Scientific-Coordination Workshop on
Non-Ideal Plasma Physics

High accuracy molecular dynamics simulations of electron-ion temperature relaxation in nonideal plasmas

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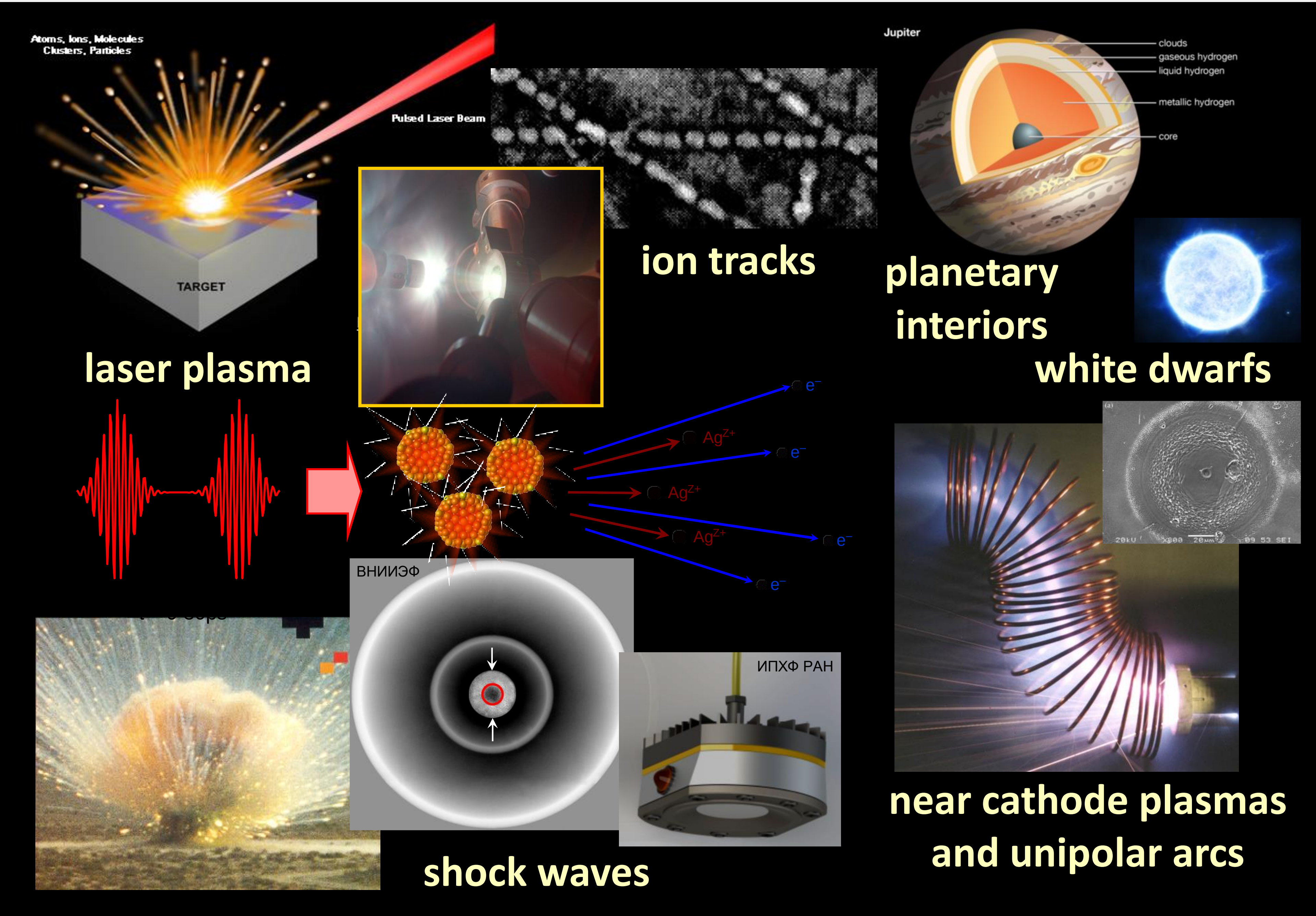
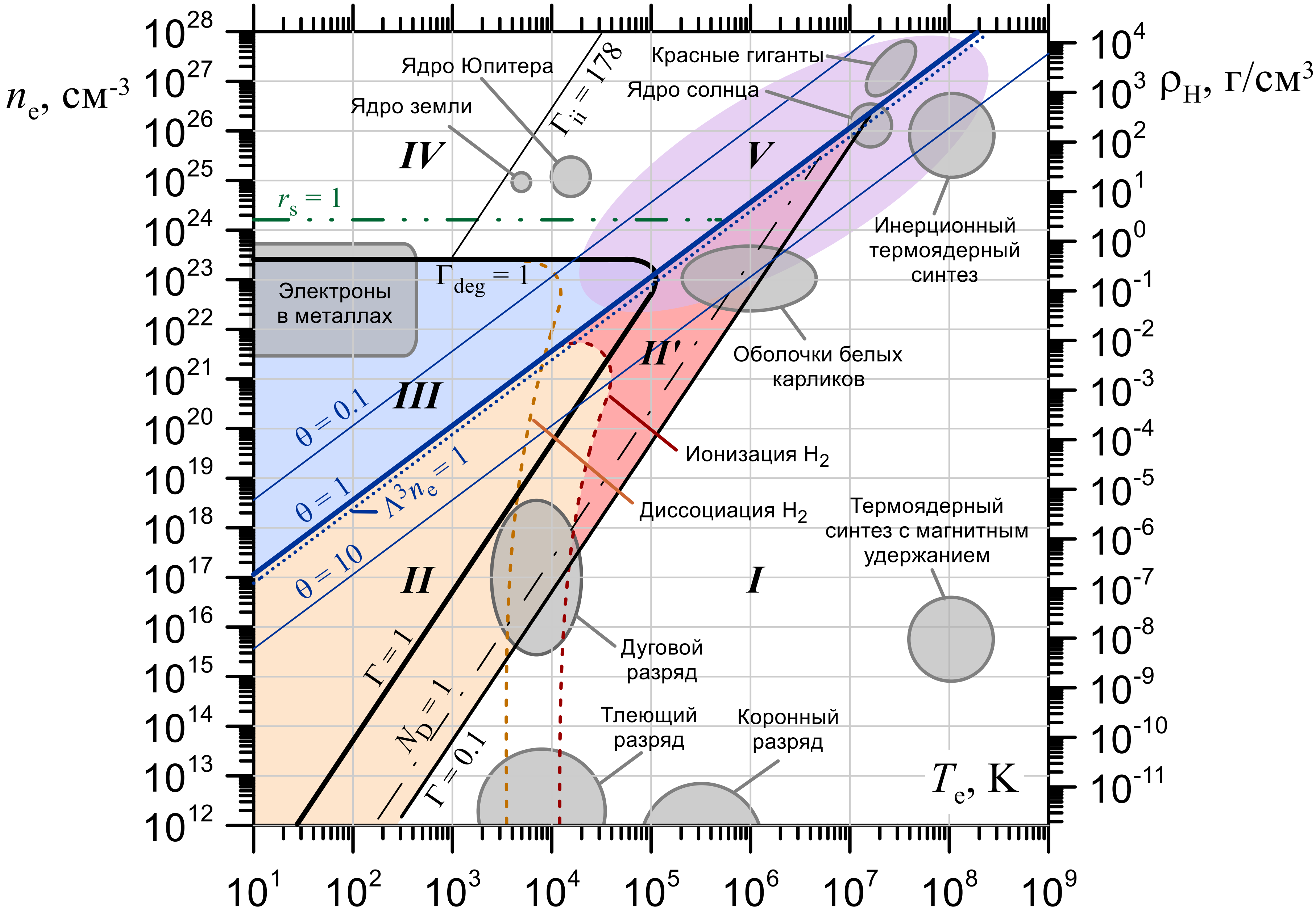
Nonideal plasmas and warm dense matter



Temperature-density diagram



Simulations of nonideal plasmas and WDM

Physical model

Plasma is considered as a mixture of electrons and ions that can form atoms and molecules

Chemical model

Plasma is considered as a mixture of ‘reacting’ electrons, ions, atoms, molecules, etc

- **Classical molecular dynamics (MD)**
- **Wave packet molecular dynamics (WPMD)**
- **Quantum molecular dynamics based on the density functional approach (QMD/DFT)**
- **Path integral Monte-Carlo/molecular dynamics (PIMC/PIMD)**
- **Classical Monte-Carlo (MC)**

Exchange-correlation effects in WPMD

Original method of WPMD

Hartree approximation for the many-electron wave function

Antisymmetrization of wave function for electrons with the same spin (AWPMD)

The method of unrestricted Hartree-Fock

Combined WPMD-DFT approach

Exchange-correlation effects are taken into account using the density functional approach (similar to DFT)

Electron force fied (eFF)

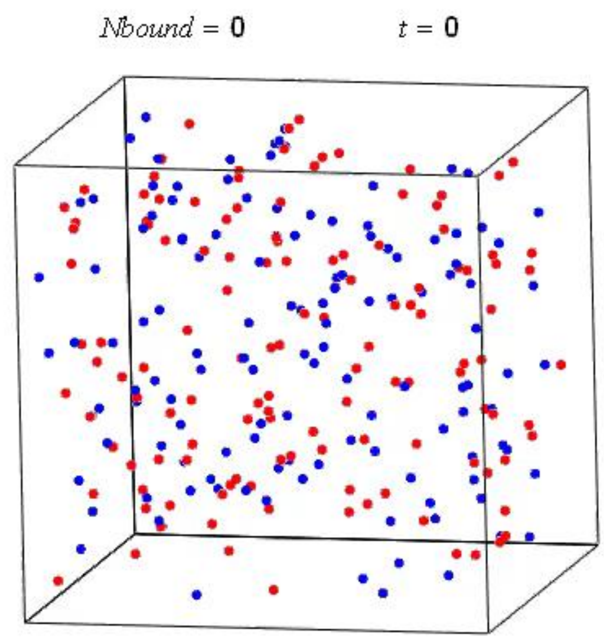
Pseudopotentials for election-electron and electron-ion interactions that account for symmetry effects

Classical molecular dynamics

Newton's equations of motion

$$\begin{cases} \vec{r}_k''(t) = \dfrac{1}{m_k}\dfrac{\partial V(\vec{r}_1,\ldots,\vec{r}_N)}{\partial \vec{r}_k}, \quad k = \overline{1,N}, \\ \vec{r}(0) = \vec{r}_0, \quad \vec{v}(0) = \vec{v}_0, \end{cases}$$

$$V(\vec{r}_1,\ldots,\vec{r}_N) = \sum_k V^{ext}(t,\vec{v}_k,\vec{r}_k) + \sum_{i<j} V(|\vec{r}_i - \vec{r}_j|)$$

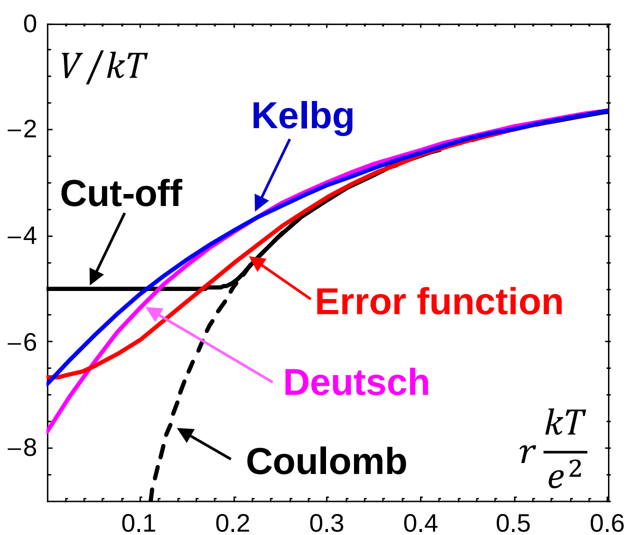


● – electron ● – ion

Electron-ion interaction pseudopotentials:

$$V_{\text{Kelbg}}(r) = \frac{1}{r}\left[F\left(\frac{r}{\lambda_{ei}}\right) + r\frac{kT}{e^2}\tilde{A}_{ei}\left(\frac{e^2}{kT\lambda_{ei}}\right)\exp\left(-\left(\frac{r}{\lambda_{ei}}\right)^2\right)\right]$$

$$F(x) = 1 - \exp(-x^2) + \sqrt{\pi}x(1 - \operatorname{erf}(x)) \qquad \lambda_{ie} = \hbar/\sqrt{2mkT}$$

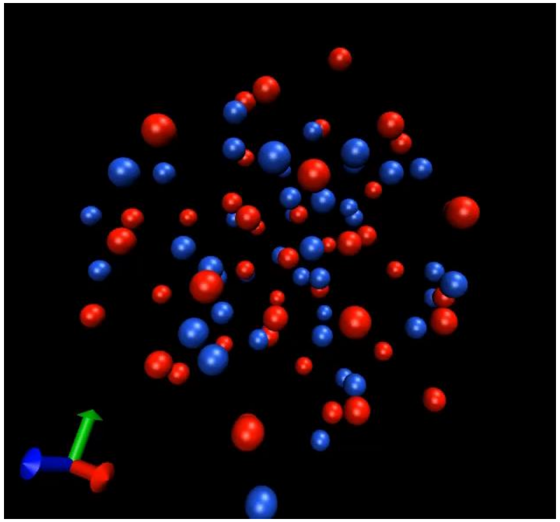


$$V_{\text{Deutsch}}(r) = \frac{1}{r}\left[1 - \exp\left(-\frac{r}{\lambda_{ei}}\right)\right]$$

