Kinetic coefficients in dense media

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EQUILIBRIUM ENERGY DISTRIBUTION FUNCTION

- In condition of "seldom" collisions
- This is followed by a sharp temperature dependence of the rate constants of barrier and adiabatic processes

- $f(\varepsilon) \sim \exp(-\varepsilon/T)$ – Maxwellian function
- $k \sim \exp[-\Delta E/T]$ (Arrenius) for barrier processes
- $k \sim \exp[-(To/T)1/3]$ (Landau-Teller) – for adiabatic processes

AS THE ELASTIC COLLISION FREQUENCY RISES THE QUANTUM UNCERTAINTY OF ENERGY INREASES

- $\Delta\varepsilon \sim \hbar\nu_{el} = \hbar N k_{el}$
- N is the density *of the medium*
- k_{el} is the elastic scattering rate constant
- The quantum corrections are notable at the condition
  - $\Delta\varepsilon \sim T$
  - or
  - $N \geq T/\hbar k_{el}$,
- i.e. at elevated pressures and moderate temperature

Momenta distribution function of particles with taking account the quantum correction

$$f(E,\mathbf{p}) = n(E)\frac{\gamma(E,\mathbf{p})}{\pi\left[\left(E-\varepsilon_{\mathbf{p}}-\Delta(E,\mathbf{p})\right)^2+\gamma^2(E,\mathbf{p})\right]} \equiv n(E)\delta_\gamma(E-\varepsilon_{\mathbf{p}})$$

- $n(E)$ is the population numbers,
- $\varepsilon_p = p^2/2m$ is the kinetic energy,
- $\gamma \sim \hbar\nu$ is the collision width,
- ν is the collision frequency,
- Δ is the density shift of the energy

Momenta distribution function of particles with taking account the quantum correction

- In particular, for electrons in equilibrium state

$$n(E)=\frac{1}{e^{\frac{E-\mu}{T}}+1},$$

Momenta distribution function of particles with quantum correction

- The momenta distribution function of particles is the result of integration of $f(E,\mathbf{p})$ over the energies:

$$f(\mathbf{p}) = \int dE f(E,\mathbf{p})$$

Momenta distribution function of particles in a rarefied gas

- In this case the collision width γ of the spectral function $\delta_\gamma(E - \varepsilon_p)$ is a negligible i. e. the function is close to the δ–function. This results in:

$$f(\mathbf{p}) = e^{\frac{\mu}{T}} e^{-\frac{\varepsilon_p}{T}}$$

- which is the maxwellian momenta distribution function of particles

Momenta distribution function (MDF) of particles in the case of a gas of a specific density

- MDF in a high momenta region $\varepsilon_{\mathbf{p}} >> \{T, \gamma, \Delta\}$ along with the resonant, maxwellian item contains also a power-like correction

$$f(\mathbf{p}) = \frac{1}{\pi \varepsilon_p^2} \int_{-\infty}^{\infty} n(E)\gamma(E,\mathbf{p})dE$$

