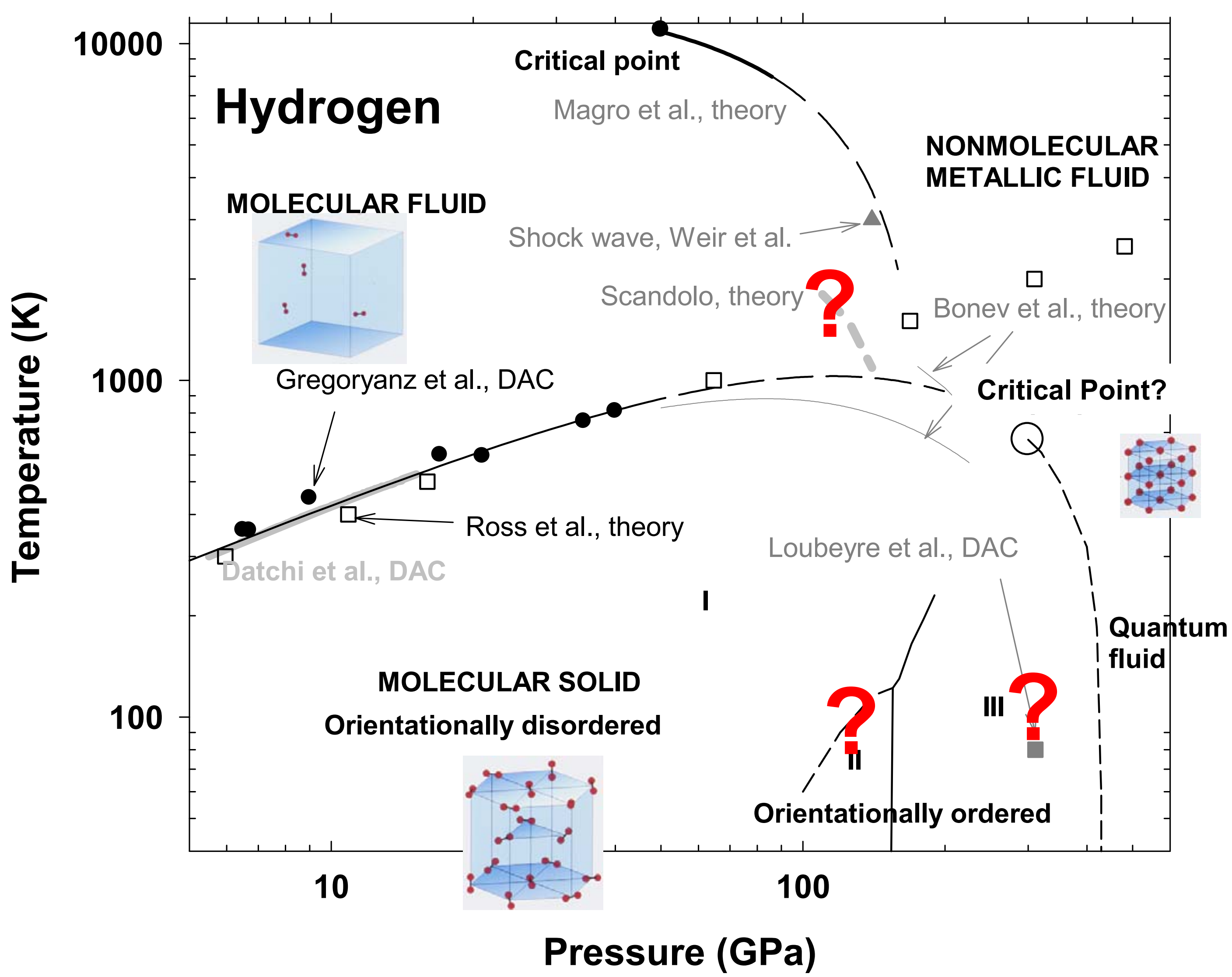
Физика вещества с высокой концентрацией энергии
Научно-координационная Сессия "Исследования неидеальной плазмы"
1 - 2 декабря 2010 г.

