Charged Clusters in Liquid Helium

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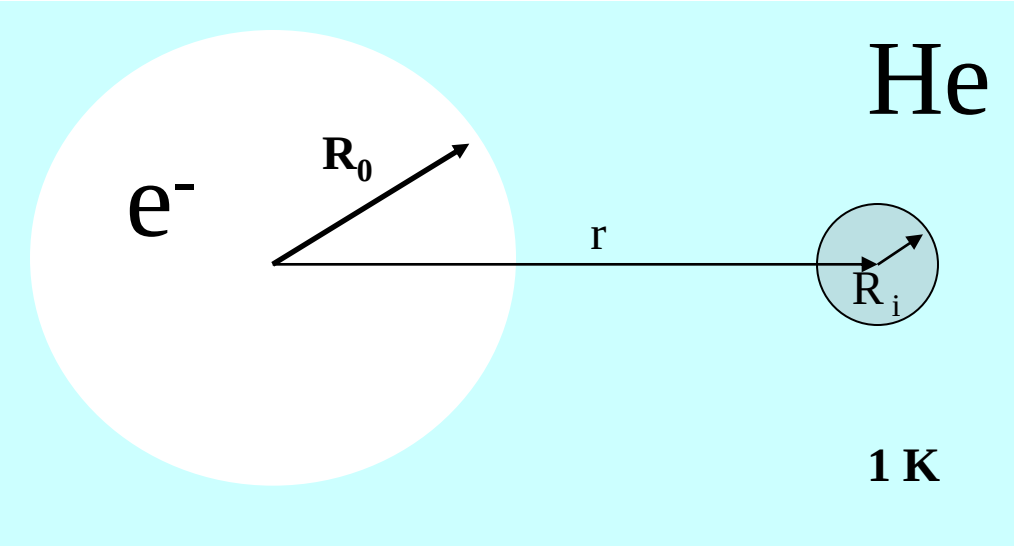
Ne , Ar, Kr, Xe, H_2, N_2



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Bound States of an Electron and a Macroscopic Cluster at a Helium Surface, JETP, 98, 2, 441-444, (2004).

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Interaction of Negative Ions with the Surface of Inert Liquids, JETP Letters, 89(3), 145 (2009).

E. V.Lebedeva, A.M. Dyugaev, and P. D. Grigoriev, Diffusion Transport of Negative Ions through the Interface between Cryogenic Liquids JETP, 110(4), 693 (2010).

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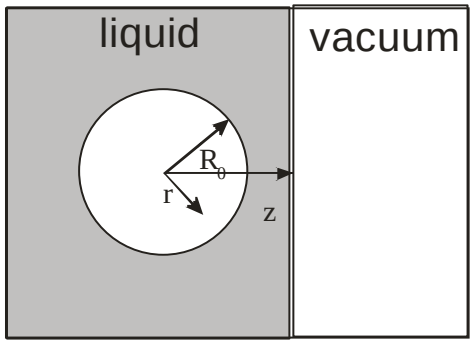
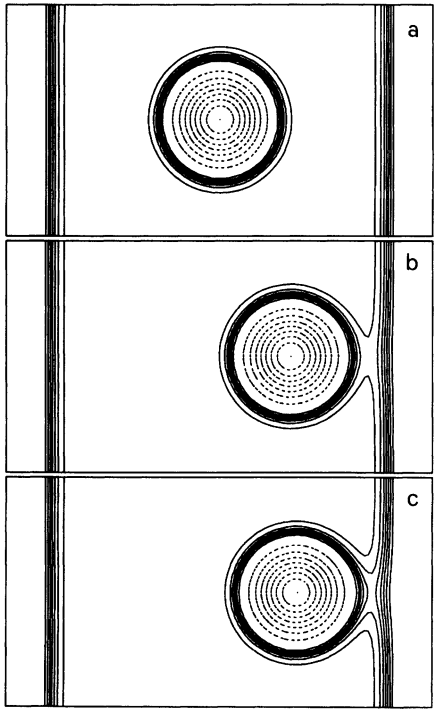
Density-functional approach for investigation of electron bubble properties near the surface of liquid helium.