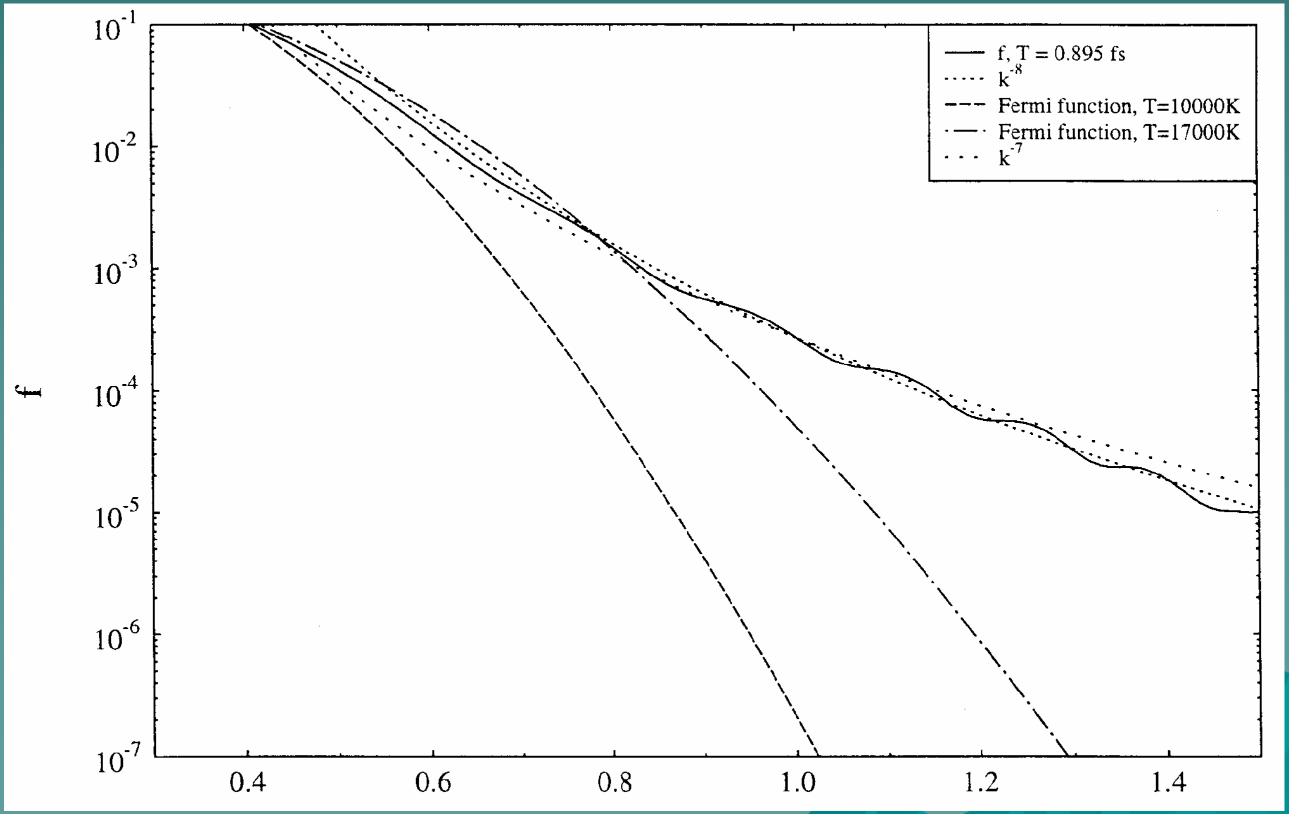
Asimptotic representation for *f*(**p**) within the frame of Lorentz gas model

$$f(p) = e^{\frac{\mu}{T}}\left(e^{-\frac{\varepsilon_p}{T}} + \frac{\hbar N T \sigma_t(p)}{2\pi\varepsilon_p^2}\sqrt{\frac{\pi T}{2m}} \right)$$

- Specifically for the electronic gas $\sigma_t \sim (\varepsilon_p)^{-2}$ so that the momenta dependence of the quantum correction has the form $\sim p^{-8}$