Cell Model of hydrogen Liquid at Megabar Pressures

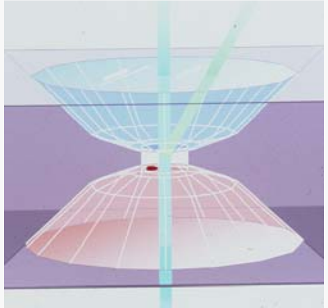
V. S. Vorob'ev[1], v. G. Novikov

*[1]Joint Institute for High Temperatures of Russian Academy of Science,
Izhorskaya 13, 125412 Moscow, Russia*

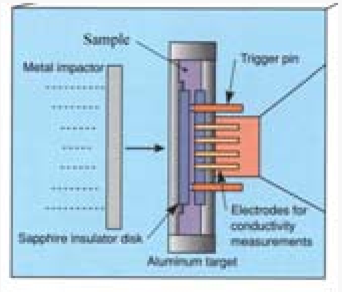
The phase diagram of dense hydrogen has been constrained by a combination of techniques



[*after* Goncharov and Crowuhurst, *Phase Trans.* (2007)]



STATIC



DYNAMIC

THEORY

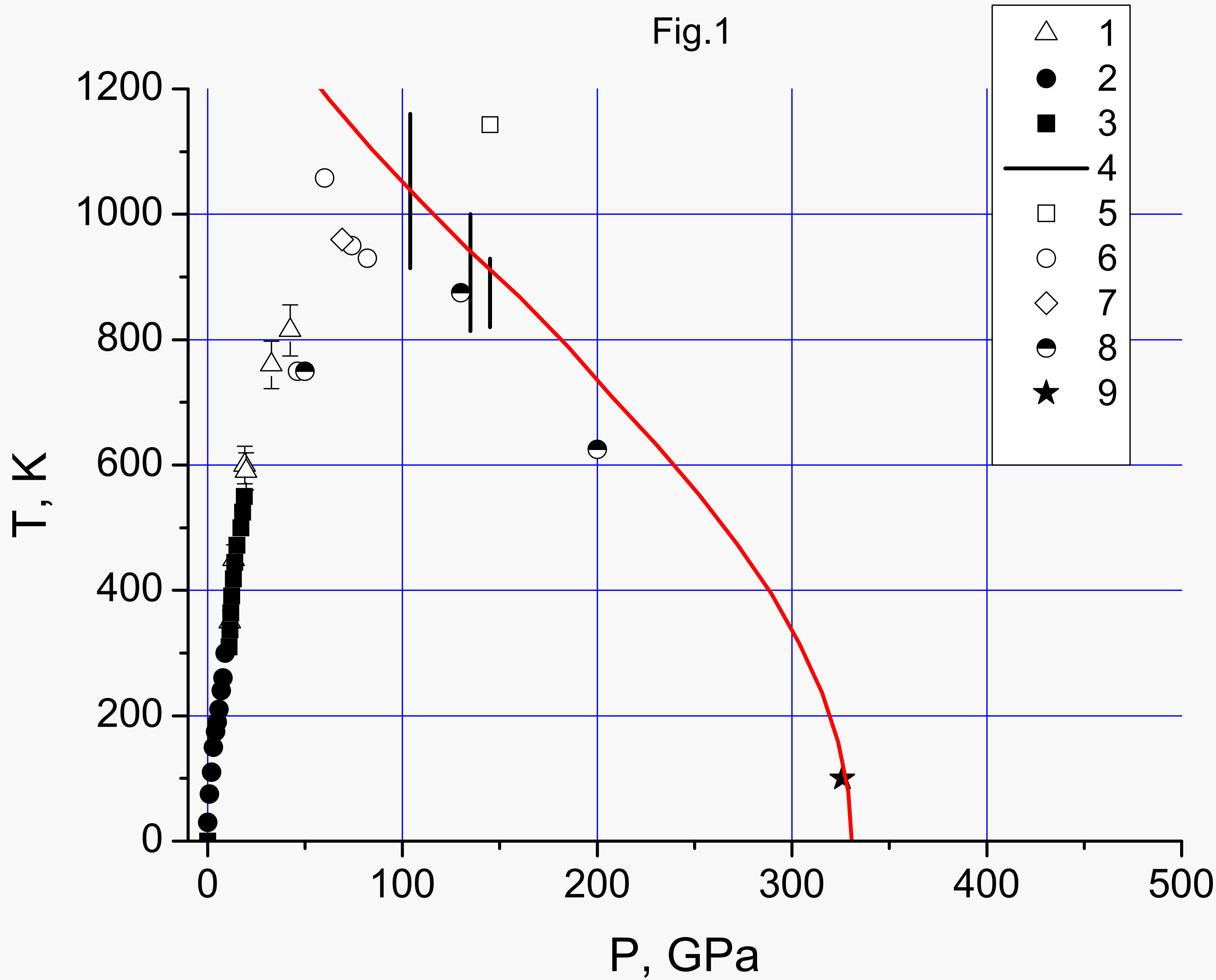


Fig.1
1200
1000
800
600
400
200
0
0
100
200
300
400
500
T, K
P, GPa
1
2
3
4
5
6
7
8
9

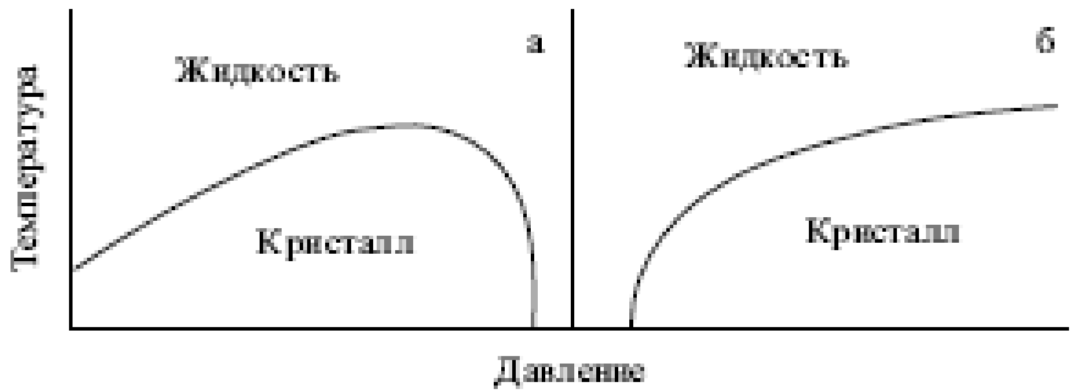
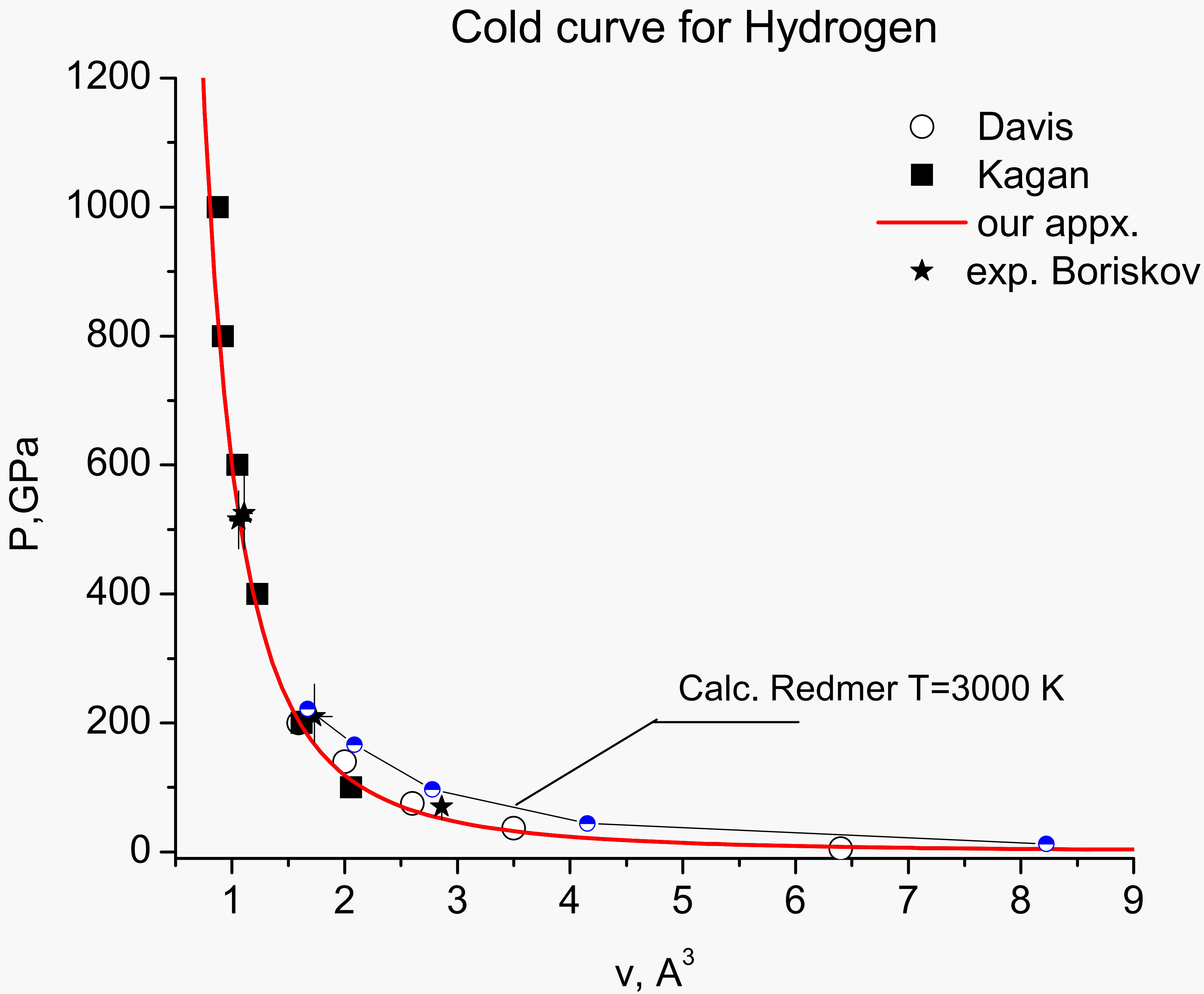