F. Ancilotto and F. Toigo, Phys. Rev. B, 50, 12820 (1994).



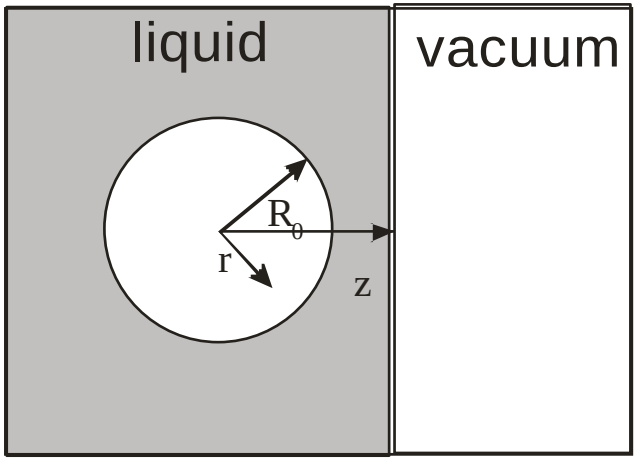


Complicated procedure of simulation.

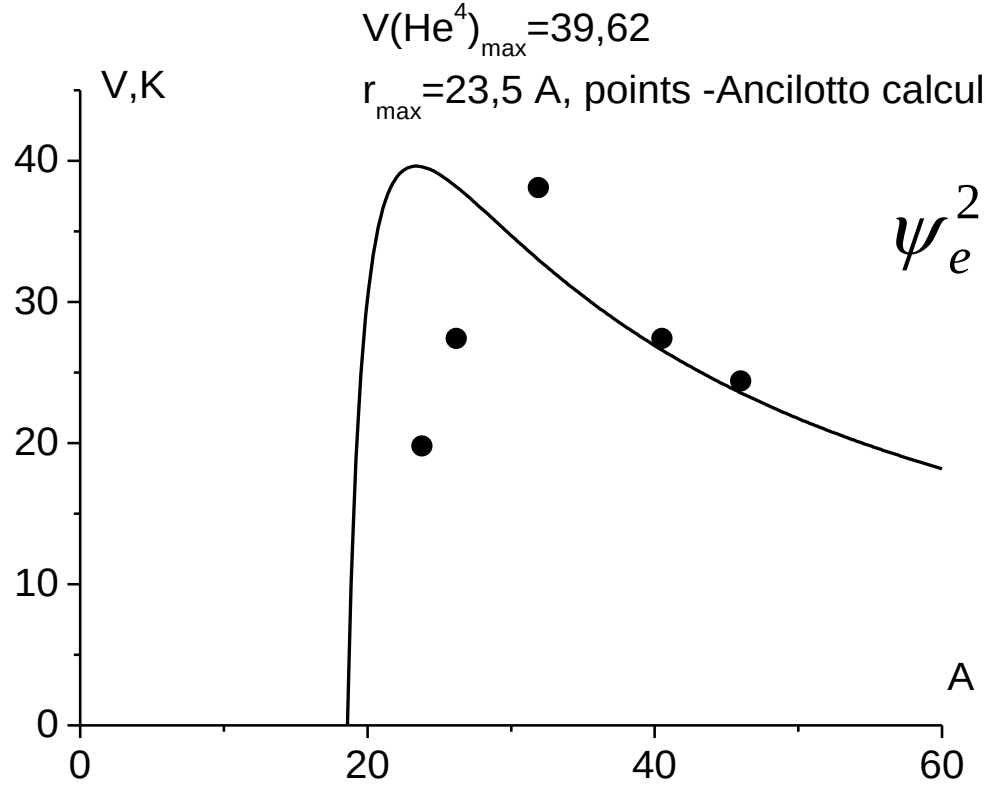
- definition of energy functional for electron and He;
- solution of nonlinear Schrödinger's equations; for electron and helium density functions
- energy minimization, laws of conservation;
- adjustment of procedure parameters to reproduce the experimental values of He constants.

Energy of helium atom: kinetic, He-He interaction, He-electron interaction.
Electron energy: kinetic, He-electron interaction.

Our approach is continuous media approximation. Instead of complicated computation we used the simple integration on the half-space.



A.M. Dyugaev, P. D. Grigor'ev and E. V.Lebedeva Interaction of Negative Ions with the Surface of Inert Liquids, JETP Letters, 89(3), 145 (2009).



$$\psi_e^2(r) = \frac{1}{4\pi}\frac{2}{R_0}\frac{\sin^2(\pi r/R_0)}{r^2}$$

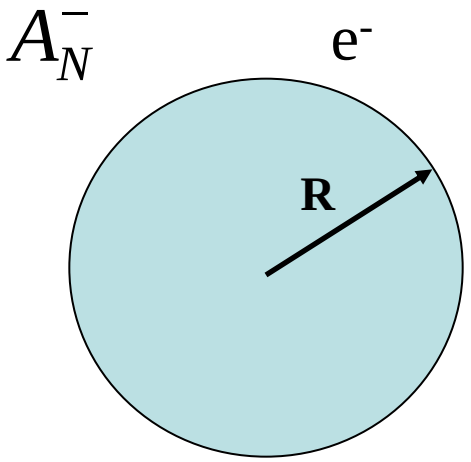
$$V(\vec{r}_1 - \vec{r}_2) = -\frac{C_6}{|\vec{r}_1 - \vec{r}_2|^6}$$

$$V_e(z) = A\int \frac{\psi_e^2(r)}{z(r)}$$

Charged cluster in vacuum (H_2, Ne, He)