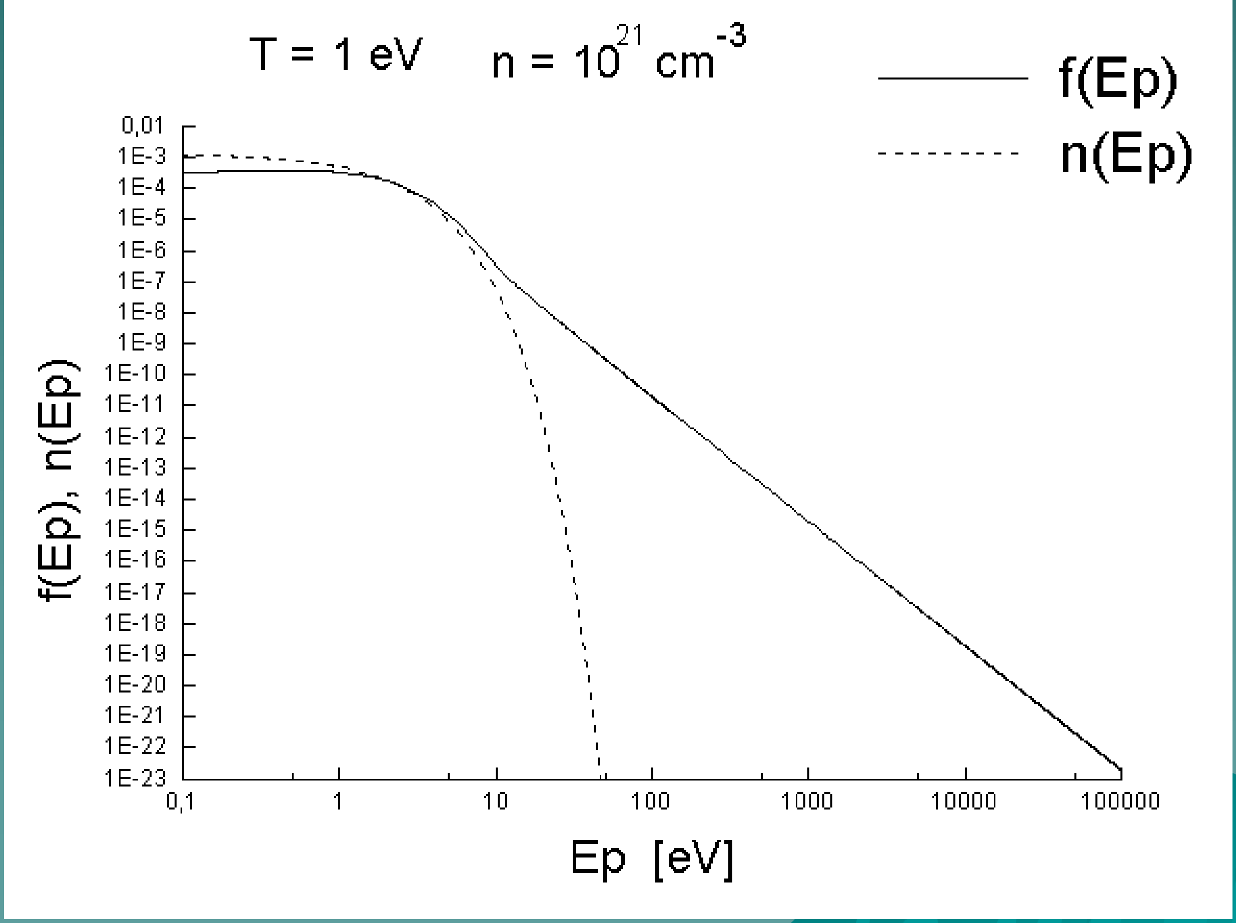
High density plasma

In Rostock university (BRD, M.Bonitz, D.Semkat) have developed numerical codes for computing distribution function, using the Kadanoff-Baym equations



High density plasma

Our calculations give the same momenta distribution of electrons for the same conditions



High density plasma

The reaction rate constant for the Lorentz gas model expression with taking into account quantum effects in high density plasmas has the following form:

$$n_e k_{ij} \sim A\int dE d\vec{p} d\vec{p}\,' n(E)\left(1-n(E\mp I)\right)\left|f_{ij}\left(\vec{p},\vec{p}\,',E\right)\right|^2 \times$$

$$\times\,\delta_\gamma(E-\varepsilon_p)\,\delta_\gamma(E\mp I-\varepsilon_{p'})$$

Here «-» or «+» correspond to the processes with the absorption or release of energy amount I;
f_{ij} is the scattering amplitude for the process *i–j*.