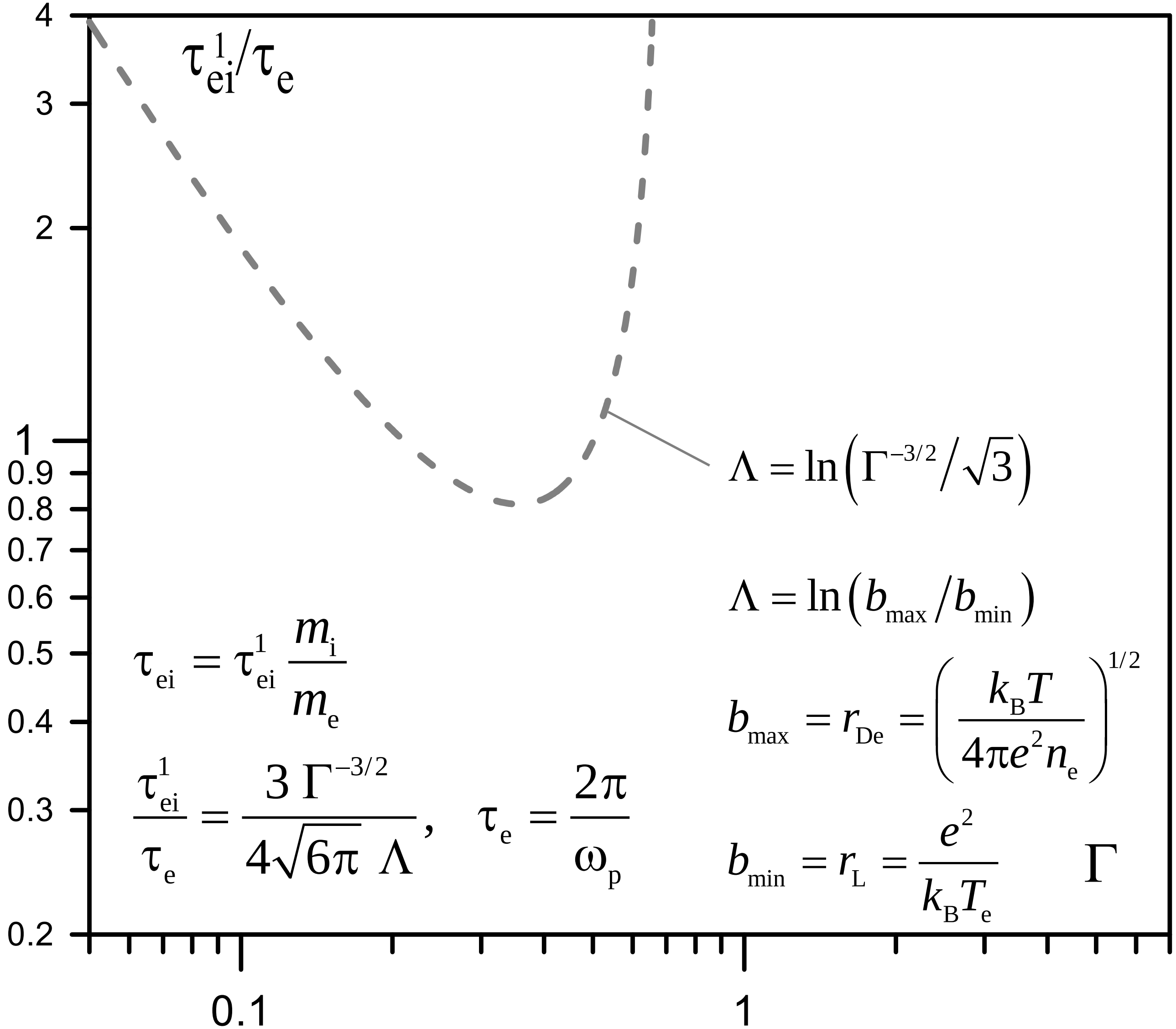
$$V_{\text{Erf}}(r) = \frac{1}{r}\operatorname{erf}\left(-\frac{r}{\lambda_{ei}}\right)$$

$$V_{\text{Cutoff}}(r) = \begin{cases} \dfrac{1}{r}, & r > \dfrac{1}{\varepsilon}; \\ -\varepsilon, & r \le \dfrac{1}{\varepsilon} \end{cases}$$

$$V_{\text{Coulomb}}(r) = \frac{1}{r}$$



Electron-ion relaxation time vs plasma nonideality



$$\Lambda = \ln\left(\Gamma^{-3/2}/\sqrt{3}\right)$$

$$\Lambda = \ln\left(b_{max}/b_{min}\right)$$

$$\tau_{ei} = \tau^1_{ei}\frac{m_i}{m_e}$$

$$b_{max} = r_{De} = \left(\frac{k_B T}{4\pi e^2 n_e}\right)^{1/2}$$

$$\frac{\tau^1_{ei}}{\tau_e} = \frac{3\,\Gamma^{-3/2}}{4\sqrt{6\pi}\ \Lambda}, \quad \tau_e = \frac{2\pi}{\omega_p}$$

$$b_{min} = r_L = \frac{e^2}{k_B T_e} \qquad \Gamma$$

$$\Gamma = \left(\frac{4\pi n_e}{3}\right)^{1/3}\frac{e^2}{k_B T_e}$$

$$\omega_p = \left(\frac{4\pi n_e e^2}{m_e}\right)^{1/2}$$

$$\tau_{ei} = \frac{3 m_i m_e}{8\sqrt{2\pi}\, n_i Z^2 e^4 \Lambda}\left(\frac{k_B T_e}{m_e}\right)^{3/2}$$

1. L. P. Pitaevskii and E. M. Lifshitz. Physical Kinetics, Vol. 10. Butterworth-Heinemann, Oxford, 2012.
2. L. Spitzer. Physics of Fully Ionized Gases. John Wiley & Sons, New York, 1962.

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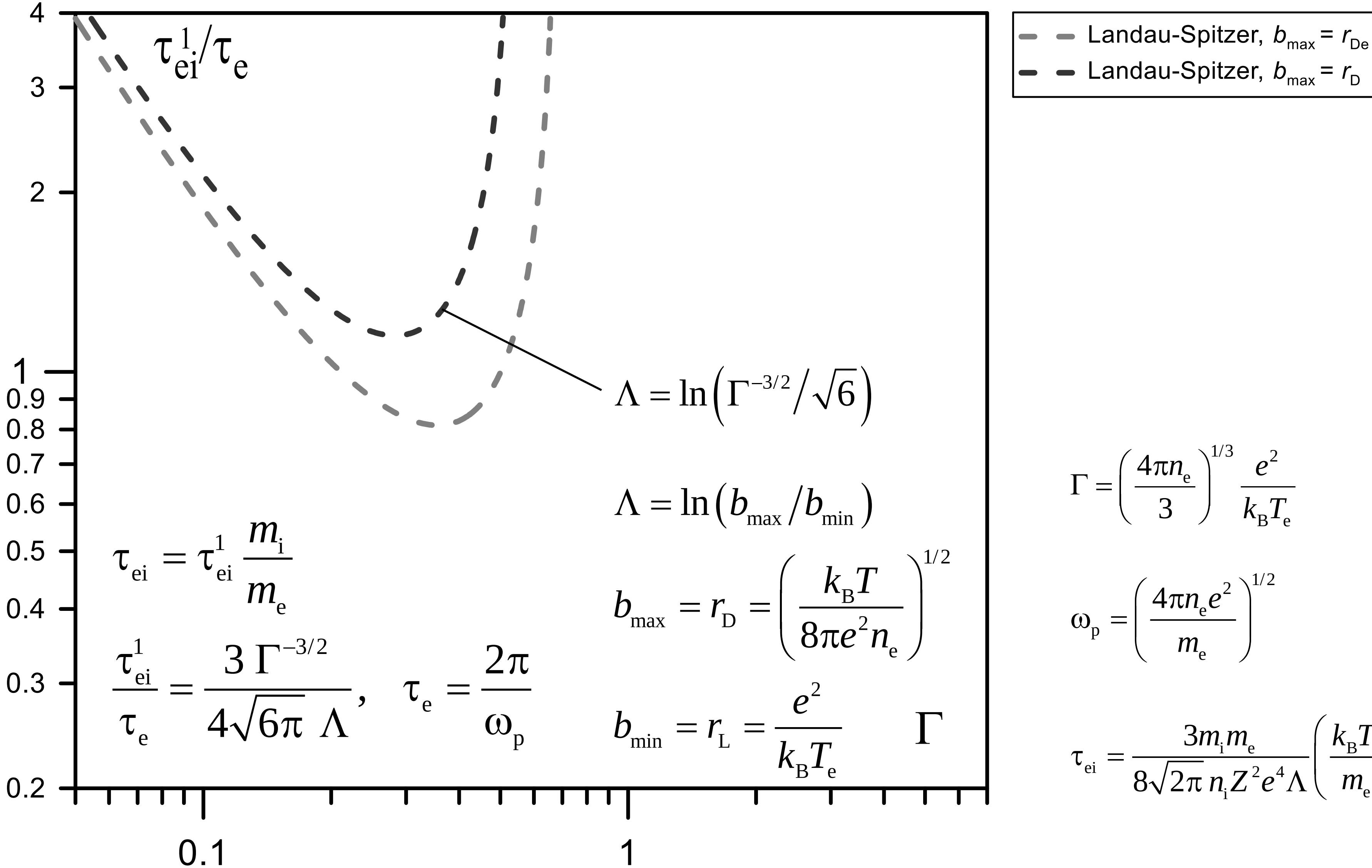

$$\Lambda = \ln\left(\Gamma^{-3/2}/\sqrt{6}\right)$$

$$\Lambda = \ln\left(b_{max}/b_{min}\right)$$

$$b_{max} = r_D = \left(\frac{k_B T}{8\pi e^2 n_e}\right)^{1/2}$$

$$b_{min} = r_L = \frac{e^2}{k_B T_e}$$

$$\tau_{ei} = \tau_{ei}^1 \frac{m_i}{m_e}$$

$$\frac{\tau_{ei}^1}{\tau_e} = \frac{3\,\Gamma^{-3/2}}{4\sqrt{6\pi}\;\Lambda}, \quad \tau_e = \frac{2\pi}{\omega_p}$$

$$\Gamma = \left(\frac{4\pi n_e}{3}\right)^{1/3} \frac{e^2}{k_B T_e}$$

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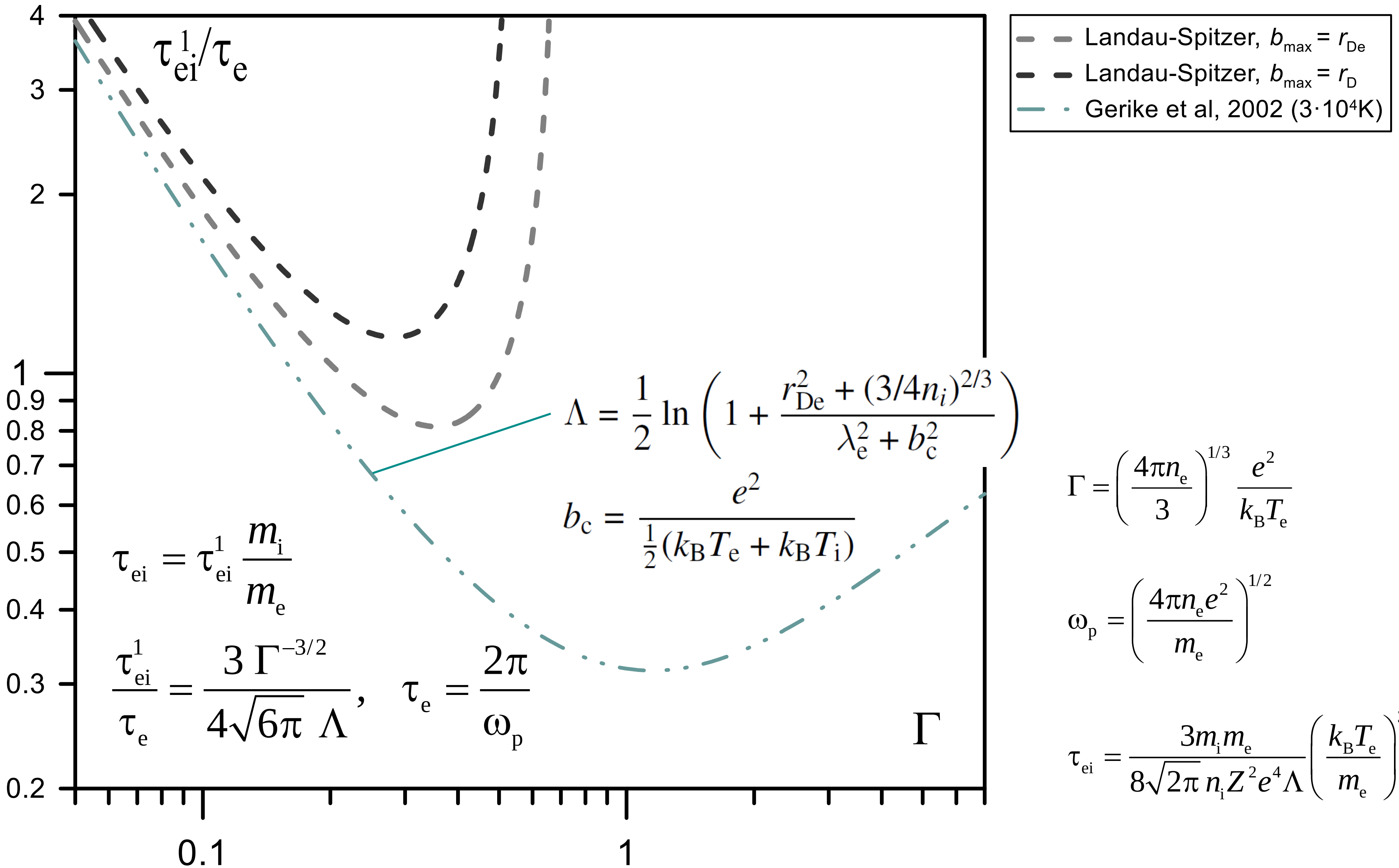

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D. O. Gericke, M. S. Murillo, M. Schlanges. // Phys. Rev. E. 2002. V. 65, no. 3. P. 036418.