V.M. Nabutovskii and D.A. Romanov, Sov. Phys. Low Temp. Phys. 11, 277 (1987)
M Rosenblit and J Jortner J. Chem. Phys. 101, 9982, (1994).
M Rosenblit and J Jortner J. Chem. Phys. 101, 8039, (1994).

- **Weakness of polarization attraction between electron and inert atom.**
- **The number N of atoms or molecules in the cluster, that could exist, is macroscopically large.**
- **Charged cluster can't exist if R<Rc.**



H_2 : R_c=35A, N_c= 4.6 ×10^3

Ne : R_c=39A, N_c= 1.5 ×10^4

He^4 : R_c=149A, N_c= 3 ×10^5

He^3 : R_c=203A, N_c= 5.7 ×10^5

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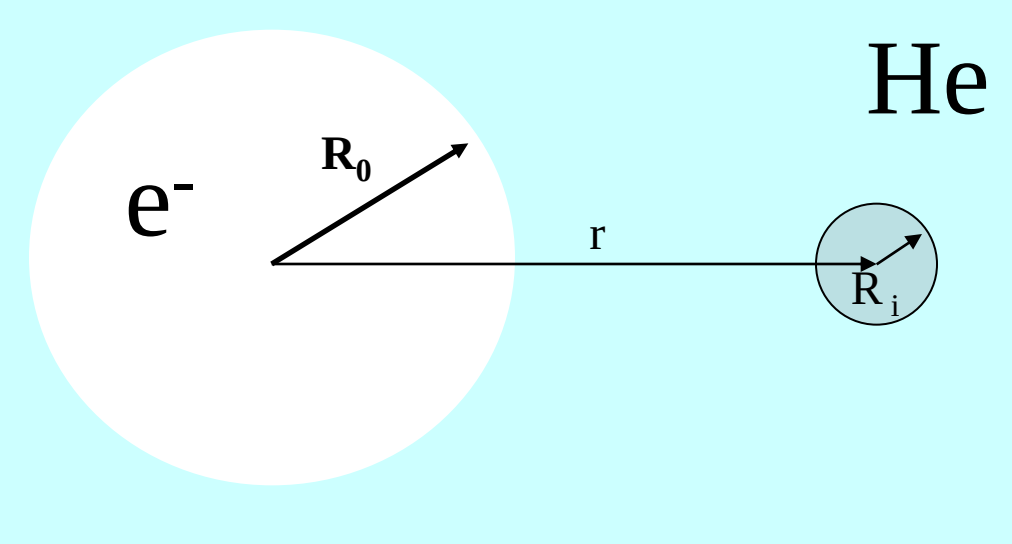
Cluster-electron interaction potential: polarization and van der Waalse parts



N_i – the number of particles in cluster,

$10<N_i<1000$

$N_0 = 450$ – the number of helium atoms, replaced by the bubble.

$M_e = 900$ a.m.u.

$R_0 = 17$A, $R_i<R_0$

Effective van der Waals repulsion potential:

$$v_{0i}(r) = \frac{e^2 c_{0i} r_B^5}{r^6}$$

Attractive potential of cluster's particle polarization by a point charge:

$$v_e = -\frac{e^2 \alpha_i r_B^3}{2r^4}$$

α_i - polarizability of cluster particles,

c_{0i} - van der Waals constant for cluster's particle-He interaction,

r_B - Bohr's radius.

