Excluded volume effects in the hadron resonance gas

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Van der Waals Equation

$$\left[P + a\left(\frac{N}{V}\right)^2\right]\left[\frac{V}{N} - b\right] = kT$$

reproduces qualitative properties the isotherms of simple gases and liquids. There is no complete theoretical justification.

Equation of state

Connects pressure, temperature, and particle density

But does not provide full information about the state. The partition function is necessary!

The simplest nontrivial case - binary interaction

$$H_N = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i>j} W|\vec{r_i} - \vec{r_j}|$$

Canonical partition function

$$Z_C = \frac{1}{N!} \left(\frac{mkT}{2\pi\hbar^2} \right)^{3N/2} \int\limits_V d^3\vec{r_1} \cdots d^3\vec{r_N}\, e^{-\beta \sum\limits_{i>j} W_{ij}}$$

The Virial Expansion

The expansion of the thermodynamic quantities in powers of the density.

$$g(r) = e^{-\beta W(r)} - 1\,; \quad f = e^{\beta\mu}\left(\frac{mkT}{2\pi\hbar^2}\right)^{1/2}$$

Grand canonical partition function

$$Z_G = \sum_N \frac{f^N}{N!}\int_V d^3\vec{r_1}\cdots d^3\vec{r_N}\prod_{i>j}(1+g_{ij})$$

$$= e^{fV}\left[1 + Vf^2B_1 + \frac{1}{2}(Vf^2B_1)^2 + 2Vf^3B_1^2 + \frac{1}{3!}(Vf^2B_1)^3\cdots\right]$$

$$B_1 = \frac{1}{2}\int d^3\vec{r}g(r)\,; \quad B_2 = \frac{1}{6}\int d^3\vec{r_1}d^3\vec{r_2}g(r_1)g(r_2)g(|\vec{r_1}-\vec{r_2}|)$$

The Virial Expansion

Then

$$\frac{\mu}{kT} \approx \ln \frac{N\lambda_T^3}{V} - 2B_1 \frac{N}{V} - 3B_2 \left(\frac{N}{V}\right)^2$$

$$\lambda_T = \left(\frac{mkT}{2\pi\hbar^2}\right)^{1/2}$$

The free energy

$$F(T, V, N) = -NkT \left[\ln \frac{V}{N\lambda_T^3} + 1 + B_1 \frac{N}{V} + B_2 \left(\frac{N}{V}\right)^2 + \cdots\right]$$

The EoS

$$P = -\frac{\partial F}{\partial V} = kT\frac{N}{V} - B_1 kT \left(\frac{N}{V}\right)^2 - 2B_2 kT \left(\frac{N}{V}\right)^3 + \cdots$$

$$\approx kT\frac{N}{V}\left(1 + b\frac{N}{V}\right) - a\left(\frac{N}{V}\right)^2$$

Hadron resonance gas with excluded volume

Hadrons are not point particles, and repulsive interactions can be implemented via an excluded-volume approximation whereby the volume available for the hadrons to move in is reduced by the volume they occupy.

- R. Hagedorn and J. Rafelski, Phys. Lett. **B 97**, 136 (1980).
- R. Hagedorn, Z. Phys. C: Part. Fields **17**, 265 (1983).
- M. I. Gorenstein, V. K. Petrov, and G. M. Zinovjev, Phys. Lett. **B 106**, 327 (1981).

Excluded volume model I

The volume excluded by a hadron is proportional to its energy with the constant of proportionality ϵ_0 (dimensions of energy per unit volume) being the same for all species. It is also assumed that hadrons are deformable so that there is no limitation by a packing factor as there would be for rigid spheres.

$$V_{ex} = \frac{1}{\epsilon_0}\left(\sum_{j=1}^{N_1} E_1(p_j) + \cdots + \sum_{j=1}^{N_n} E_n(p_j)\right)$$

The pressure in the exclude volume approximation is expressed in terms of the point particle pressure

$$P_{ex}(T,\mu) = \frac{P_{pt}(T_*,\mu_*)}{1 - P_{pt}(T_*,\mu_*)/\epsilon_0}\,;$$

Excluded volume model I

Also

$$T = \frac{T_*}{1 - P_{pt}(T_*, \mu_*)/\epsilon_0}\,; \quad \mu = \frac{\mu_*}{1 - P_{pt}(T_*, \mu_*)/\epsilon_0}$$

The model is solved by picking specific values for T_* and μ_*, calculating the point particle properties with these values, and using them to calculate the true T and μ and thermodynamic properties in the excluded-volume approximation. The chemical potential for each species has the same multiplicative factor.