VT relaxation of diatomic molecules

The probability of a VT transition is expresse
through the Massey parameter *Me*

$P_{VT}(v) \sim \exp(-cMe) = \exp(-cb\omega/v) << 1.$

Here

$Me \sim b\omega/v \sim (b\mu^{1/2})/(m^{1/2}T^{1/2}) >> 1$, if $\mu/m \sim$

ω is the molecular vibration frequency,

b is the range of action of inter-molecular forces

v is the collision velocity

The relative contribution of the quantum correction into the VT relaxation rate constant

- The total VT relaxation rate constant

$$k_{VT} = k_0 \left[e^{-3\left(\frac{\theta'}{T}\right)^{1/3}} + C_t \right].$$

- The quantum correction

$$C_t = \frac{1}{4}\left(\frac{T}{\theta}\right)^{1/3}\left(\frac{T}{\theta}\right)^{1/2} e^{-\frac{\theta}{2T}} \frac{\Gamma(2+2k)}{\pi 2^{2+2k}} \sqrt{\frac{3}{4}} \frac{\hbar N \sigma_p^k v_T}{2\theta}$$

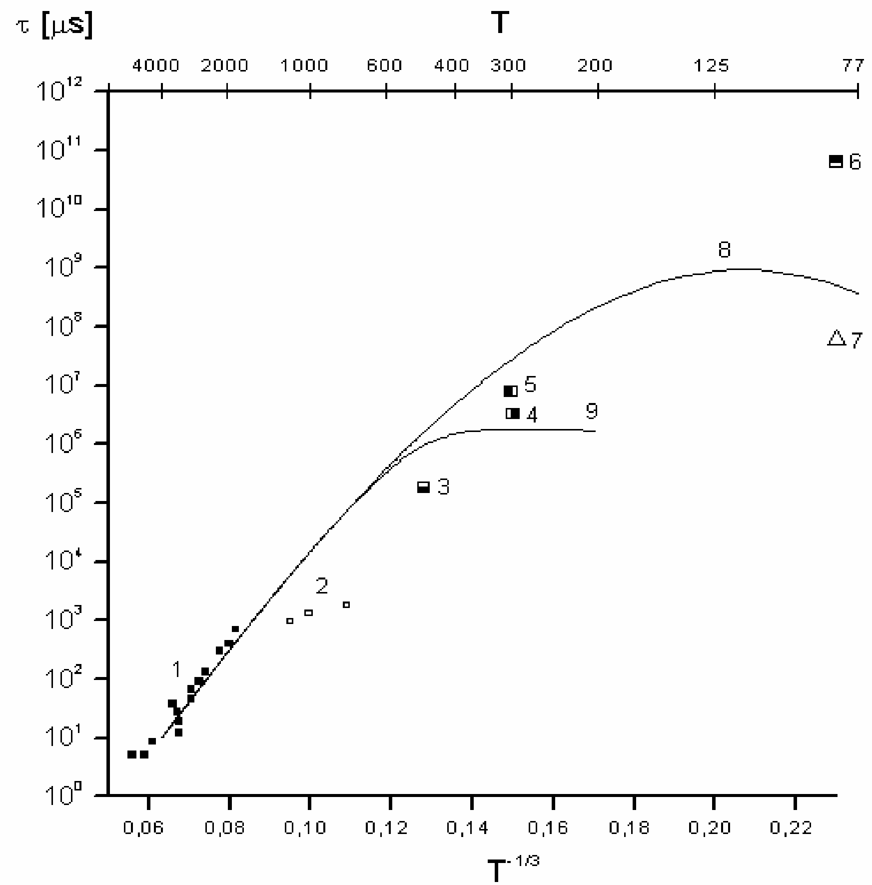
The relative contribution of the quantum correction into the VT relaxation rate constant