Reduced interaction potential of cluster and electron.

$$V(r) = E_i V_-^*(x), \quad x = r/R_0, \qquad E_i = \frac{e^2 N_i \alpha_i {r_B}^3}{2{R_0}^4}$$

$$V_-^*(x) = f_e(x) + \lambda f_b(x)$$

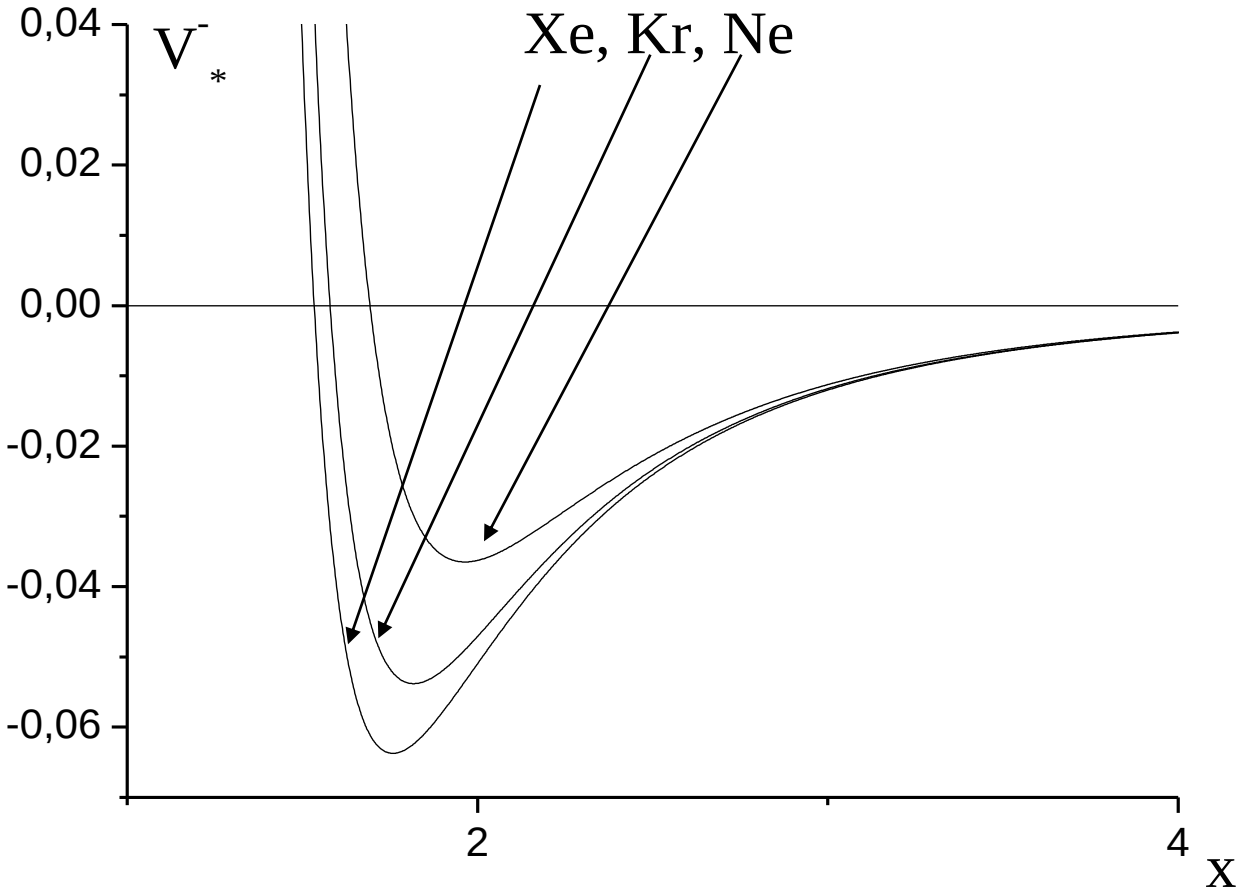
$$V_-^* = -\int_0^1 \frac{2\sin^2 \pi y dy}{(x^2 - y^2)^2} + \frac{\lambda}{(x^2 - 1)^3}$$