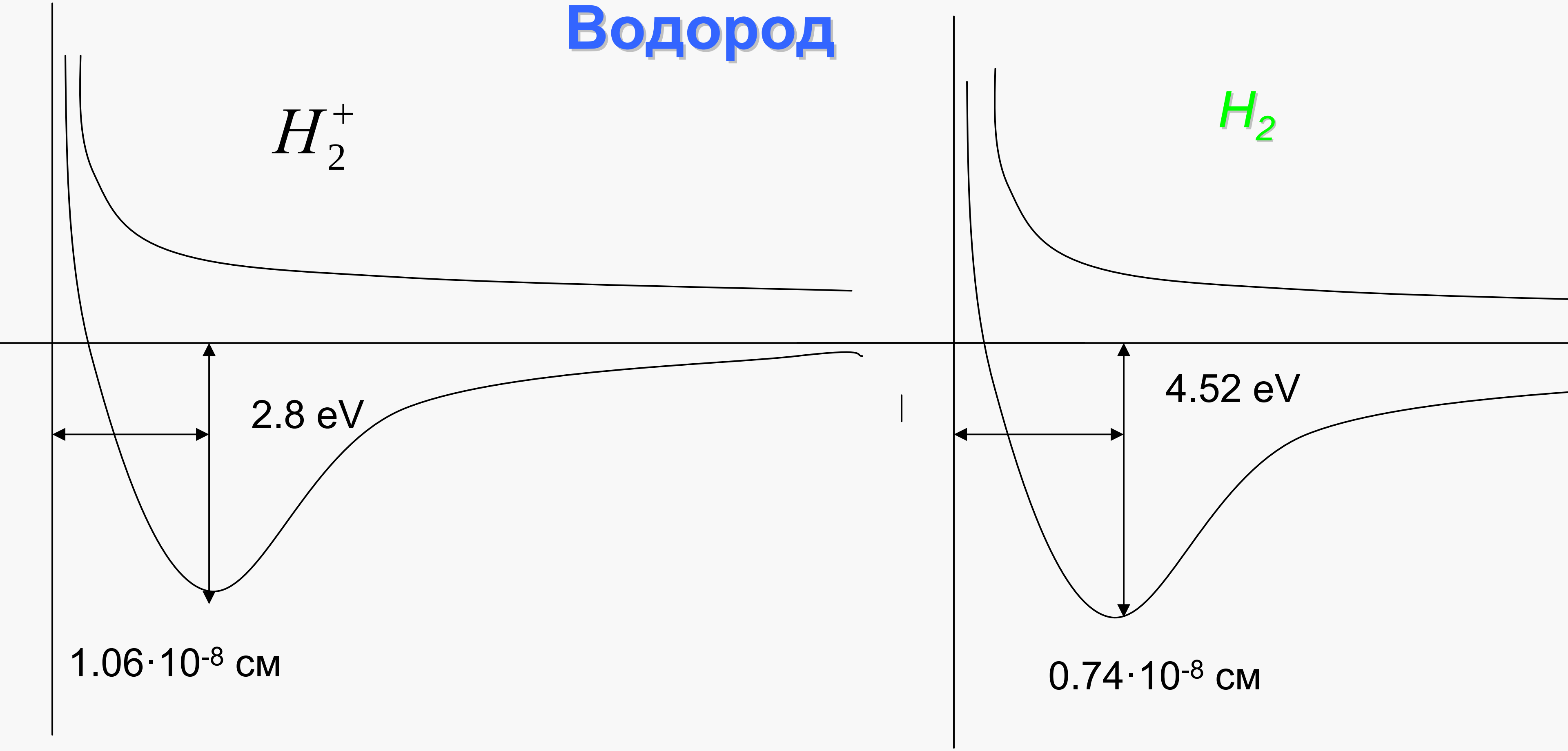
Рис. 1. Влияние квантовых эффектов на кривую плавления: (а) случай кулоновского взаимодействия; (б) случай короткодействующего отталкивания.