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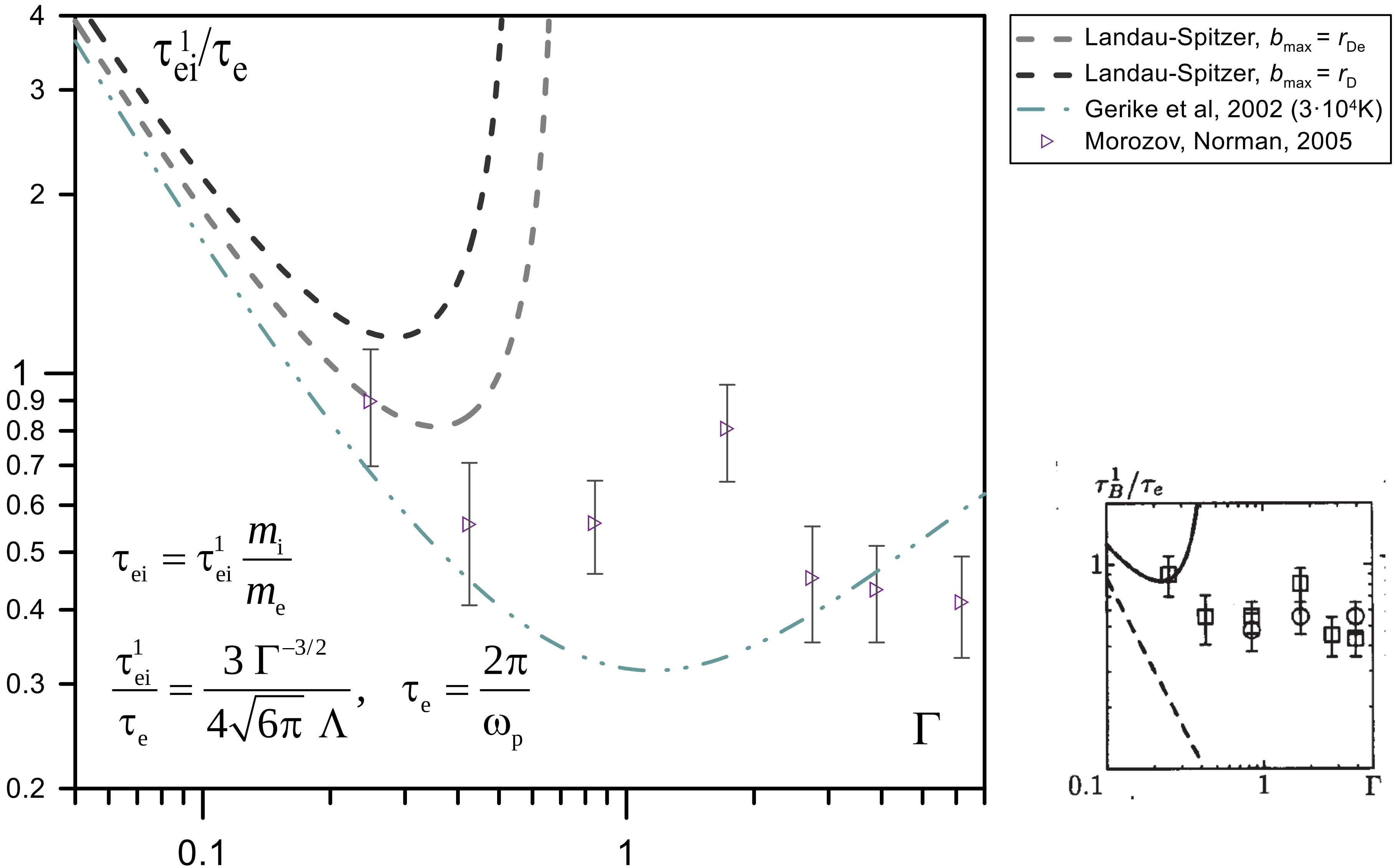

Morozov I.V., Norman G.E. // J. Exp. Theor. Phys. 2005. V. 100. No. 2. P. 370-384.

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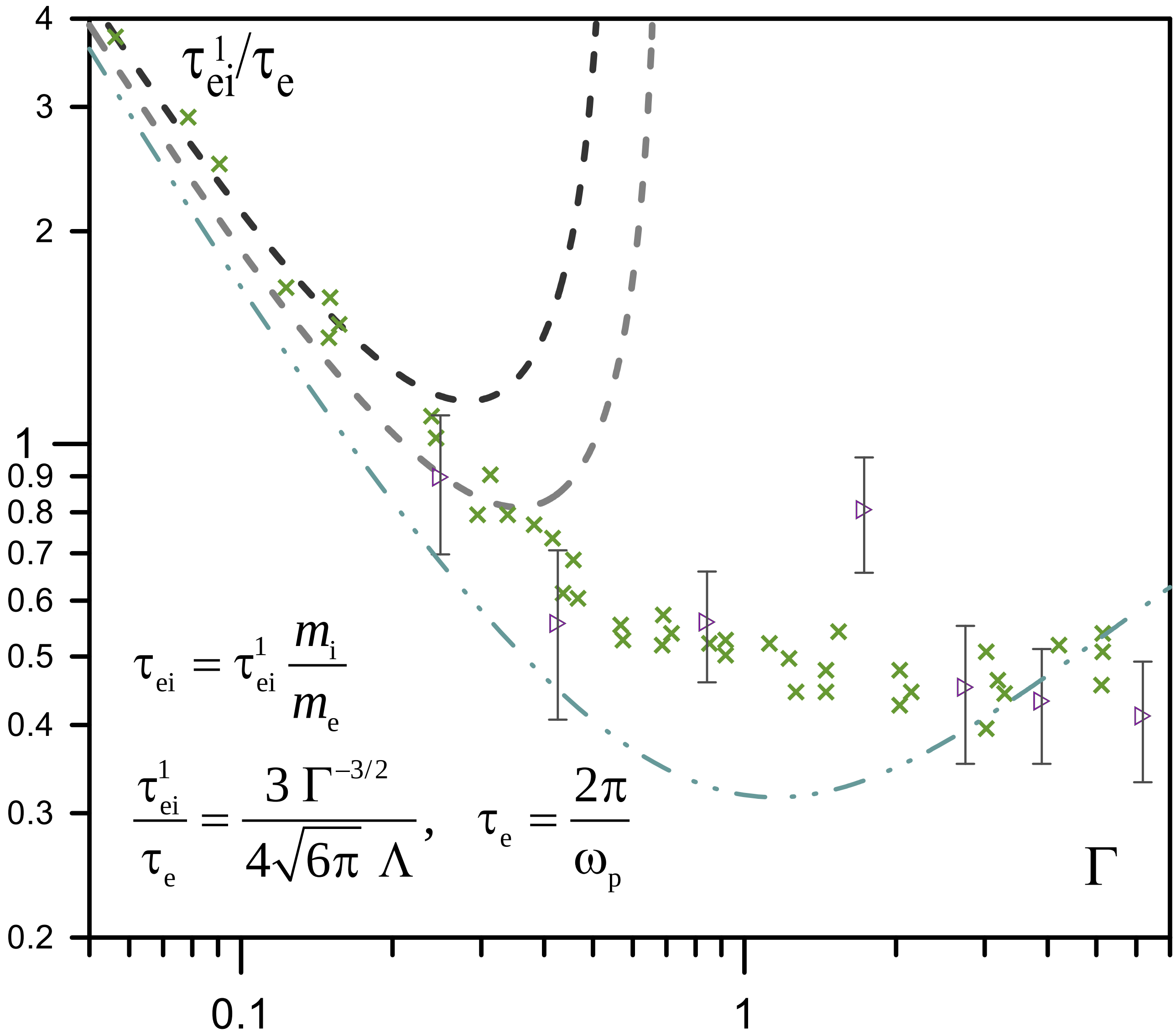

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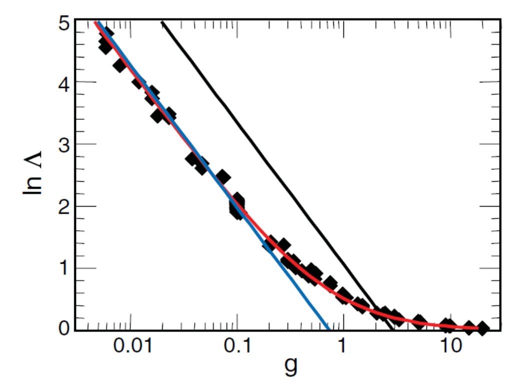
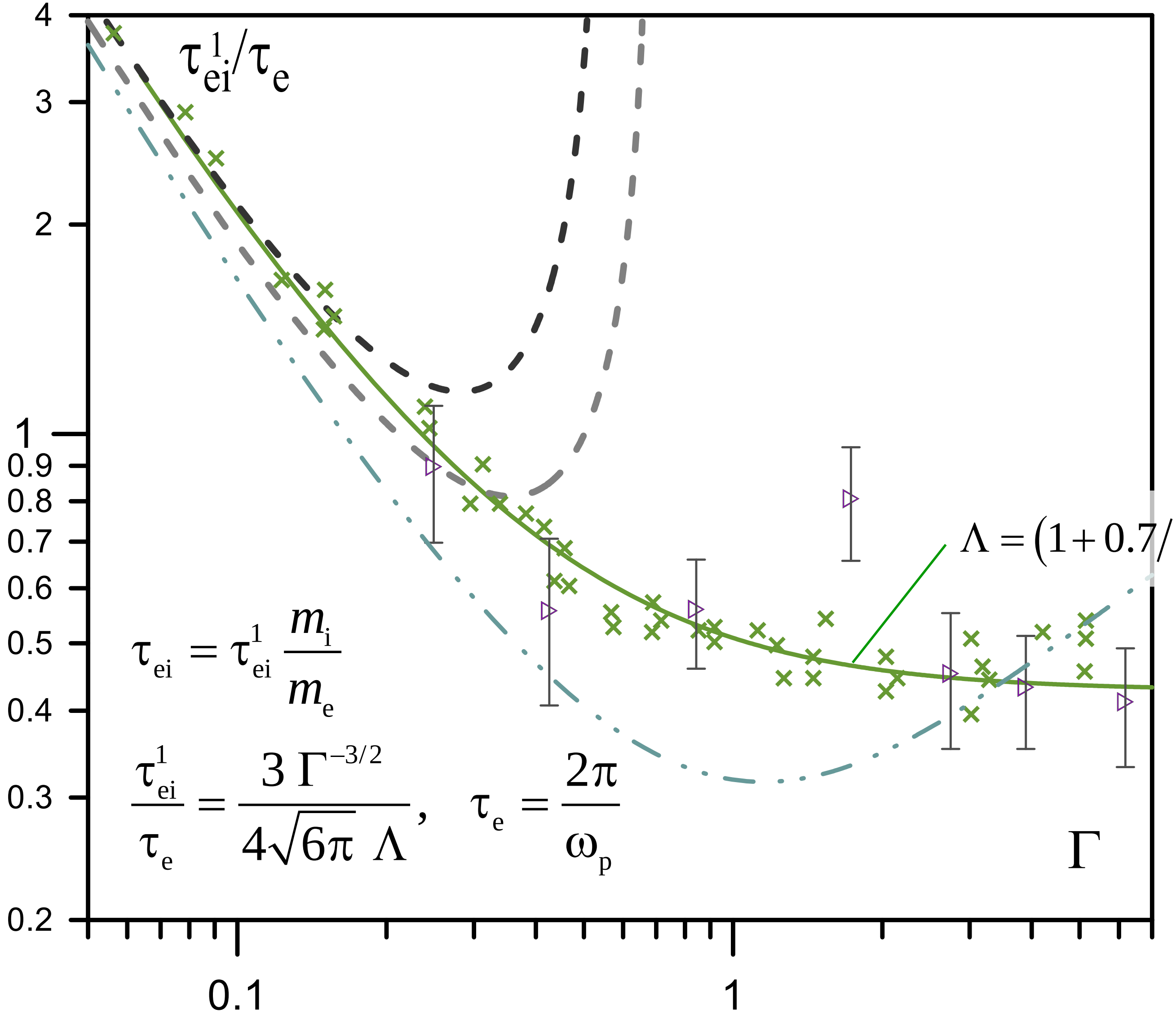


FIG. 3 (color). Coulomb log vs plasma parameter. The diamonds are from MD simulations, while the black line is the Spitzer ($C = 3$) result, the blue line is the KA and BPS theories, and the red line is a numerical fit [Eq. (15)] to the data.

Dimonte G., Daligault J. // Phys. Rev. Lett. 2008. V. 101, no. 13. P. 135001.

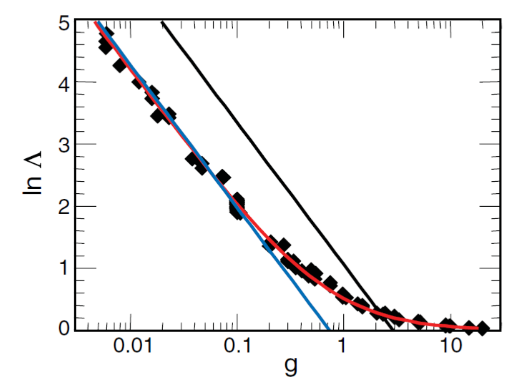
Electron-ion relaxation time vs plasma nonideality



$$\Lambda = (1 + 0.7/g) = \ln\left(1 + 0.7\Gamma^{-3/2}/\sqrt{3}\right)$$

$$\tau_{ei} = \tau_{ei}^1 \frac{m_i}{m_e}$$

$$\frac{\tau_{ei}^1}{\tau_e} = \frac{3\,\Gamma^{-3/2}}{4\sqrt{6\pi}\;\Lambda}, \quad \tau_e = \frac{2\pi}{\omega_p}$$



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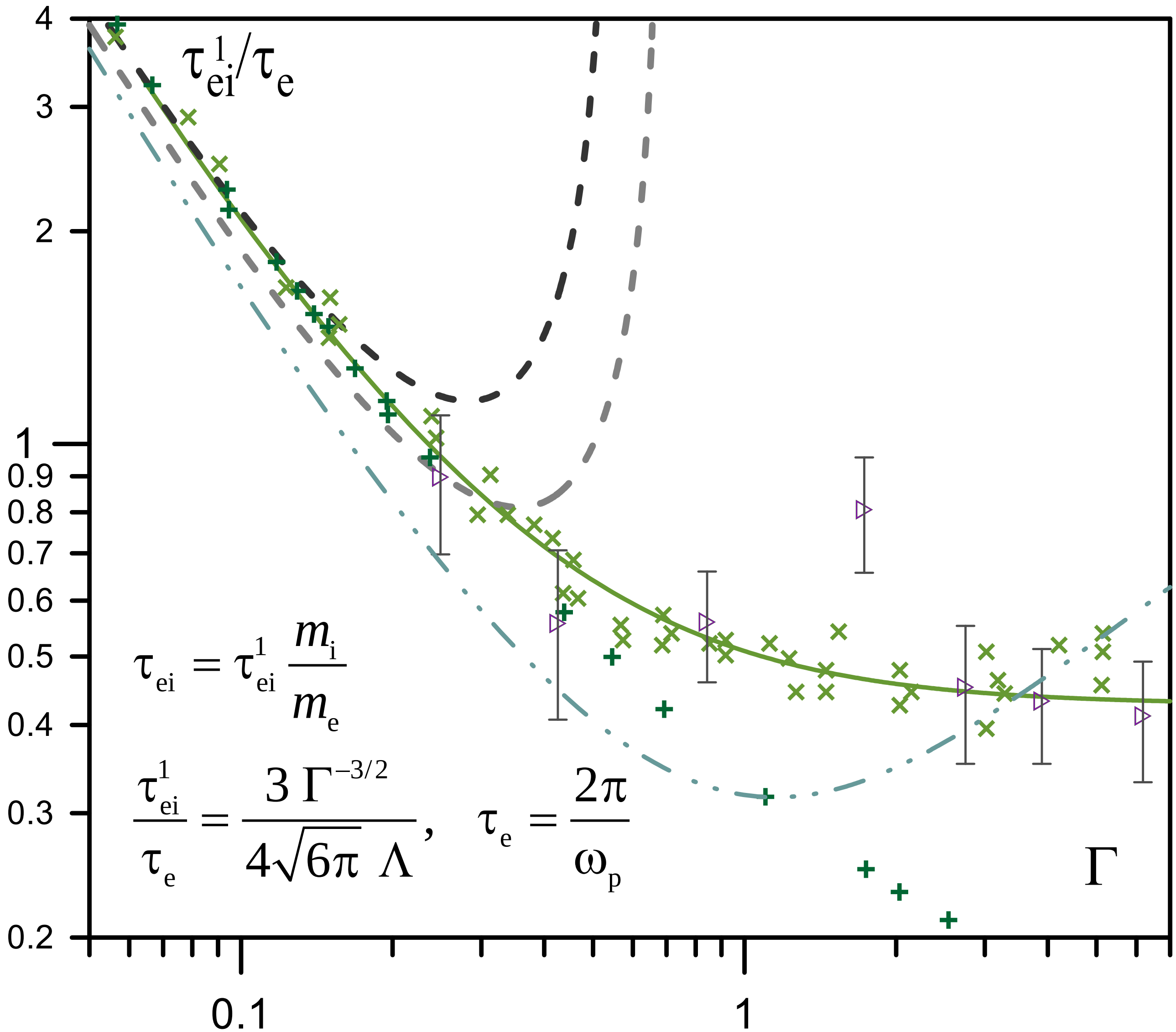