$$\lambda = \frac{2N_0 {r_B}^2 c_{0i}}{{R_0}^2 \alpha_i} \approx 0.6 - 1.$$

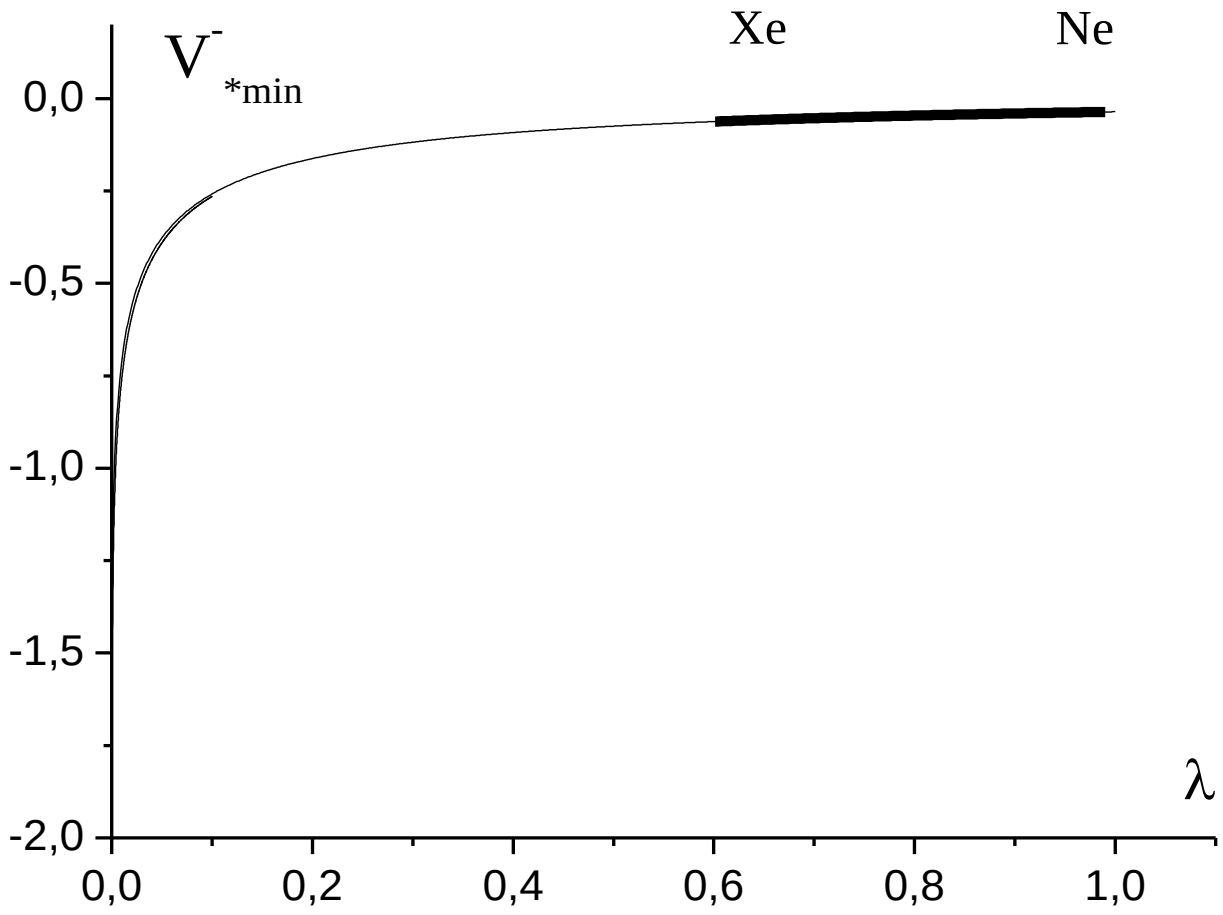
$$\frac{c_{0i}}{\alpha_i} \sim \frac{\Delta_i}{\Delta_i + \Delta_0} : 0.33\text{–}0.47$$