Д. А. Киржниц

С. М. Стишов, УФН , 171,№3, 2001


Cold curve for Hydrogen
P,GPa
v, A^3
0
200
400
600
800
1000
1200
1
2
3
4
5
6
7
8
9
Davis
Kagan
our appx.
exp. Boriskov
Calc. Redmer T=3000 K

Водород



$$T = 0 \quad ; \quad N = (0.05 \div 10) \cdot 10^{24}\ см^{-3} \quad ;$$

$$Среднее\ \ расстояние \quad R = (0.3 \div 1.7) \cdot 10^{-8}\ см^{-3}$$

$$a_0 = 0.53 \cdot 10^{-8}\ см^{-3} \quad Давления \quad (100 \div 600)\ ГПа$$

Cell model of quantum liquid

Every ion localizes in the W-Z cell

$$R = \left(\frac{3}{4\pi}\right)^{1/3} \frac{1}{N^{1/3}}$$

Electron density in the cell

$$n(r) = n_b(r) + n_f$$

Density of localized states is

$$N_b(r, T, \mu) = \frac{1}{\pi} \frac{\exp(-2r)}{1 + \exp\left[-\left(E - \mu\right)/T\right]}$$

The cell is neutral , there are continuous state over the cell, distributed uniformly over the cell , their density equals

The

$$N_f(T, \mu) = \frac{(2T)^{3/2}}{2\pi^2} I_{1/2}\left(\mu / T\right)$$

$$I_{1/2}(x) = \int_0^\infty y^{1/2} dy \Big/ \left(1 + e^{(y-x)/T}\right)$$

Cell is electrically neutral

$$4\pi\int_0^R r^2 dr\left[n_b(r)+n_f\right]=1$$

$$\frac{1-e^{-2R}\left(1+2R+2R^2\right)}{1+\exp\left(\frac{-1-\mu}{T}\right)}+\frac{\left(2T\right)^{3/2}}{2\pi^2 n}I_{1/2}\left(\mu/T\right)=x_b+x_f=1$$

$T\to 0$

$$N_b(r)=e^{-2r}/\pi \quad ; \quad N_f=e^{-2R}\left(1+2R+2R^2\right)n$$

$$x_b=1-e^{-2R}\left(1+2R+2R^2\right)\ ;\ x_f=e^{-2R}\left(1+2R+2R^2\right)$$

$$\mu=\frac{p_F^2}{2}=\frac{\left(3\pi^2\right)^{2/3}}{2}(x_f\, n)^{2/3}$$

Kinetic energy of localized electrons

$$T_b = \left\langle \frac{p^2}{2} \right\rangle = 4\pi \int_0^R r^2 dr R_{10}(r) \nabla^2 R_{10}(r) = -4 \int_0^R r^2 dr e^{-r} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} e^{-r} \right) =$$

$$= \left[1 - e^{-2R} \left(1 + 2R + 2R^2 \right) \right]$$

Kinetic energy of delocalized electrons

$$T_f = \frac{\left(3\pi^2\right)^{2/3} 3 n_f^{5/3}}{5} 4\pi \int_0^R r^2 dr = \frac{\left(3\pi^2\right)^{2/3} 3 N^{2/3}}{5} \left[e^{-2R} \left(1 + 2R + 2R^2 \right) \right]^{5/3}$$