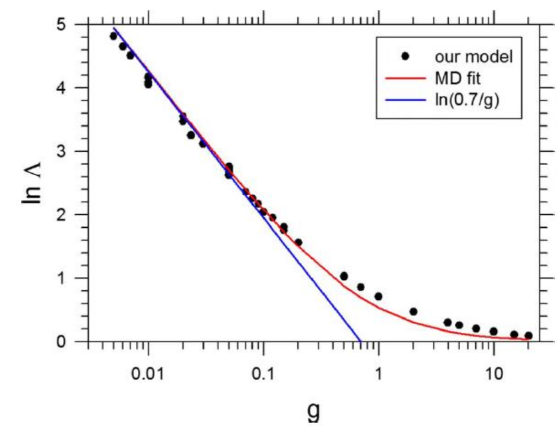

J. Daligault, G. Dimonte. // Phys. Rev. E. 2009. V. 79, no. 5. P. 056403.

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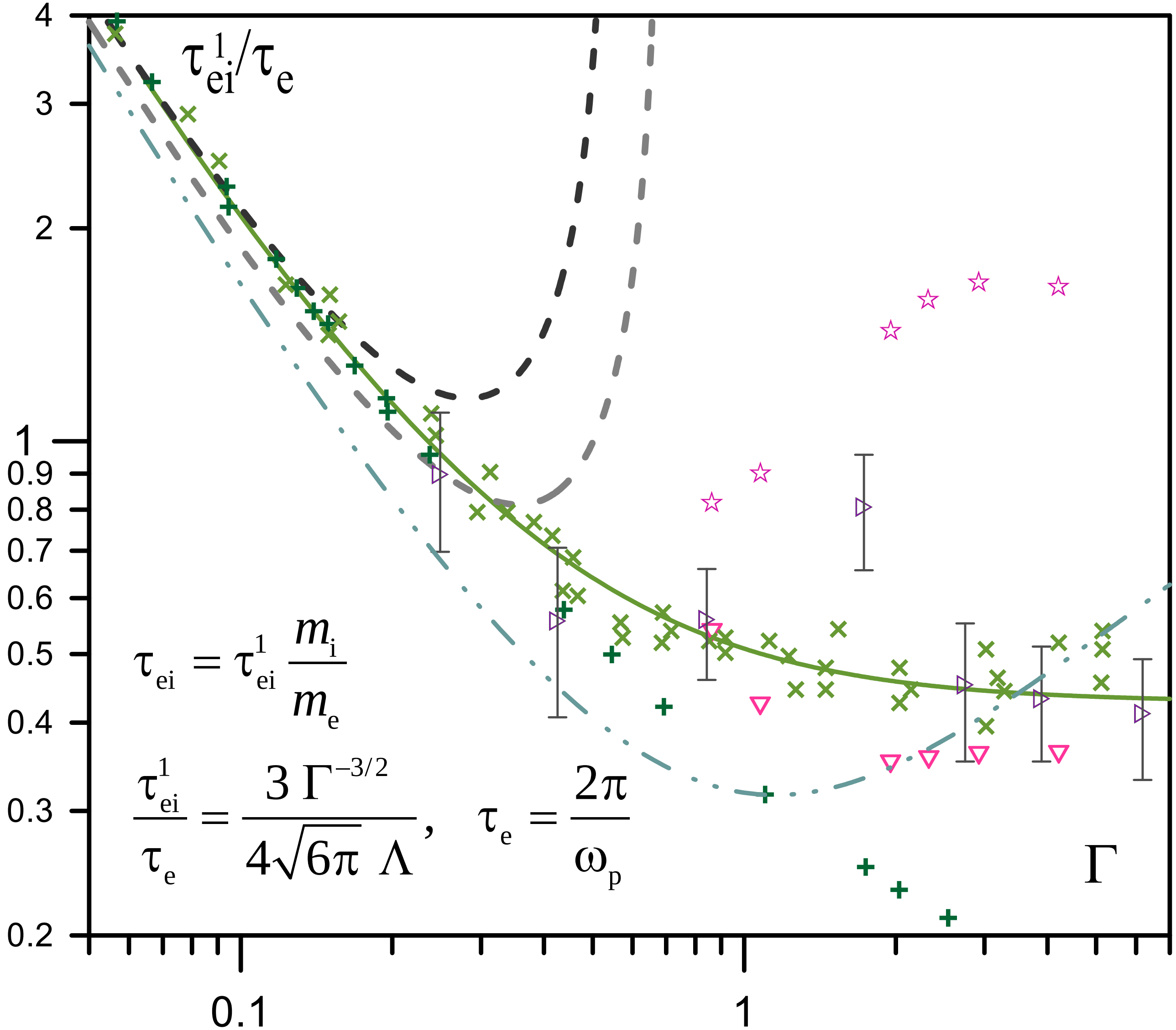
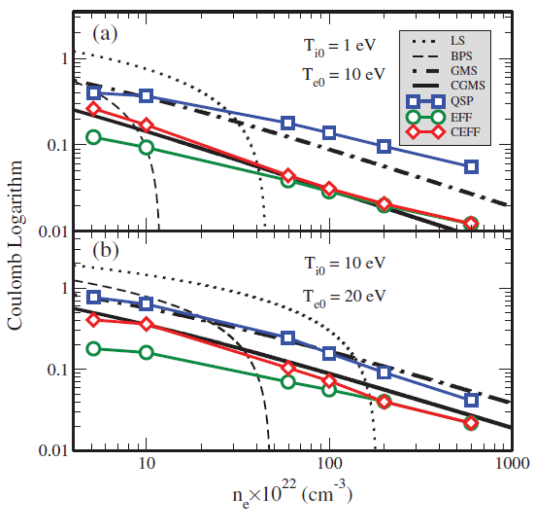




Interaction models

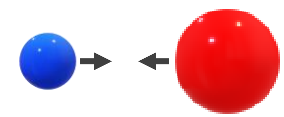
1. Like charges interacting via the repulsive Coulomb potential[1]

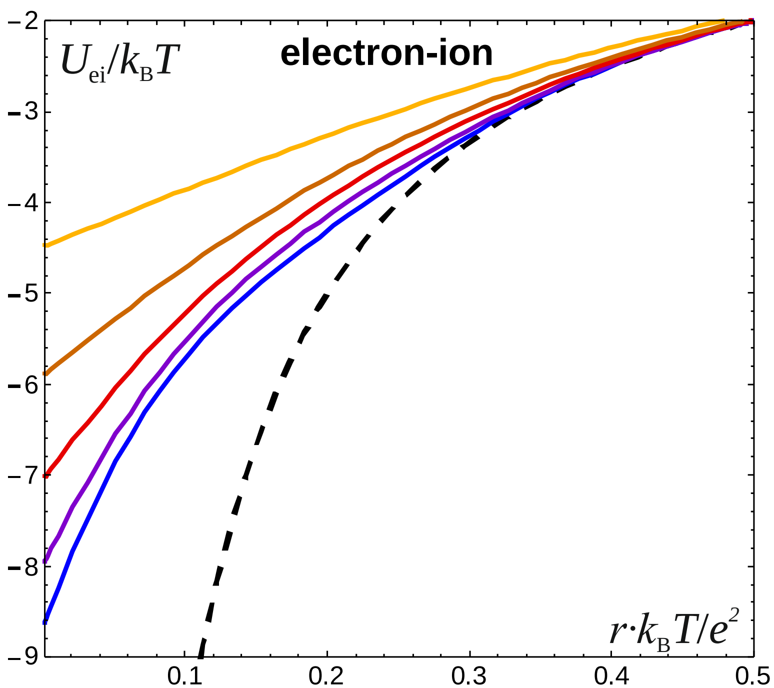
$$U_{cd}(r) = \frac{e^2}{r}$$

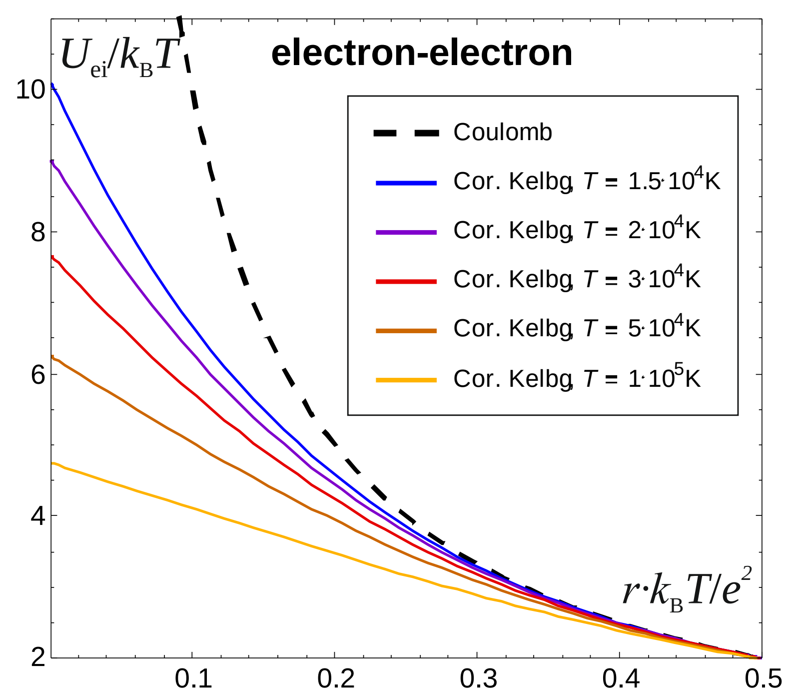
2. Electrons and ions interacting via the Corrected Kelbg potential[2]

$$U_{cd}(r) = \frac{q_c q_d}{r}\left[F\left(\frac{r}{\lambda_{cd}}\right) - r\frac{k_B T}{q_c q_d}\tilde{A}_{cd}(\xi_{cd})\exp\left(-\frac{r^2}{\lambda_{cd}^2}\right)\right],$$

$$F(x) = 1 - \exp\left(-x^2\right) + \sqrt{\pi}x\left(1 - \mathrm{erf}(x)\right),$$