- Here $$\theta' = \frac{m}{2}\left(\frac{\pi\omega}{a}\right)^2 >> T$$ is the characteristic temperature; $\theta = \hbar\omega$.
- For nitrogen the contribution of the correction is

$$\frac{I_2}{I_1} \approx 2.9 \cdot 10^{-17} \cdot T^{4/3}\left(\frac{N}{N_L}\right) e^{-\frac{1690}{T}} e^{\frac{277.8}{T^{1/3}}}$$

Comparison with experiment for N_2

- 1-7 are the experimental data;
- 8 is calculation by the Landau-Teller model
- 9 is the temperature dependence of k_{VT} with taking account the quantum correction



Thermonuclear fusion reaction

- d + d → t + p
- In this case the reaction proceeds through the under-barrier tunneling and the velocity dependence of the cross section has the following form:

$$\sigma_1(\varepsilon_p) = \frac{S(\varepsilon_p)}{\varepsilon_p} \exp\{-2\pi\eta(\varepsilon_p)\}$$

Thermonuclear fusion reaction

- Here

$$\eta(\varepsilon_p) = \frac{Z_1 Z_2 e^2}{\hbar v}$$ is the Gamov factor;

- $S(\varepsilon_p)$ is the astrophysical factor
- The correction is calculated by the averaging the cross section over the MDF

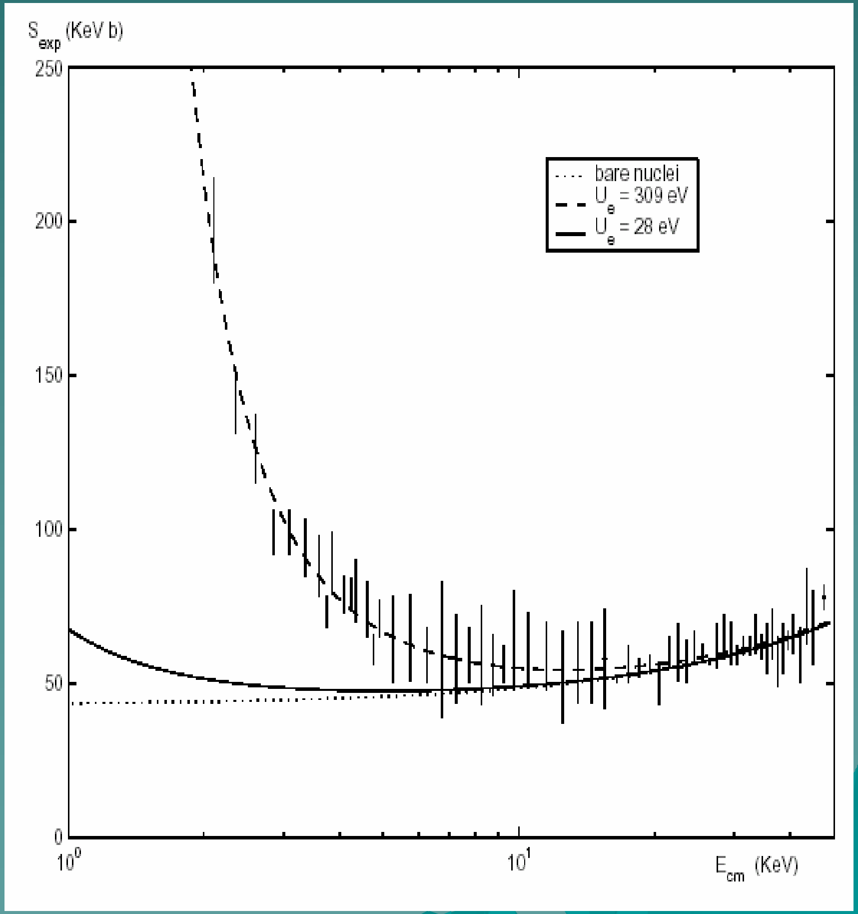
Momenta distribution function of particles in dd experiment

$$f(p)=\frac{1}{(2\pi mT)^{3/2}}\left[e^{-\frac{\varepsilon_p}{T}}+\frac{\sqrt{\pi}N\hbar T}{(\varepsilon_p)^4}\sqrt{\frac{2T}{m_a}}\right],$$