Electron-ion energy of interaction

$$U_{ei} = -4\pi \cdot 2 \int_0^R r^2 dr \frac{n(r)}{r} = -2 \left[1 - e^{-2R} \left(1 + 2R \right) \right]$$

$$U_f = -4\pi \cdot 2 \int_0^R r^2 dr \frac{N_f(r)}{r} = -4\pi \left(\frac{3}{4\pi} \right)^{2/3} x_f n^{1/3}$$

$$I = T_b + U_b = -1 + e^{-2R} \left(1 + 2R + 2R^2 \right)$$

Electon-electron and exchange interactions

Self-consistent potential, formed by all charge particles

$$\Phi(r) = \frac{1}{r} - \int \frac{n(r')r'^2\,dr'\,d\Omega'}{|r-r'|}$$

$$\Phi(r) = \frac{1}{r} - 4\pi \cdot \left[\frac{1}{r}\int_0^r r'^2\,dr'\,n(r') + \int_r^R r'\,n(r')\,dr' \right] = \frac{1}{r} - V_b(r) - V_f(r)$$

Middle electron interaction energy

$$U_{ee} = -4\pi \int_0^R \left[V_b(r) + V_f(r) \right] n(r) r^2 dr$$

Exchange addition to potential

$$\Phi_{ex}(r) = \left(\frac{3}{\pi} \right)^{1/3} n(r)^{1/3}$$

Exchange potential energy

$a = 1.15$ Is fitting parameter

$$U_{ex} = 8\pi a \left(\frac{3}{\pi} \right)^{1/3} \int_0^R r^2 dr n(r)^{4/3}$$

$$R = U_{ee} + U_{ex} = W = 4\pi \int_0^\infty [V_b(r) + V_f(r)] N(r) r^2 dr - 8\pi a \left(\frac{3}{\pi}\right)^{1/3} \int_0^\infty r^2 dr N(r)^{4/3}$$

