

It is sufficient that the increase of $\langle \alpha | O_i | \alpha \rangle$ with α be faster than logarithmic, i.e. [3]

$$\lim_{\alpha \rightarrow \infty} \frac{\langle \alpha | O_i | \alpha \rangle}{\ln \alpha} \rightarrow \infty. \quad (5)$$

For example, if the set of observables O_i , $i = 1 \dots n$ are all projection operators [2] $P_\alpha = |\alpha\rangle\langle\alpha|$ where $\alpha = 0, 1 \dots n-1$, then condition (4) is not satisfied and $Z(\lambda_1 \dots \lambda_n) = \infty$ and $\rho = 0$. However, if one observable in the set satisfies conditions (4) and (5), as the Hamiltonian does, for example, then Z and ρ are finite for arbitrary

observables in the rest of the set.

In conclusion, it should be noted that conditions (4) and (5) are necessary restrictions only in infinite dimensional vector spaces.

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QUANTUM CORRECTIONS FOR SECOND VIRIAL COEFFICIENTS USING DIFFERENT LENNARD-JONES ($m-n$) POTENTIALS AND APPLICATION TO HELIUM

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Using the Slater sum we get an expression for the second virial coefficient and its quantum corrections [1]. For the Lennard-Jones ($m-n$) potential

$$U = \alpha \epsilon \left\{ \left(\frac{\sigma}{r} \right)^n - \left(\frac{\sigma}{r} \right)^m \right\}, \quad \alpha = \frac{1}{n-m} \left(\frac{n}{m} \right)^{n-m} \quad (1)$$

the integration over the coordinate space gives:

$$B = \frac{2\pi N \sigma^3}{3} \sum_{\nu=0}^3 \sum_{s=0}^{\infty} \left\{ \frac{h}{\sigma(M\epsilon)^{\frac{1}{2}}} \right\}^{2\nu} b_{\nu}^{(s)}(m, n) \left\{ \frac{\epsilon}{kT} \right\}^{\frac{s(n-m) + \nu(n-2) + 3}{n}},$$

$$b_{\nu}^{(s)}(m, n) = \frac{k_{0\nu} + k_{1\nu}s + k_{2\nu}s^2 + k_{3\nu}s^3}{d_{\nu} n \pi^{2\nu} s!} \alpha^{\frac{s(n-m) - 2\nu + 3}{n}} \Gamma \left(\frac{ms - 3 + 2\nu}{n} \right). \quad (2)$$

$k_{\mu\nu} = 0$ ($\mu = 0, 1, 2, 3$) for $\mu > \nu$; $d_{\nu} = \text{const}$. $k_{\mu\nu}$ depend on m and n only.

Using $b_{\nu}^{(s)}(6, 8)$ ($0 \leq s \leq 51$), $b_{\nu}^{(s)}(6, 9)$ ($0 \leq s \leq 60$) and $b_{\nu}^{(s)}(6, 12)$ ($0 \leq s \leq 40$) [1] the second virial coefficient, its derivatives with respect to temperature and the zero-pressure Joule-Thomson coefficient are calculated with their first three quantum corrections in the

temperature range $0.30 \leq T^* \leq 400$.

Applying eq. (2) to helium we use firstly experimental values of White [2] ($45 < T < 300^{\circ}\text{K}$: case 1) and secondly of White [2] and Yntema [3] ($45 < T < 1473^{\circ}\text{K}$: case 2) to fit the theoretical values. This is possible up to about 900°K . We have used the method of least squares. For more detailed information another method is used: We rewrite eq. (2), so that we get σ as a

function of ϵ with the parameter T . This method takes into account that the quantum corrections are also functions of σ and ϵ , so that it becomes an iterative method. For some temperatures of case 1 one finds a comparison of the calculated and the experimental values in table 1. Figure 1 shows the Lennard-Jones (6-9) and (6-12) potentials and an exp - six potential (MR 5) [4]. For heli-

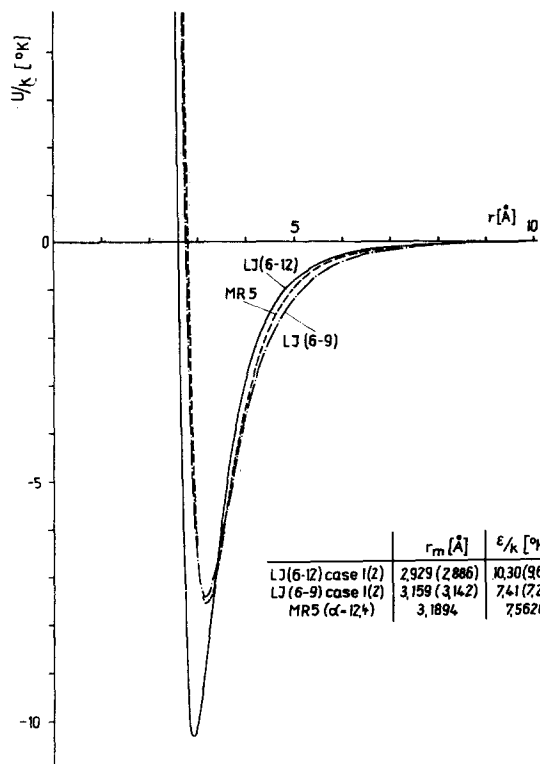


Fig. 1. Different potential curves for helium.

um the Lennard-Jones (6-9) potential seems to be more appropriate than the commonly used (6-12) potential. Using the Lennard-Jones (6-8) potential (case 1 (2): $r_m = 3.279$ (3.272) Å; $\epsilon/k = 6.34$ (6.29)°K in case 2 the deviations are even something more smaller. We have found a similar

Table 1
Experimental and calculated B [cm³/mole] for He⁴

T [°K]	B (exper.)	B (6-9)	B (6-12)	B (6-8)
45.10	7.48	7.37	7.60	7.28
60.03	9.55	9.56	9.52	9.57
75.01	10.70	10.72	10.60	10.77
100.02	11.85	11.68	11.55	11.74
200.11	12.23	12.30	12.34	12.29
273.16	12.08	12.09	12.25	12.02
299.99	11.99	11.99	12.19	11.90
Maximum deviation 1 (2)		0.22(0.50)	0.32(0.65)	0.20(0.43)
Average deviation 1 (2)		0.11(0.23)	0.19(0.48)	0.11(0.15)

situation for hydrogen and deuterium. It would be of interest to check this result for further physical quantities, e.g. transport coefficients.

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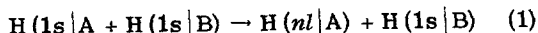
EXCITATION OF H-ATOMS BY FAST ATOM IMPACT

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Bates and Griffing [1] have investigated the excitation and ionization of ground state H-atoms by fast atom impact, using the Born approximation. They considered first the reaction



(A labels the target atom, and B the incident atom) to find the cross-section $\sigma(1s - nl; 1s - 1s)$ when the incident atom is unchanged. Secondly they found the total cross-section for exciting the target atom into the state nl , allowing for all transitions in the incident atom. This total cross-