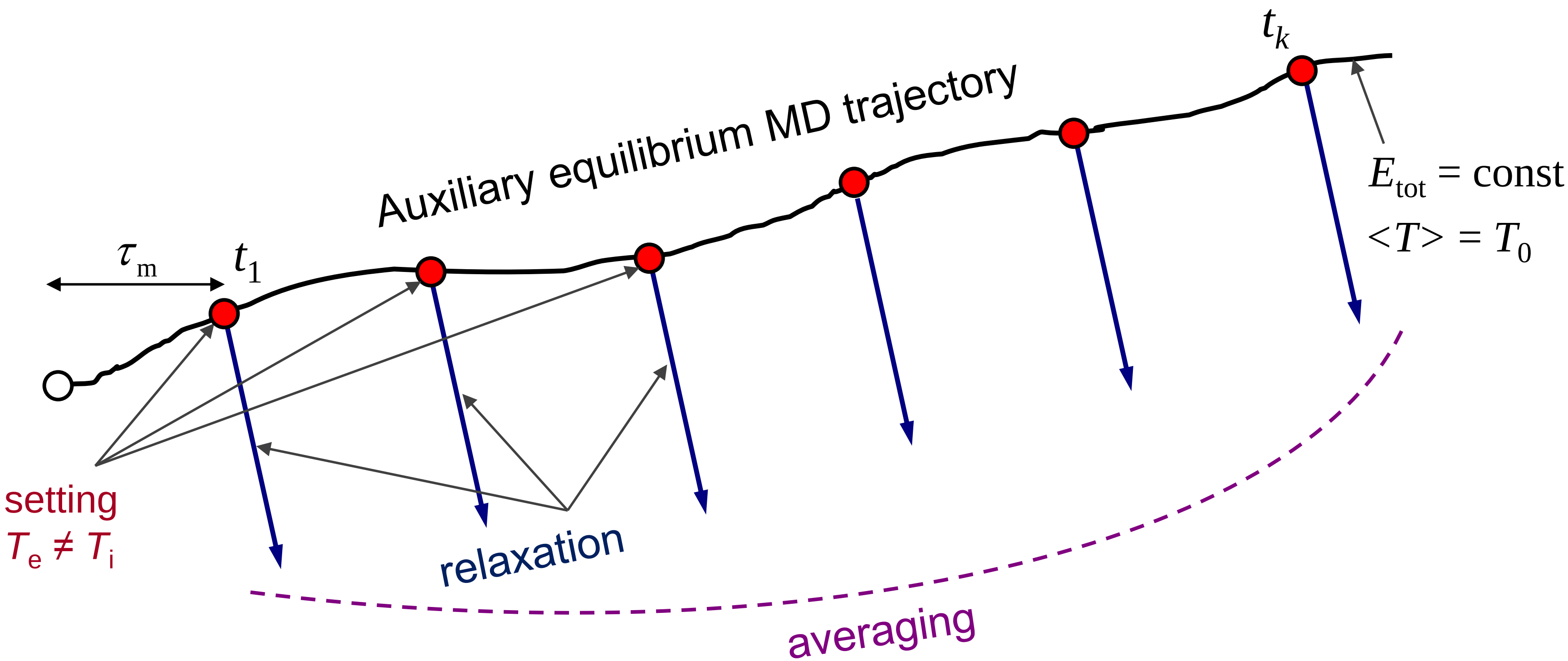






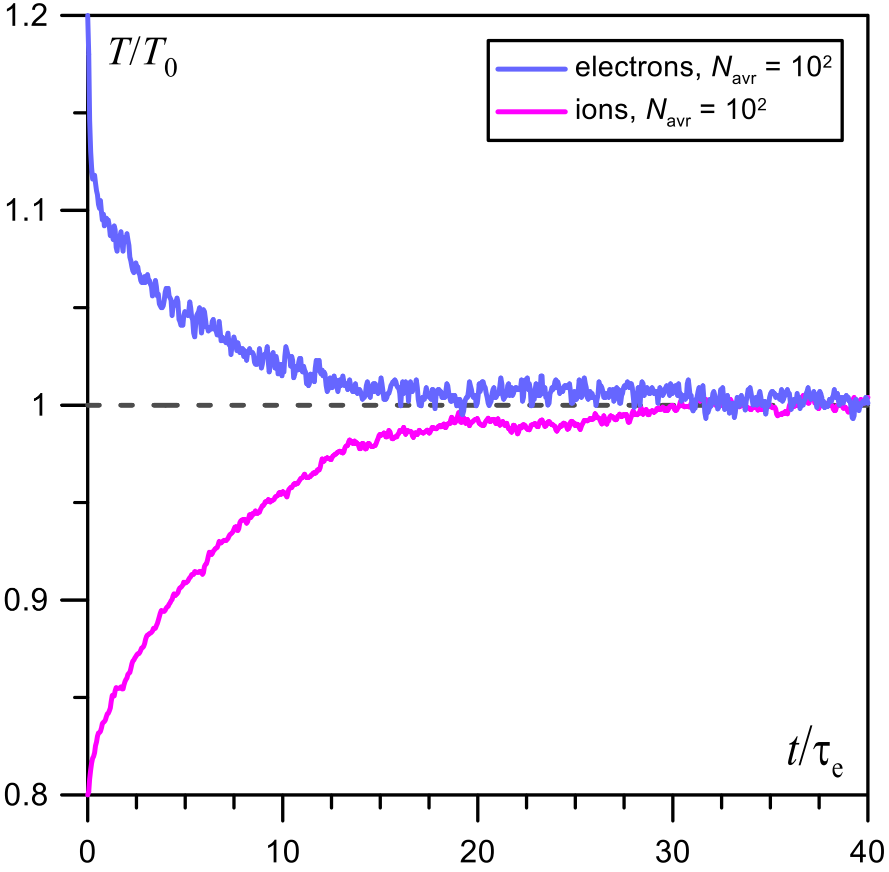
1. Dimonte G., Daligault J. // Phys. Rev. Lett. 2008. V. 101, no. 13. P. 135001.
2. J. Ortner, I. Valuev, W. Ebeling // Contrib. Plasma Phys. 1999. V. 39, no. 4. P. 311.

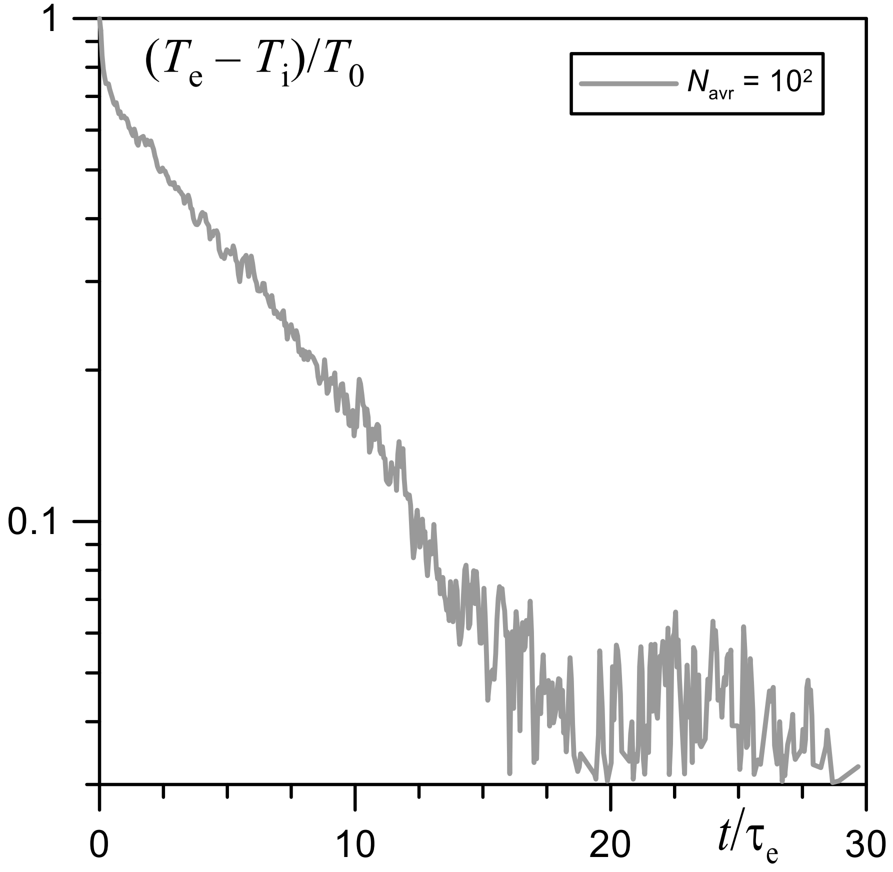
Simulations of the electron-ion equilibration



1. Kuksin A.Yu., Morozov I.V., Norman G.E., Stegailov V.V., Valuev I.A. // Molecular Simulation. 2005. V. 31. № 14–15. P. 1005-1017.

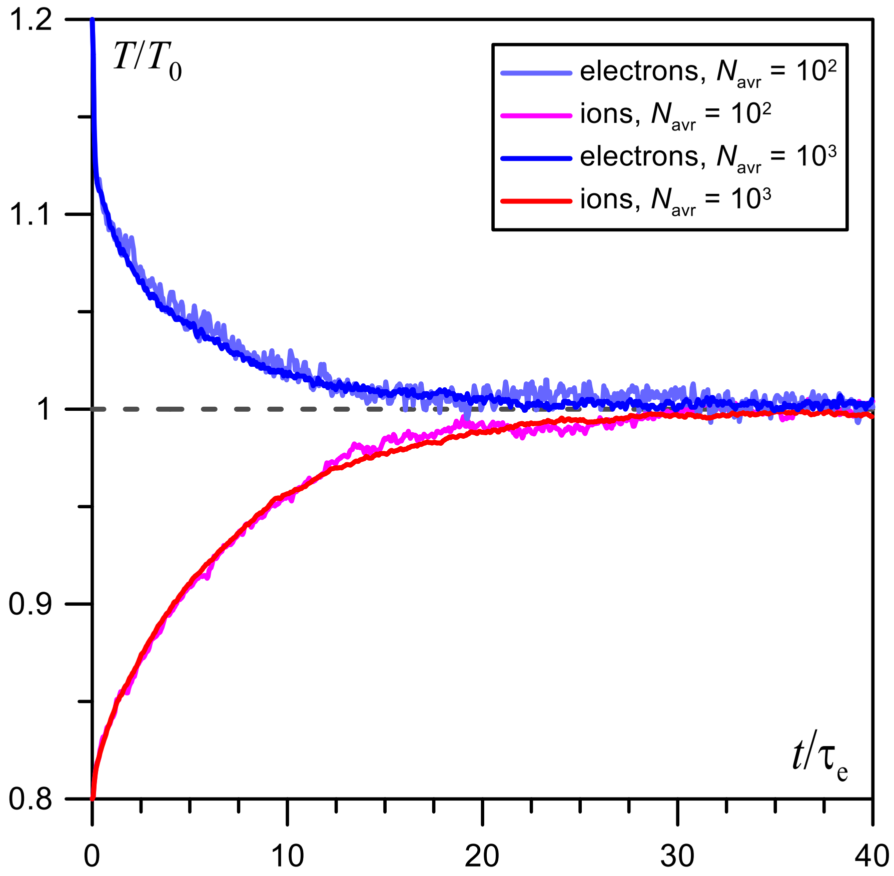
Averaging over initial nonequilibrium states

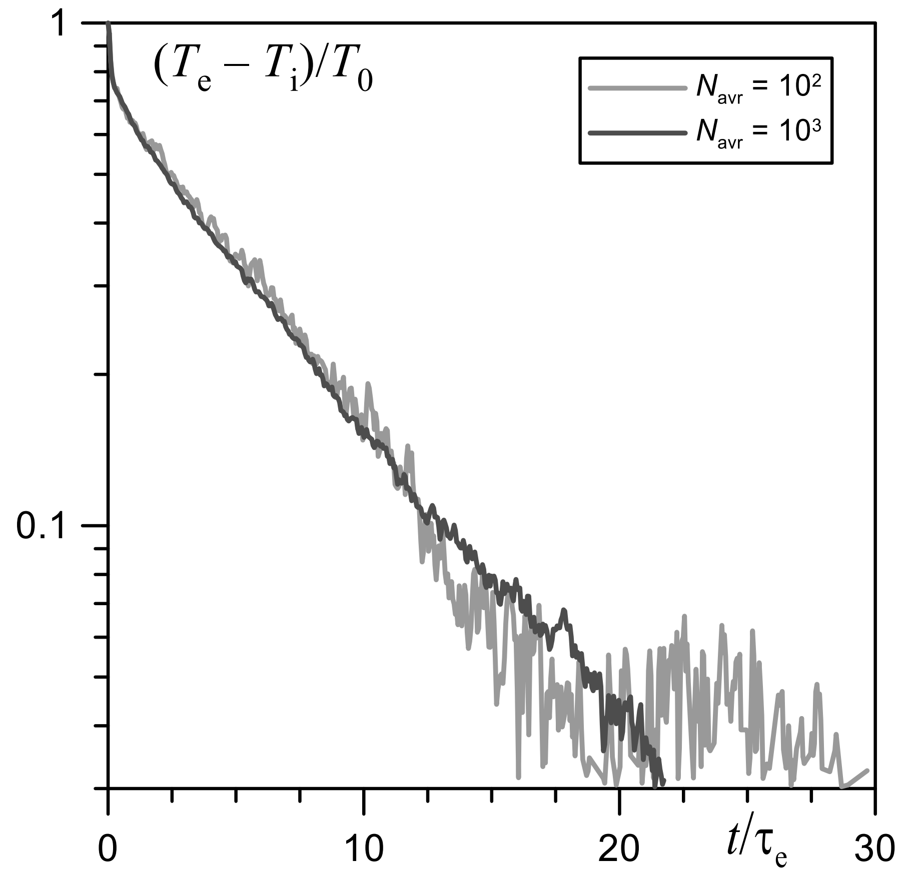




Corrected Kelbg potential, $\Gamma = 1$, $T_0 = 3{\cdot}10^4$ K, ***M*/*m* = 20**