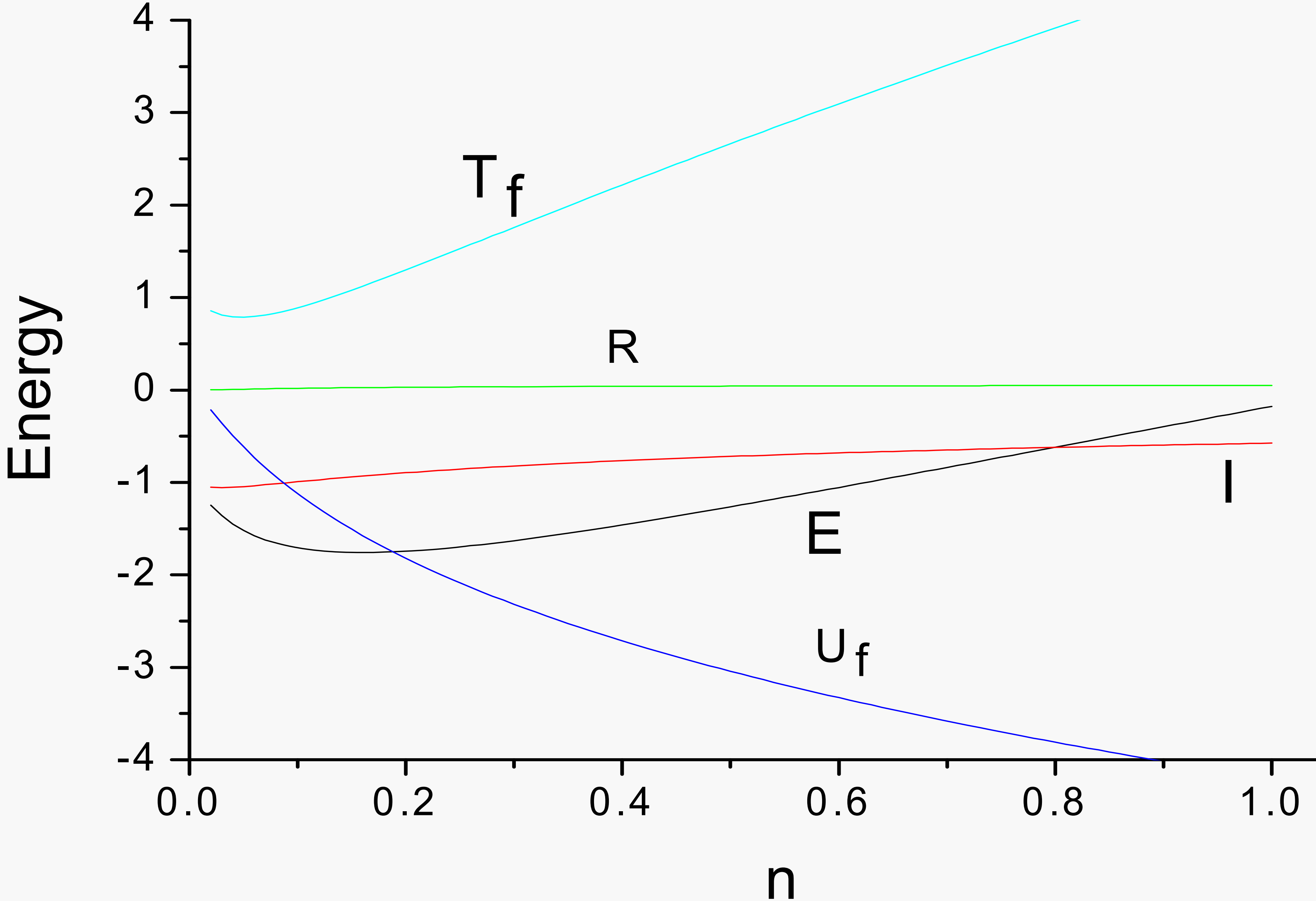
In the limit $N \to 0, R \to \infty, \quad U_{ex} + U_{ee} \to 0$ Like as in hydrogen atom

Total Energy $$E = I + R + T_f + U_f$$

$$E = I(n) + R + \frac{(3\pi^2)^{2/3} 3}{5} n^{2/3} x_f^{5/3} - \alpha(n) n^{1/3}$$

$$\alpha(n) = (36\pi)^{1/3} x_f \quad (*)$$

Contribution of different terms in full cell energy



Proton contribution

Both electrons and protons are degenerate at T = 0. Their wave length in this limit is .

$$\lambda = \hbar / p_F = 1/(3\pi^2)^{1/3} n^{1/3}$$

The relation of this wave length to the cell radius equals to

$$\lambda / R = \frac{1}{(3\pi^2)^{1/3} n^{1/3}} \left(\frac{4\pi}{3} \right)^{1/3} n^{1/3} = \left(\frac{4}{9\pi} \right)^{1/3} \approx 0.52$$

This constant does not depend on density. The proton wave length and the relation at finite temperature are and (here T and n are expressed in K and Å-3 correspondingly). The latter relation equals to ~0.42 at n = 0.1 and T = 1000 K. So we have degenerate protons over the entire domain of our consideration.

This atomic – like structure of diameter $2Ra$ and mass M (proton) is confined to move in a space with characteristic dimension

$$\Delta(n) = 2R(1 - 4\pi n R_a^3 / 3)$$

, the mean – proton spacing with the correction due to the own size of the atomic-like structure