$$c_{0i} : 3 - 10 \quad \alpha_i : 3 - 27$$

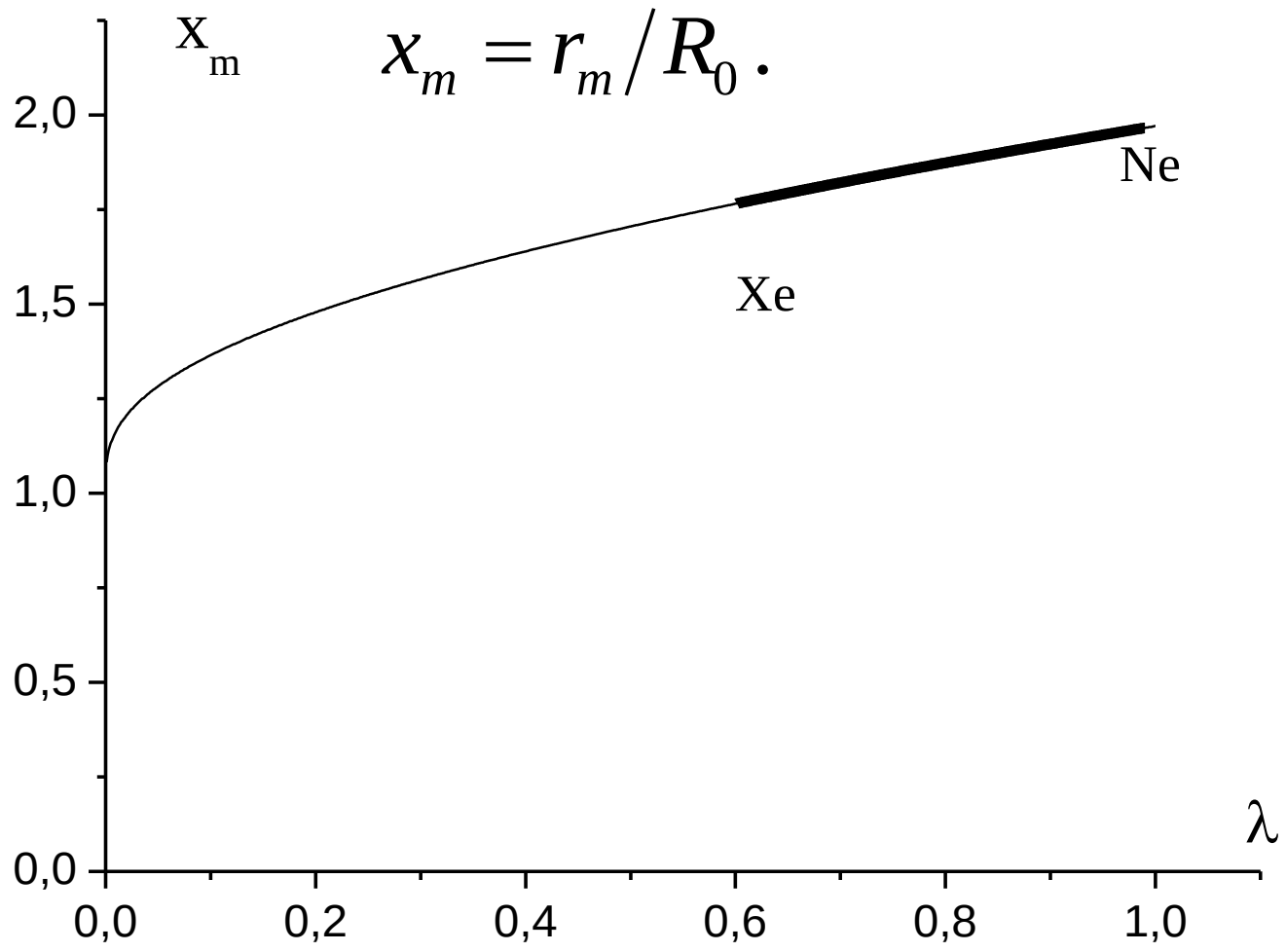
H. Margenau,
Rev. Mod. Phys. 11, 1-35 (1939).


0,04
0,02
0,00
-0,02
-0,04
-0,06
V*-
Xe, Kr, Ne
2
4
x

The dependence of reduced potential minimum on λ-parameter



The dependence of reduced potential minimum position on λ-parameter



Charged cluster's characteristics in liquid helium

	α	c_{0i}	λ	$V^{-}_{*\min}$	$\mathbf{r_{min}}$	N_1	f_l	f_s
Ne	2,66	3,04	0,99	-0,036	33,4	70	0,119	0.036
Ar	11,1	9,60	0,752	-0,049	31,4	12	0,140	0,046
Kr	16,7	13,4	0,698	-0,054	30,9	7	0,146	0,049
Xe	27,3	18,6	0.593	-0,063	29,9	4	0,159	0,056
H_2	5,33	4,22	0,689	-0,054	30,9	23	0,147	0,049
N_2	11,9	10,14	0,741	-0,050	31,3	11	0,142	0,047

Number of states N_s and number of levels N_l

$$N_l = \frac{1}{8} N_i \frac{M_i^*}{m_e} \alpha_i \frac{r_B^{\,2}}{R_0^{\,2}} f_l, \quad f_l = \int \left(-V_*^{-}(x)\right) x\, dx$$