Averaging over initial nonequilibrium states





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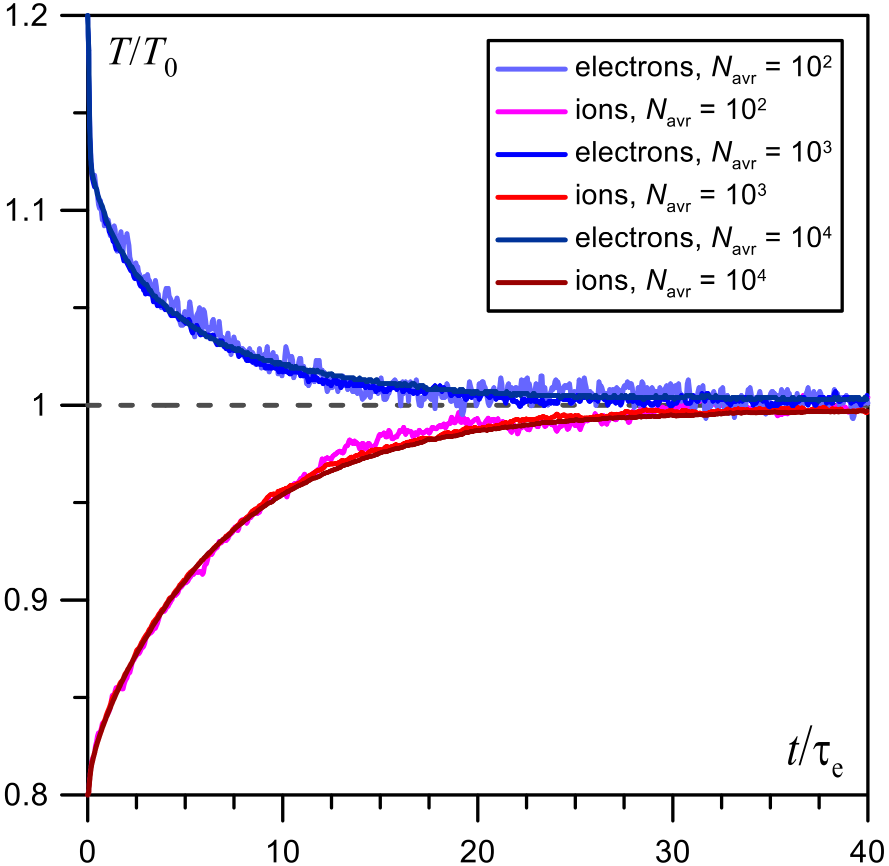
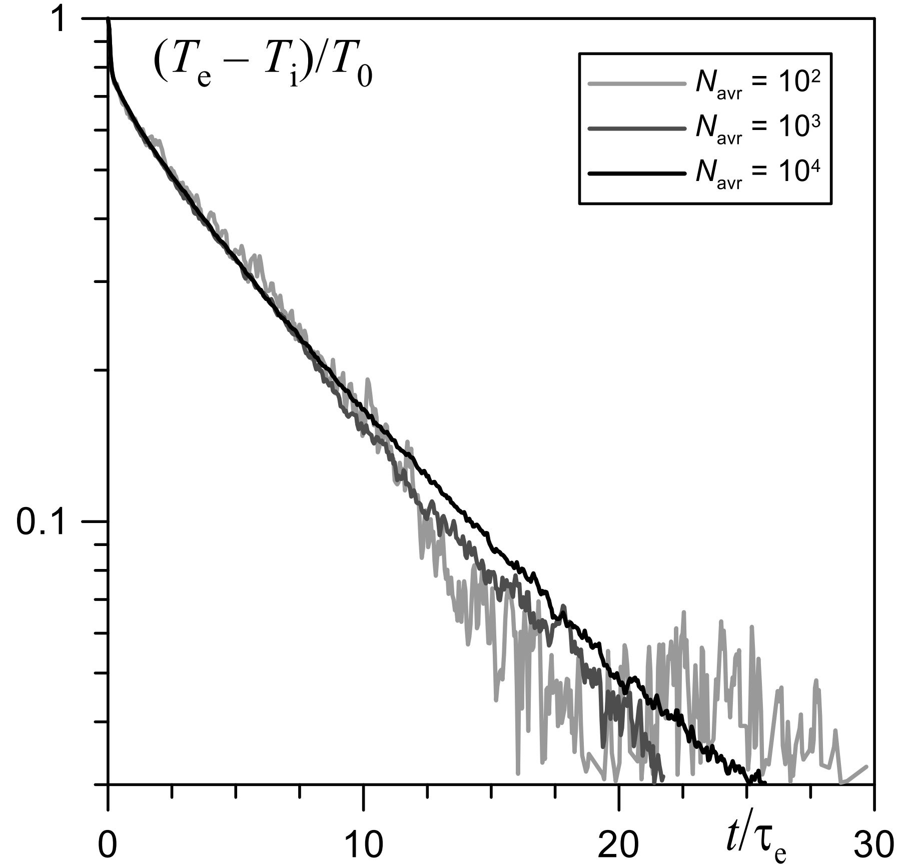
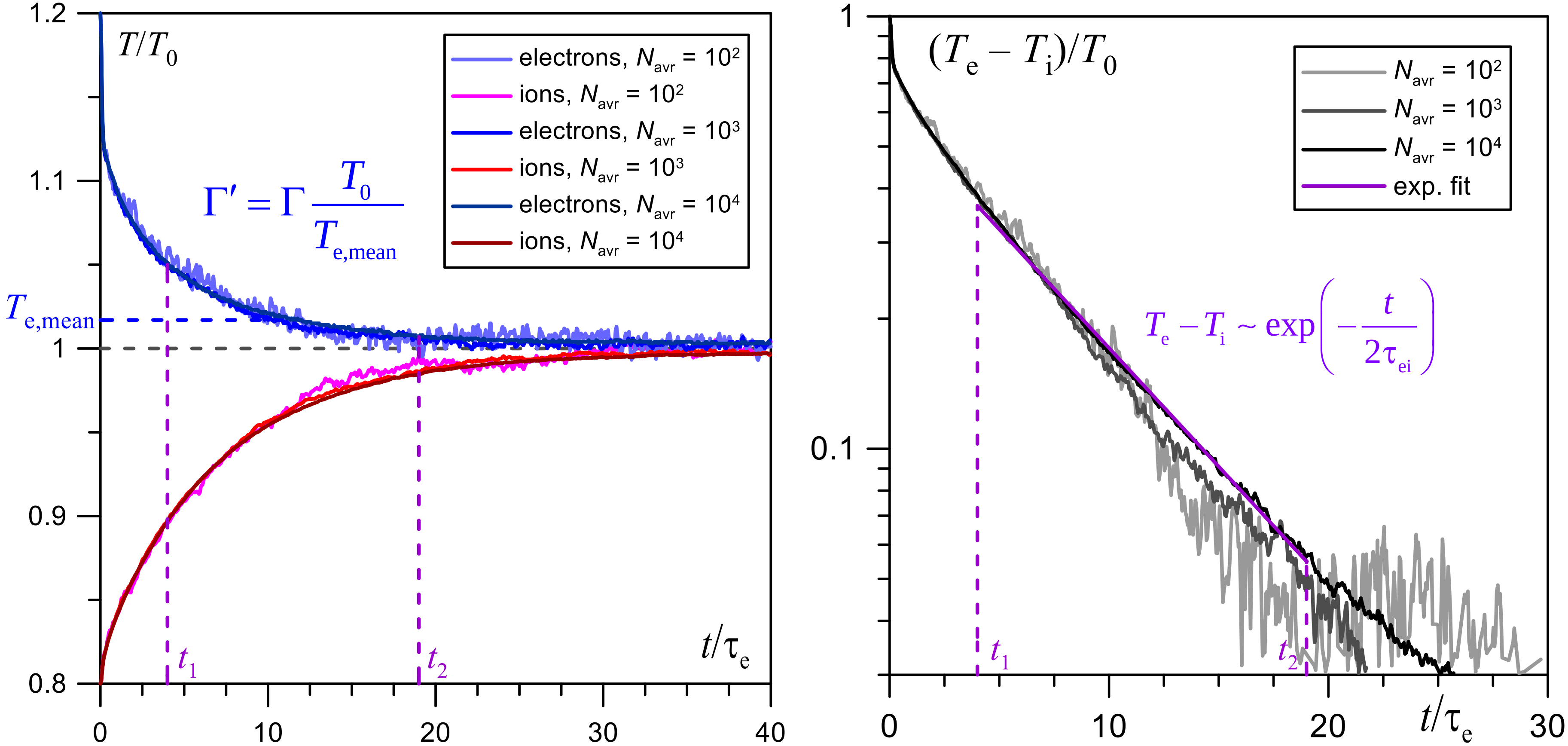
Averaging over initial nonequilibrium states





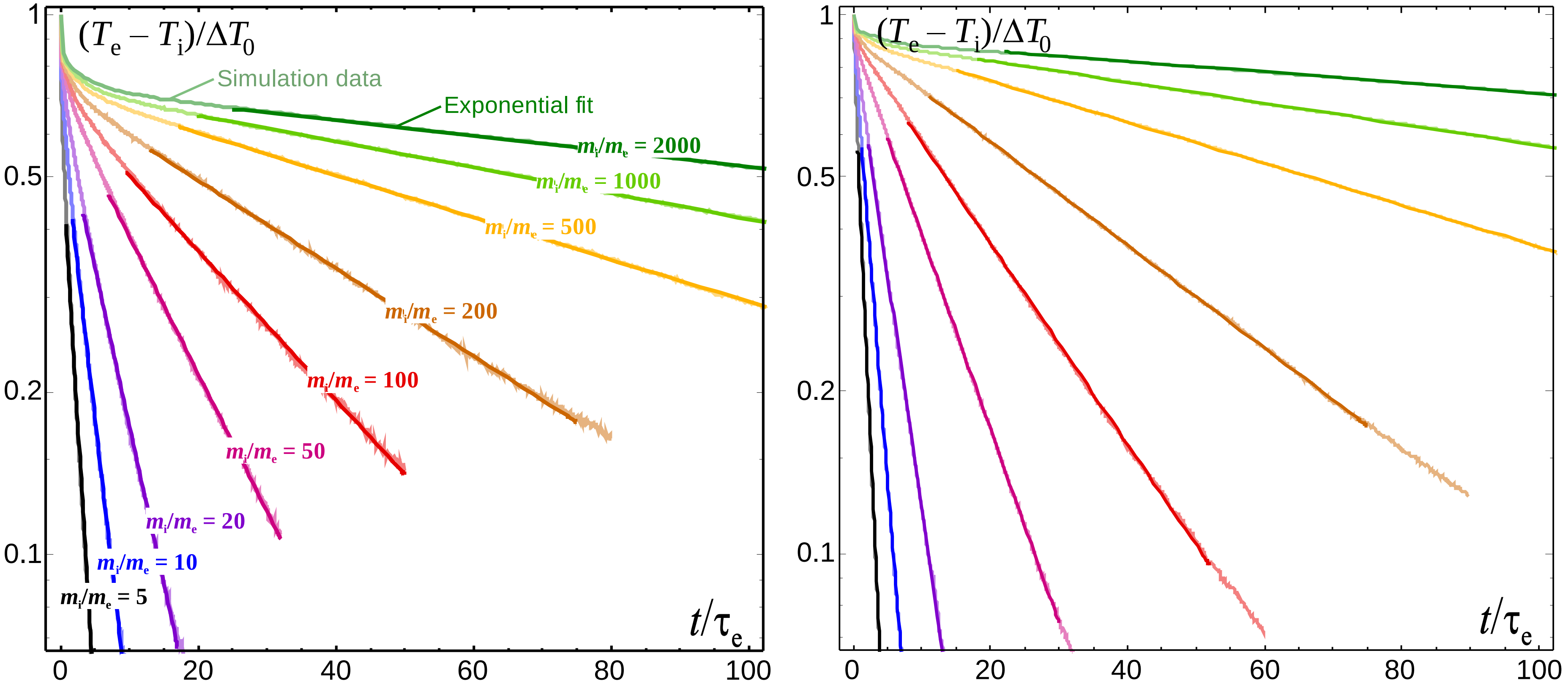
Corrected Kelbg potential, Γ = 1, T_0 = 3·10^4 K, ***M/m* = 20**

Averaging over initial nonequilibrium states



Corrected Kelbg potential, $\Gamma = 1$, $T_0 = 3\cdot10^4$ K, $\boldsymbol{m_i/m_e = 20}$

Equilibration rate depending on the e-i mass ratio

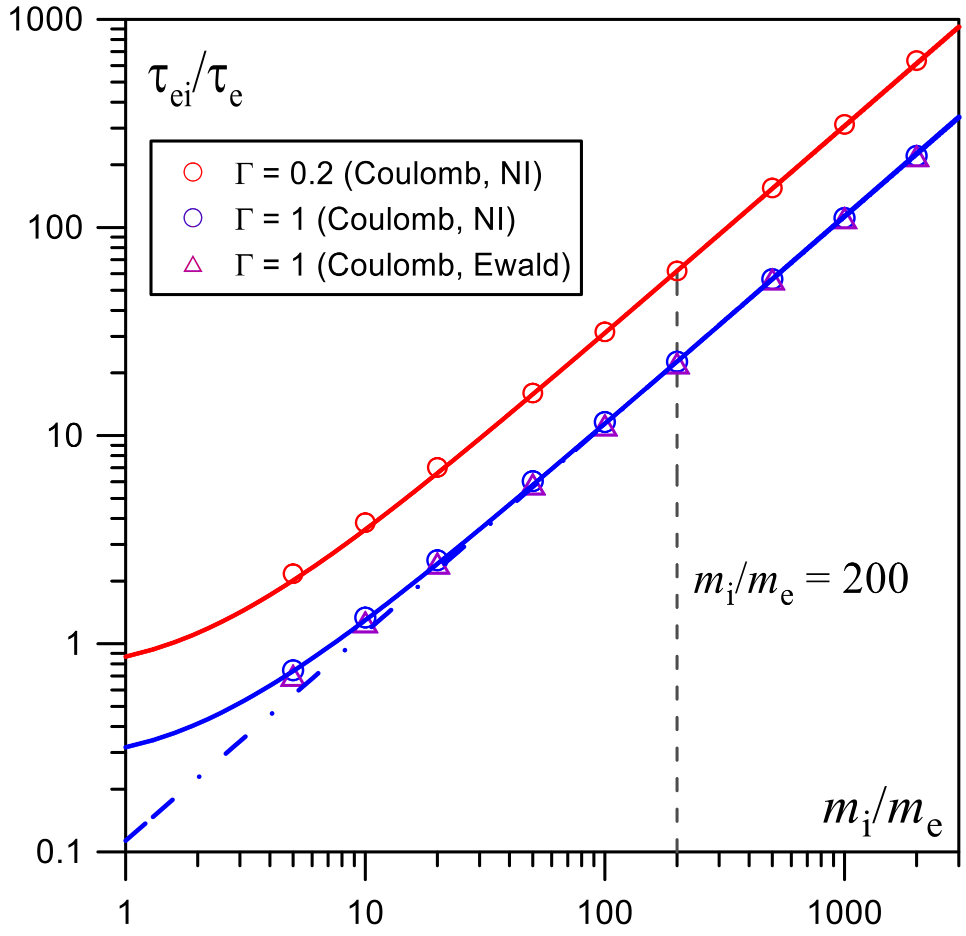


Cor. Kelbg potential, $T_0 = 3 \cdot 10^4$ K

Coulomb potential

$\Gamma = 1, \quad N_{avr} = 10^4$

Equilibration rate depending on the e-i mass ratio

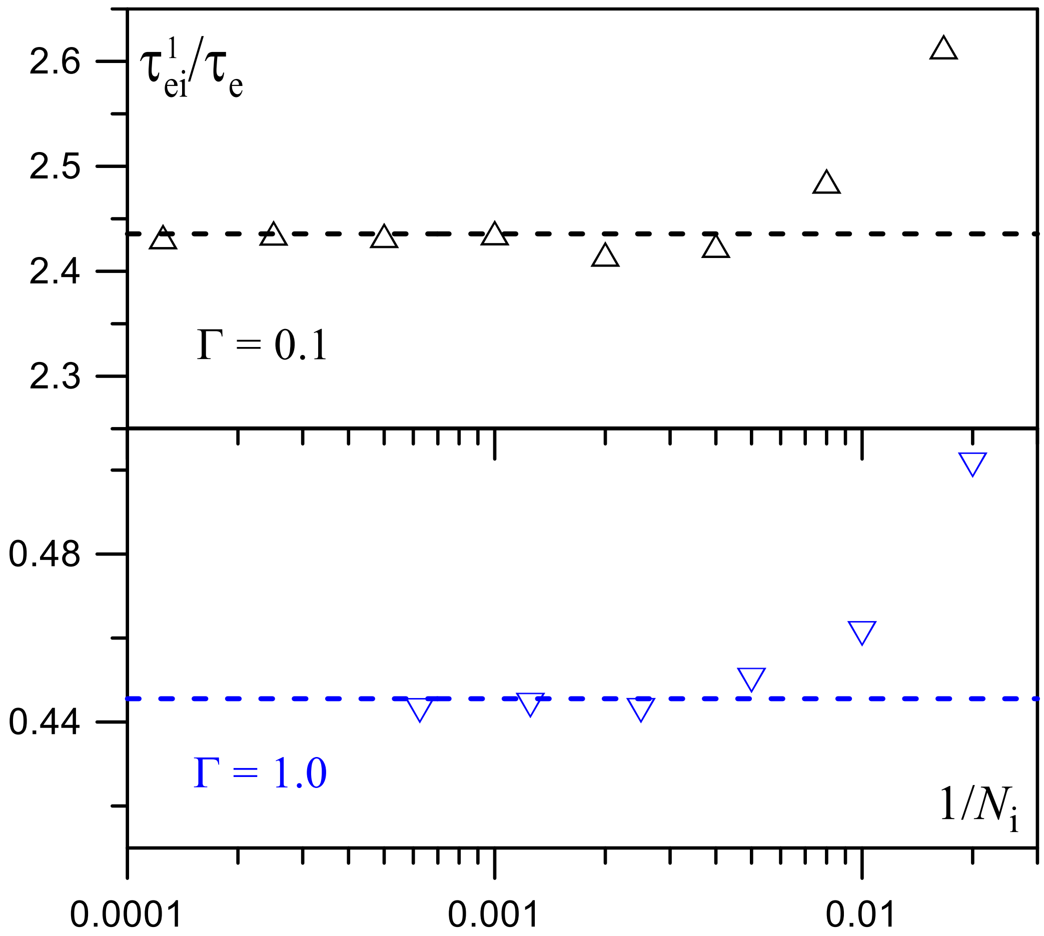


Definition of the mass-independent relaxation time

$$\frac{\tau_{\mathrm{ei}}}{\tau_{\mathrm{e}}} = \frac{3}{4\sqrt{5\pi}\,\Gamma^{3/2}\Lambda}\,\frac{m_{\mathrm{i}}}{m_{\mathrm{e}}}\left(1+\frac{T_{\mathrm{i}}}{T_{\mathrm{e}}}\frac{m_{\mathrm{e}}}{m_{\mathrm{i}}}\right) = \frac{\tau_{\mathrm{ei}}^{1}}{\tau_{\mathrm{e}}}\frac{m_{\mathrm{i}}}{m_{\mathrm{e}}}\left(1+\frac{T_{\mathrm{i}}}{T_{\mathrm{e}}}\frac{m_{\mathrm{e}}}{m_{\mathrm{i}}}\right)$$