The free energy of degenerate proton gas at low temperatures can be presented as

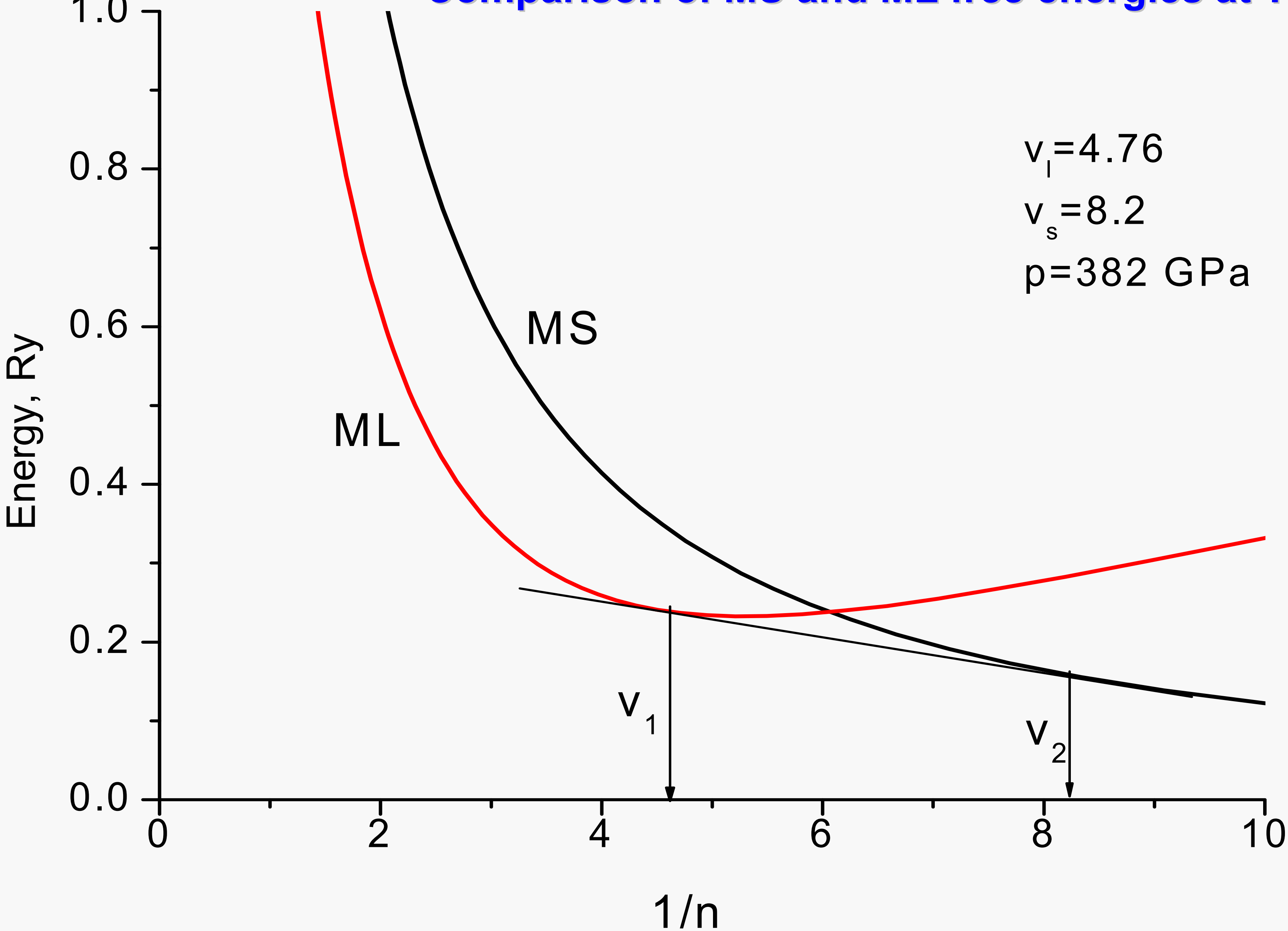
$$F_p = \frac{(3\pi^2)^{2/3}3}{5}\frac{m}{M}\frac{1}{\Delta(n)^2} - \left(\frac{\pi}{3}\right)^{2/3}\frac{M}{4m}\Delta(n)^2 T^2 ; Ry$$

COMPARISON MS AND AS FREE ENERGIES AT *T* = 0

$$E' = I + R + T_f + U_f + 2 + D/2$$

D is the energy of dissociation of the molecule (0.165 Ry/atom)

Comparison of MS and ML free energies at T=0



Conclusion

If it is possible to get a quantum metastable hydrogen liquid as molecular hydrogen solid is subjected to melting at megabar pressure

Reference

1. Vorob'ev V. S., Novikov V. G. EPL, 89, 40014 (2010).