- The quantum correction is represented by the second item

Energy dependence of the astrophysical factor of dd-reaction

- The theoretical dependences have been obtained with taking account the quantum correction and the effect of screening of deuterium nuclei with free electrons of the metal target



Monte-Carlo simulations

The Monte Carlo simulation had been carried out for real particles fusion reactions rates calculation.

$$n_a n_b \langle \sigma v \rangle = C \int_{-\infty}^{\infty} dE_a \int \mathbf{dp}_a \int_{-\infty}^{\infty} dE_b \int \mathbf{dp}_b \int_{-\infty}^{\infty} d\omega \int \mathbf{dq} \;\; n(E_a)\, \delta\gamma_a (E_a - \varepsilon_a) \times$$
$$\left(1 - n(E_a + Q_a - \omega)\right) \delta\gamma'_a \left(E_a + Q_a - \omega - \varepsilon_{p_a - q}\right) \cdot n(E_b) \;\; \cdot$$
$$\delta\gamma_b (E_b - \varepsilon_b) \left(1 - n(E_b + \omega + Q_b)\right) \, \delta\gamma'_b \left(E_b + \omega + Q_b - \varepsilon_{p_b + q}\right) \cdot |f|^2$$

$$\gamma_a (E_a, \varepsilon_a) = \frac{\hbar}{2} \sum_c N_c \sqrt{\frac{2E_a}{m_{ac}}} \left\langle \frac{4\pi \;\; e^4 Z_a^2 Z_c^2}{(\varepsilon_{ac} + E_a + E_{De})^2 - 4E_a \varepsilon_{ac}} \right\rangle_c$$

$$\varepsilon_a = \frac{p^2}{2m_a}$$

$$E_{De} = \frac{\hbar^2}{2m_e R_{De}^2}$$

C is the fitting constant

The relative contribution of the quantum correction into the rate constant of dd reaction

Energy, keV	K_{qu}/k_{tot}, %
15	<1
5	3
2	8,3
1,8	10,7
1,5	30
1,2	95,4
1	99,7

Simplifications of the expression for the reaction rate constant

In the case of mono-energy beam:

$$n_a K' = C\int_0^\infty dE_a \int d\vec{p}_a \int n(E_a)\, a(E_a - \varepsilon_a, \varepsilon_a)\sqrt{\frac{2\varepsilon_p}{\mu}}\,\sigma(\varepsilon_p)$$

In the case of ideal plasma:

$$n_a K_2 = C\int_0^\infty dE_a \int d\vec{p}_a \int n(E_a)\,\delta(E_a - \varepsilon_a)\sqrt{\frac{2\varepsilon_p}{\mu}}\,\sigma(\varepsilon_p) \sim \int_0^\infty d\varepsilon_a\, n(\varepsilon_a)\,\varepsilon_p\,\sigma(\varepsilon_p)$$

Quantum correction in the case of non-Maxwellian distribution function:

The momenta distribution function asymptotically contains the power-like tail:

$$f(\varepsilon) = C'\int_0^\infty dE_a n(E_a) a(E_a - \varepsilon_a, \varepsilon_a) \sim \exp\left\{-\frac{\varepsilon_a}{T}\right\} + \frac{C_a(T)}{\varepsilon_p^4}$$

Using this expression, it is possible to calculate the reaction rate for non-Maxwellian distribution function:

$$K_3 = C_3\int_0^\infty d\varepsilon_a f(\varepsilon_a)\sqrt{\frac{2\varepsilon_a\varepsilon_p}{\mu}}\sigma(\varepsilon_p)$$

Conclusions

- The quantum power-like tails of the MDF accelerate the processes
- VT relaxation in molecular gases,
- Thermonuclear fusion,
- High pressure chemical reactions.
- A new approach to calculation of the reaction rate constants has been proposed