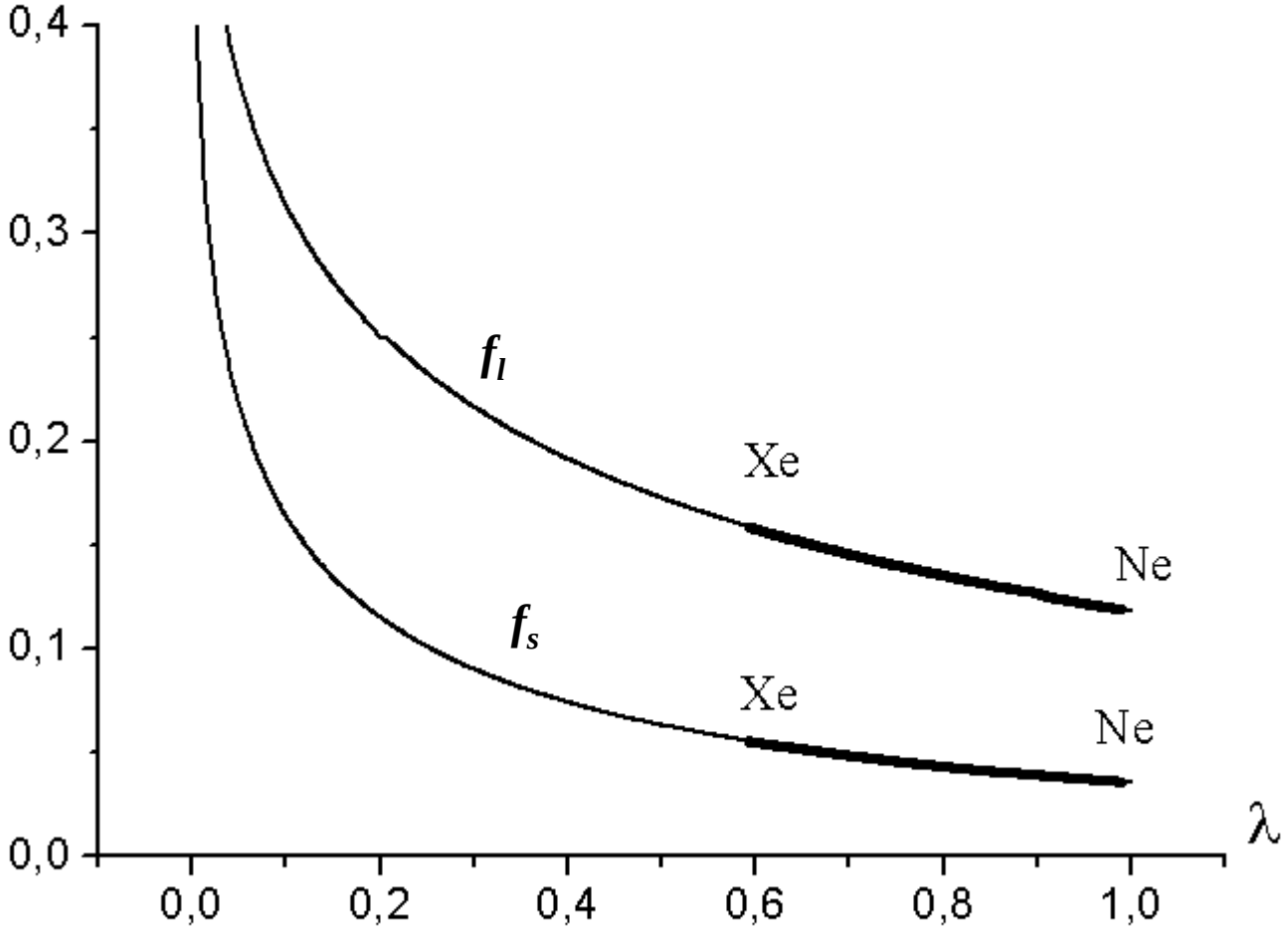
$$N_S = \frac{2}{3\pi}\left(N_i \frac{M_i^*}{m_e} \alpha_i \frac{r_B^{\,2}}{R_0^{\,2}} \right)^{3/2} f_S, \quad f_S = \int \left(-V_*^{-}(x)\right)^{3/2} x^2\, dx$$

$$M_i^* = \frac{M_e M_i}{M_e + M_i}, \quad \frac{M_e}{m_e} = 1.64 \cdot 10^6, M_e = 900\, amu$$

Example.

Xe: N_i=13, M_i=1700 amu. , N_S=2.67×10^6, N_l =7350.