Dependence on the number of particles

Dependence of the relaxation time on the number of particles

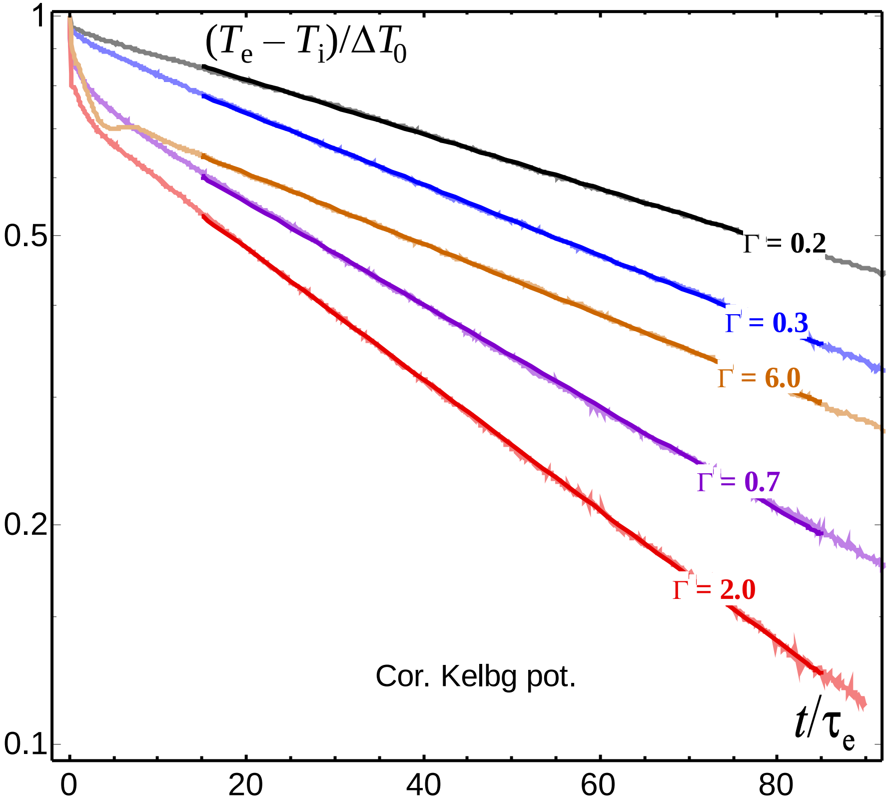


Coulomb potential

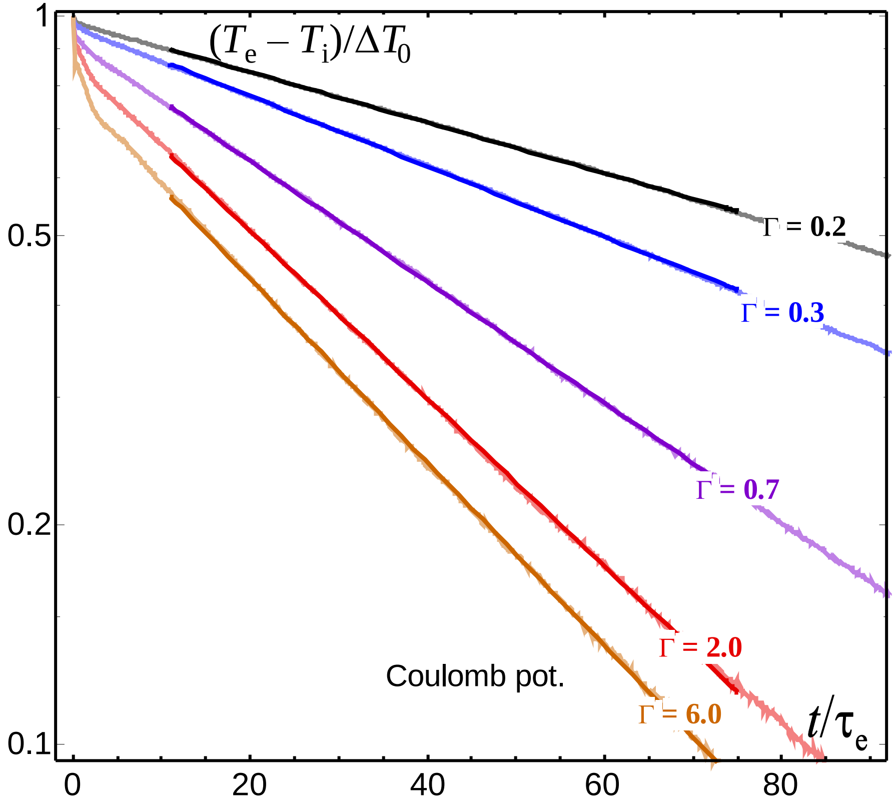
Optimal number of ions depending on the nonideality parameter

Γ	N_i
0.05	4000
0.07	2800
0.1	2000
0.15	1400
0.2	1000
0.3	650
0.5	400
0.7	300
1	250
1.5	250
2	250
3	250
4.5	250
6	250

Equilibration rate depending on the nonideality parameter



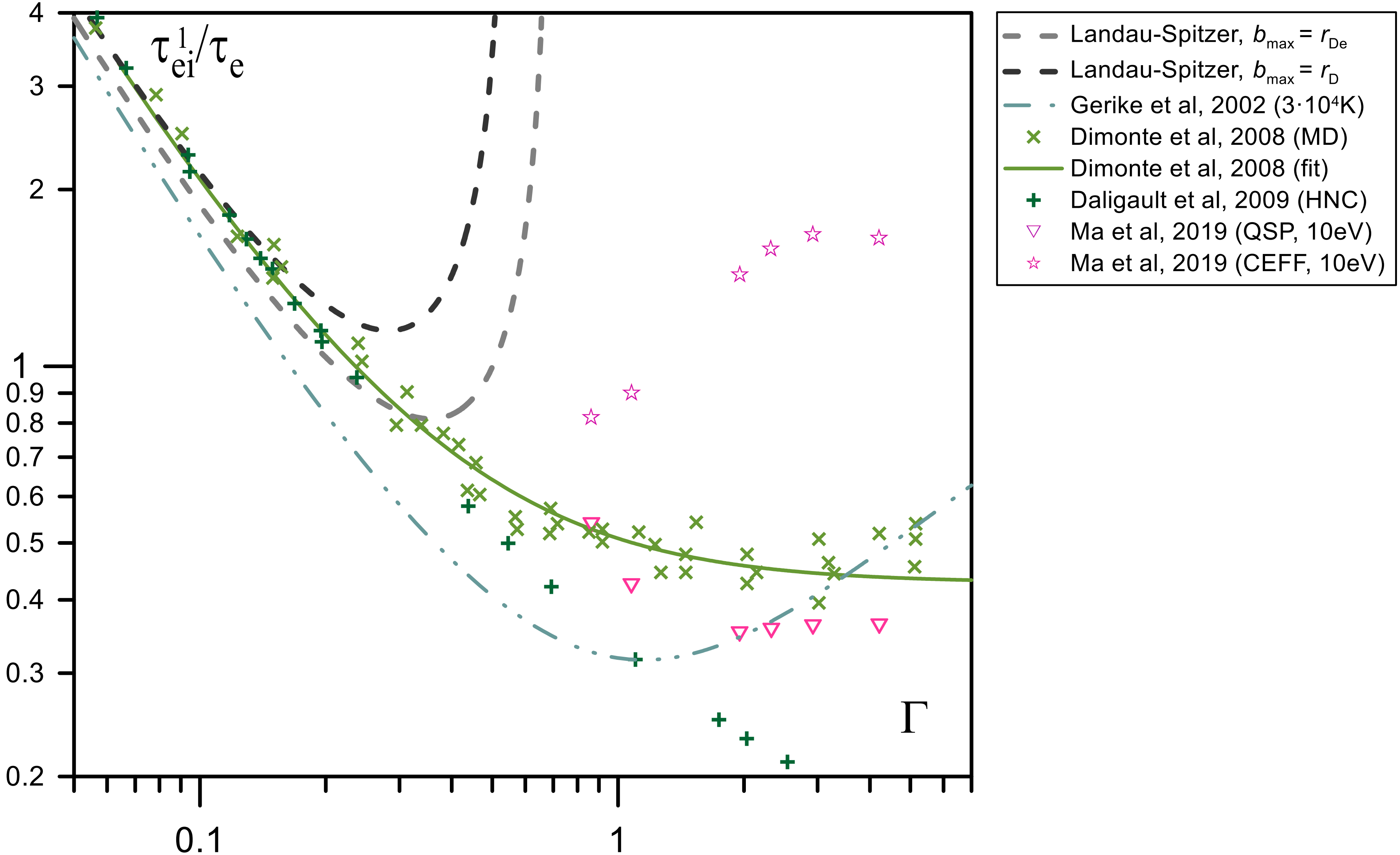
Cor. Kelbg potential, $T_0 = 3{\cdot}10^4$ K



Coulomb potential

$m_i/m_e = 200$

Electron-ion relaxation time vs plasma nonideality



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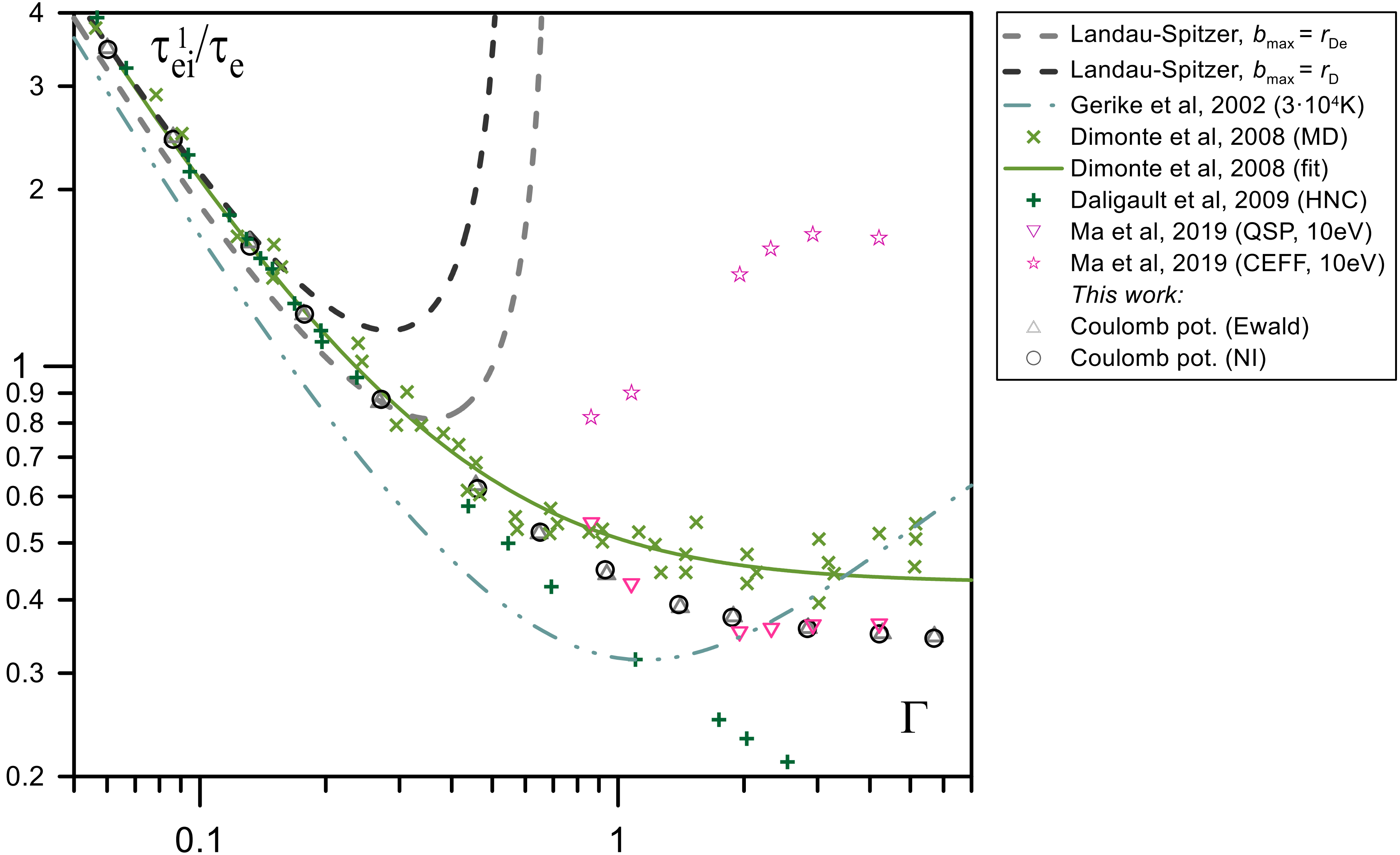