Excluded volume model II

A hadron species α has volume v_α. The chemical potential for species α is shifted by the amount

$$\mu_\alpha \to \mu_\alpha - v_\alpha P_{ex}(T, \mu)$$

Volumes v_α are chosen to be proportional to the mass; $v_\alpha = m_\alpha/\epsilon_0$ where ϵ_0 is a constant

Excluded volume in the box

1-dimensional one-particle partition function

$$\sum_{n=1}^{\infty} \exp\left(-a\, n^2\right) = \frac{1}{2}\left(\vartheta_3\left(0, e^{-a}\right) - 1\right); \qquad a = \frac{\pi^2}{2mTL^2}$$

Point like particle of mass m in the impenetrable well of size L

$$Z_1(T, L, V) = \frac{1}{2}\left(\vartheta_3\left(0, e^{-\frac{\pi^2}{2mTL^2}}\right) - 1\right);$$

Particle has a size d.
Assumption: well becomes narrower, of size $L - d$. For N particles the well shrinks to the effective size $L - N\,d$.

$$Z_N(T, L, N, d, V) = \frac{1}{2}\left[\vartheta_3\left(0, \exp\left(-\frac{\pi^2}{2mT(L - Nd)^2}\right)\right) - 1\right]$$

3-dimensional partition function

$$\mathcal{Z}_1(\mathrm{a}) = \frac{1}{8}\left(\vartheta_3\left(0, e^{-a}\right) - 1\right)^3$$

δ - volume occupied by a particle
For N particle system

$$a = \frac{\pi^2}{2Tm(V - \delta N)^{2/3}}$$

Partition function

$$\mathcal{Z}_N(T, V, \delta) = \frac{1}{8N!}\left[\vartheta_3\left(0, e^{-\frac{\pi^2}{2Tm(V-N\delta)^{2/3}}}\right) - 1\right]^{3N} =$$

$$\frac{1}{N!}\left[\sum_{n=1}^{\infty} \exp\left(-\frac{\pi^2 n^2}{2Tm(V - \delta N)^{2/3}}\right)\right]^{3N}$$

Equation of state

Pressure is given by

$$P = k_B T \frac{\partial}{\partial V} \log \mathcal{Z}_N(T, V) = -\frac{\partial \mathcal{F}(T, V, N)}{\partial V} =$$

$$k_B T N \frac{\partial}{\partial V} \log \mathcal{Z}_1(T, V - N\delta)$$

Poisson Sum Formula - quite general, just for partition function

$$\sum_{n=-\infty}^{\infty} f(\alpha n) = \frac{\sqrt{2\pi}}{\alpha} \sum_{m=-\infty}^{\infty} F\left(\frac{2m\pi}{\alpha}\right)$$

where F is the Fourier transform of f

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{ikx}\, dx$$

Pressure

Poisson sum formula in the box

$$2\sum_{n=1}^{\infty} \exp\left(-a\, n^2\right) = \sqrt{\frac{\pi}{a}} - 1 +$$

$$2\sqrt{\frac{\pi}{a}}\sum_{n=1}^{\infty} \exp\left(-\frac{\pi^2 n^2}{a}\right)$$

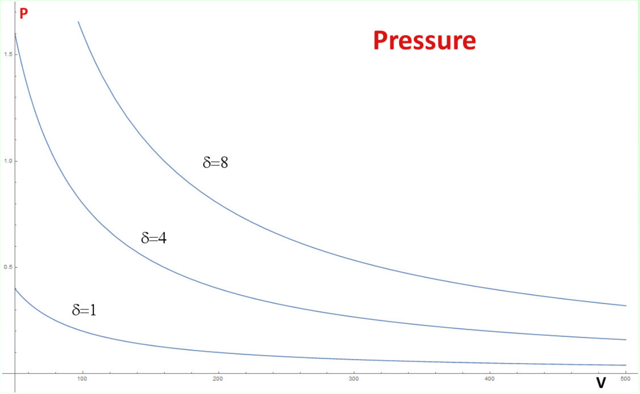
$a \approx 0$

$$\sum_{n=1}^{\infty} \exp\left(-a\, n^2\right) \approx \frac{1}{2}\sqrt{\frac{\pi}{a}}$$

This leads to

$$P = \frac{NT}{V - \delta N} = \frac{NT}{V}\left(1 + \frac{\delta N}{V} + \frac{\delta^2 N^2}{V^2} + \cdots\right)$$

Pressure



Pressure

$a > 4$

$$\sum_{n=1}^{\infty} \exp\left(-a\, n^2\right) \approx e^{-a}$$

$$P \approx N \, \frac{\pi^2}{m(V - \delta N)^{5/3}}$$

Standard limits: T large or small are replaced by limits $T(V - \delta N)^{2/3}$ large or small.
More possibilities, particle density factor becomes as important as a temperature.