The dependence of reduced potential's parameters f_l f_s on λ



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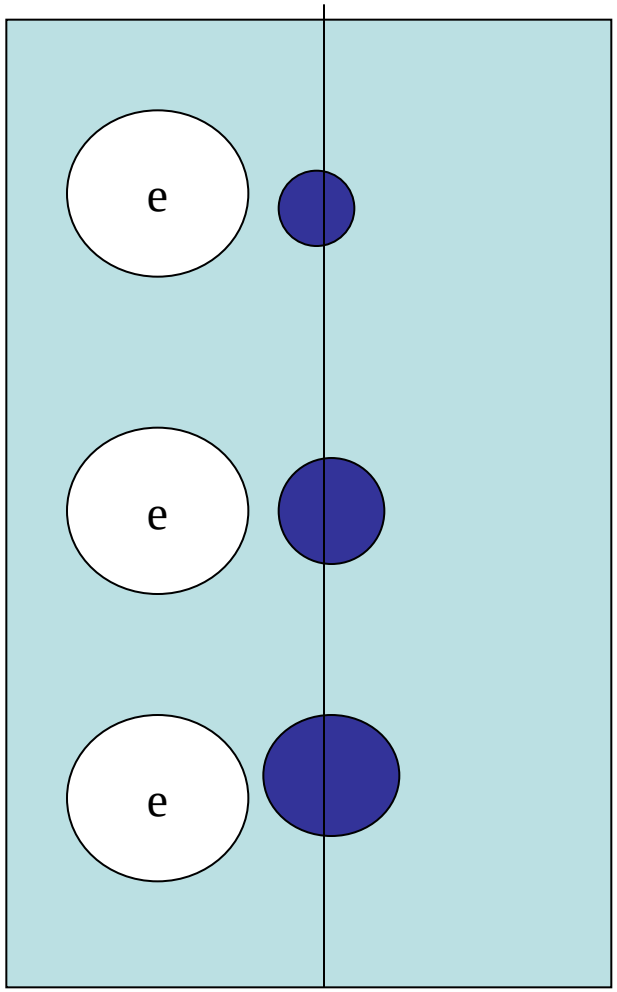
$R_l = 13 - 16A$



Ground state energy of charged cluster:

$$\varepsilon_{i0} = E_i V^*_{-\min}$$

Ne: $R_i = 16\,A$

$N_i \approx 1000$

$\varepsilon_{i0} \approx 15K$

H_2: $R_i = 14\,A$

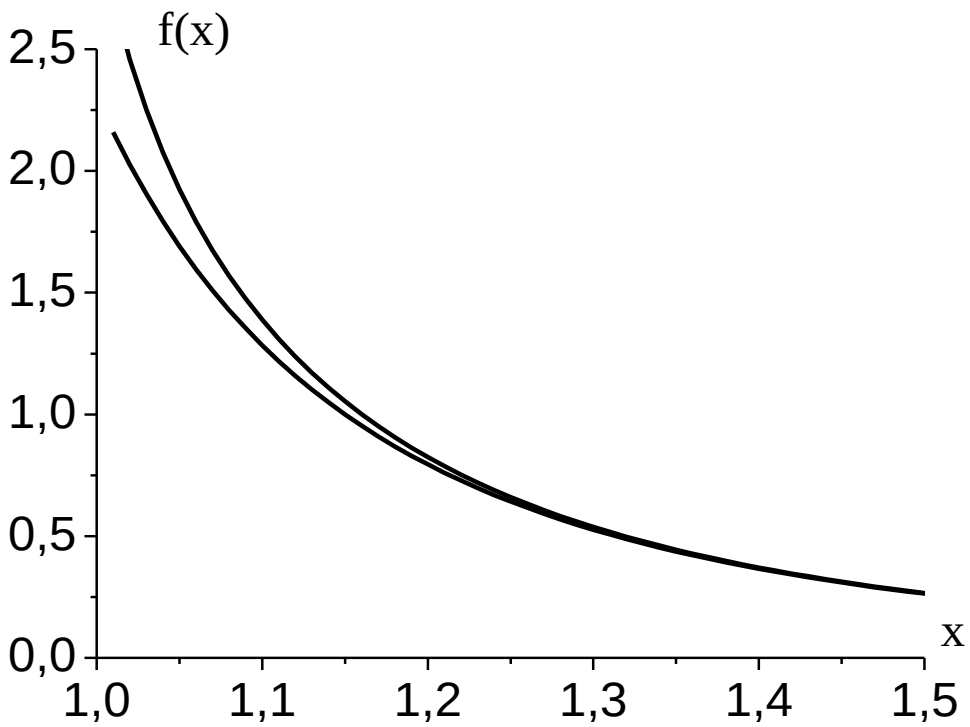
$N_i \approx 300$

$\varepsilon_{i0} \approx 13K$

Internal energy of electron: $\varepsilon_e = \dfrac{\pi^2 \hbar^2}{m_e R_0^2} \approx 2 \cdot 10^3\,K$

Summary

- **The existence of small charged inert clusters formed by Ne, Ar, Kr and Xe atoms and H_2 and N_2 molecules had been proved.**
- **The properties of these clusters had been semi-classically described.**
- **The scaling behavior of cluster parameters had been found out.**


f(x)
2,5
2,0
1,5
1,0
0,5
0,0
x
1,0
1,1
1,2
1,3
1,4
1,5