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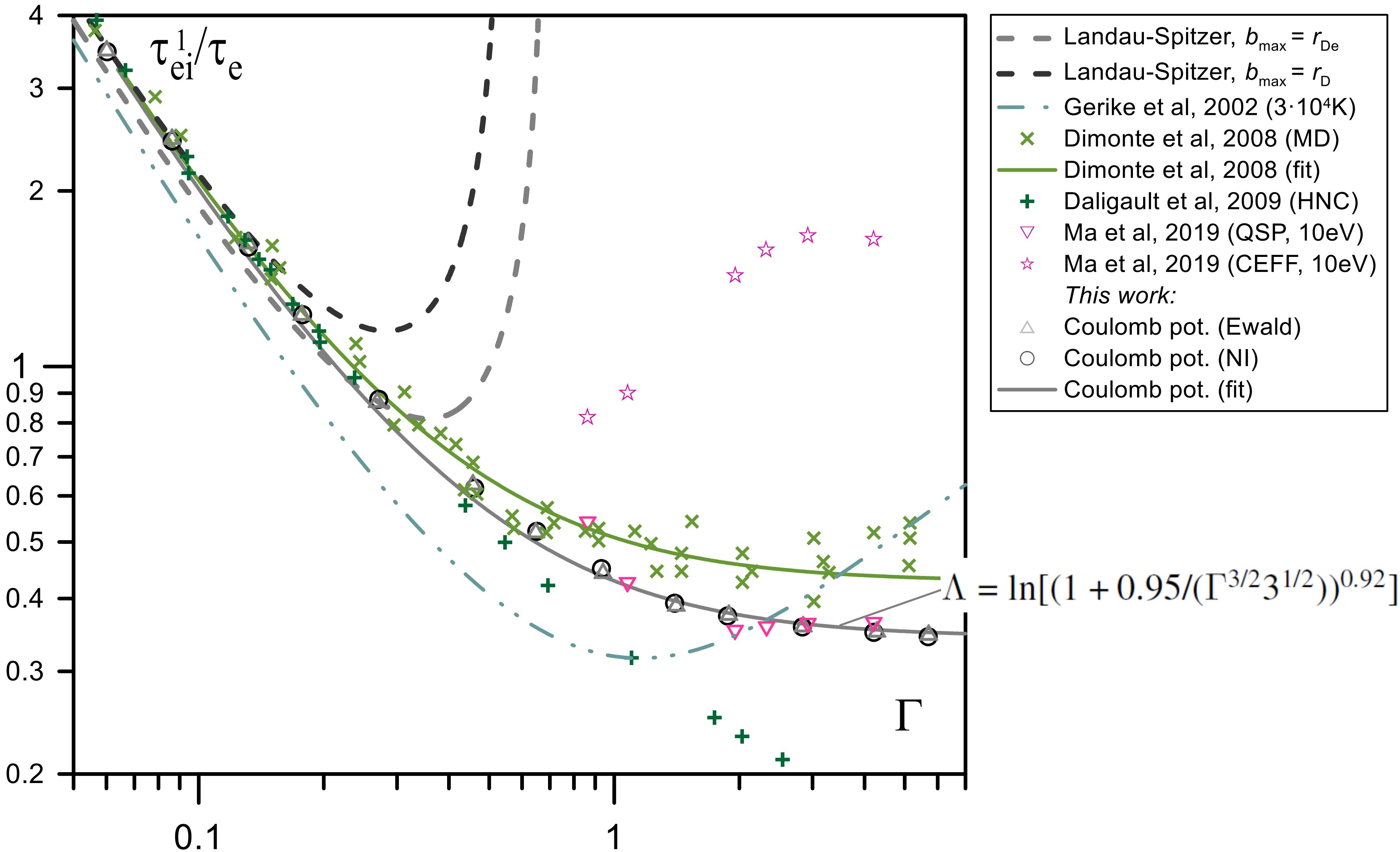

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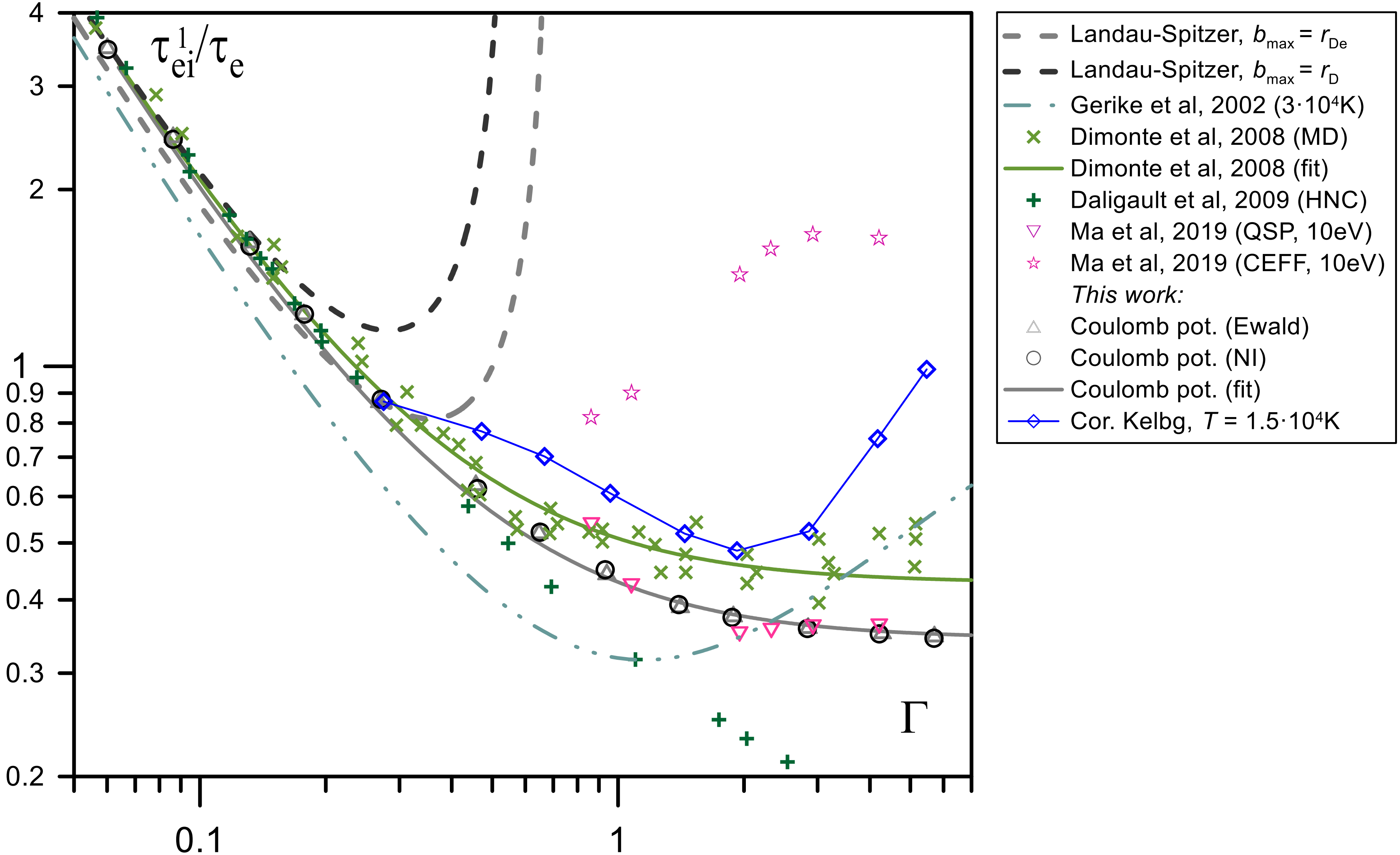

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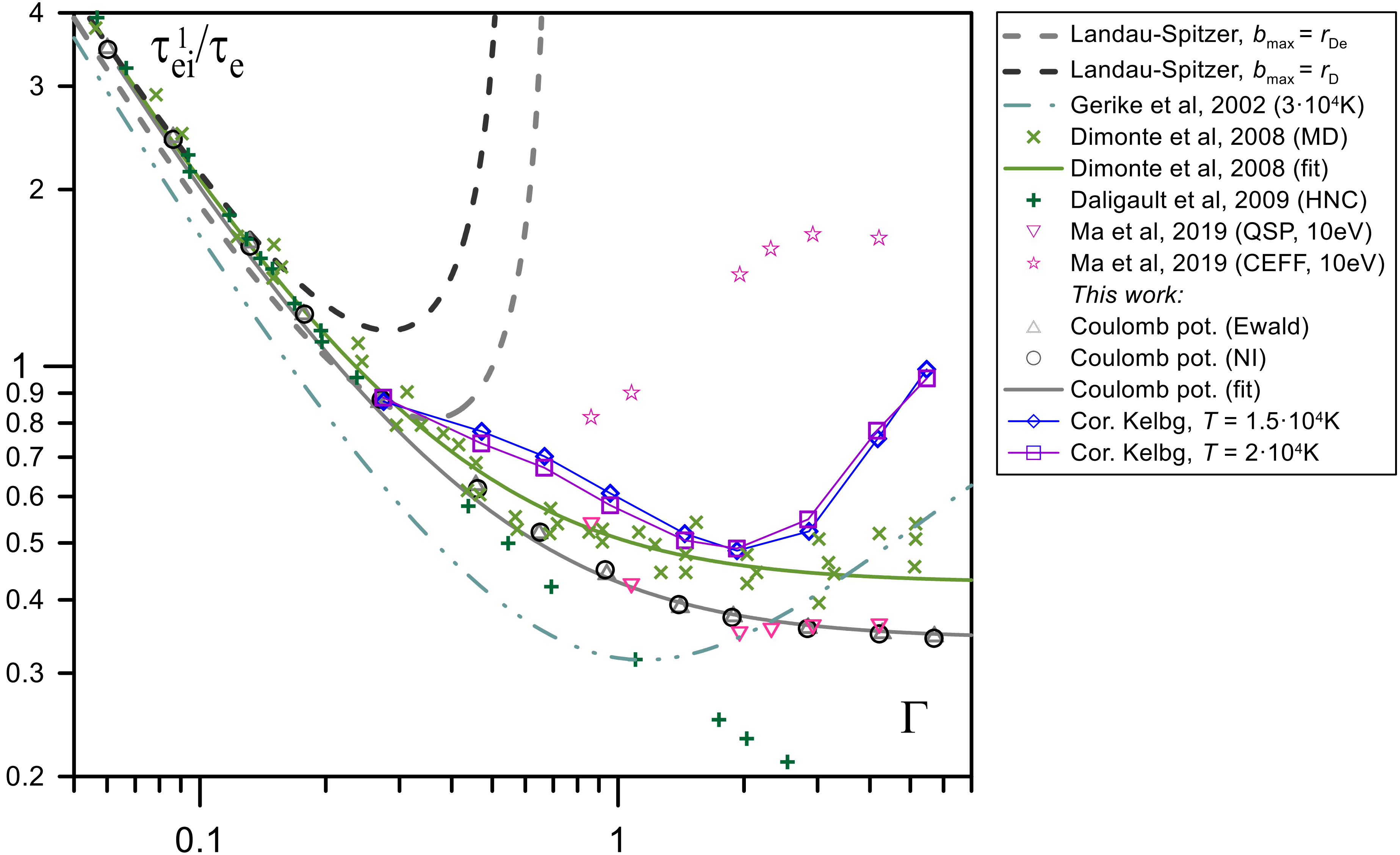

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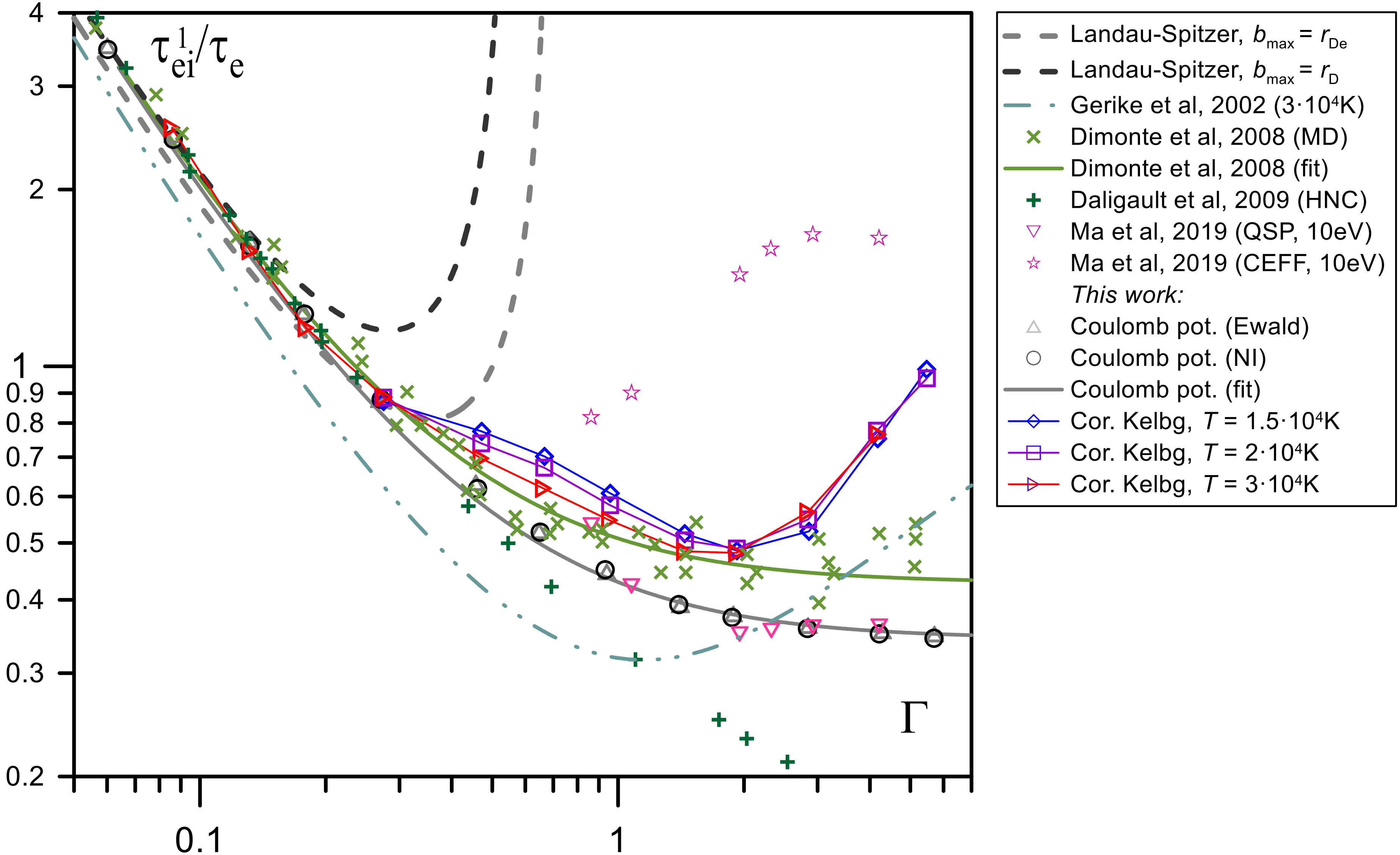

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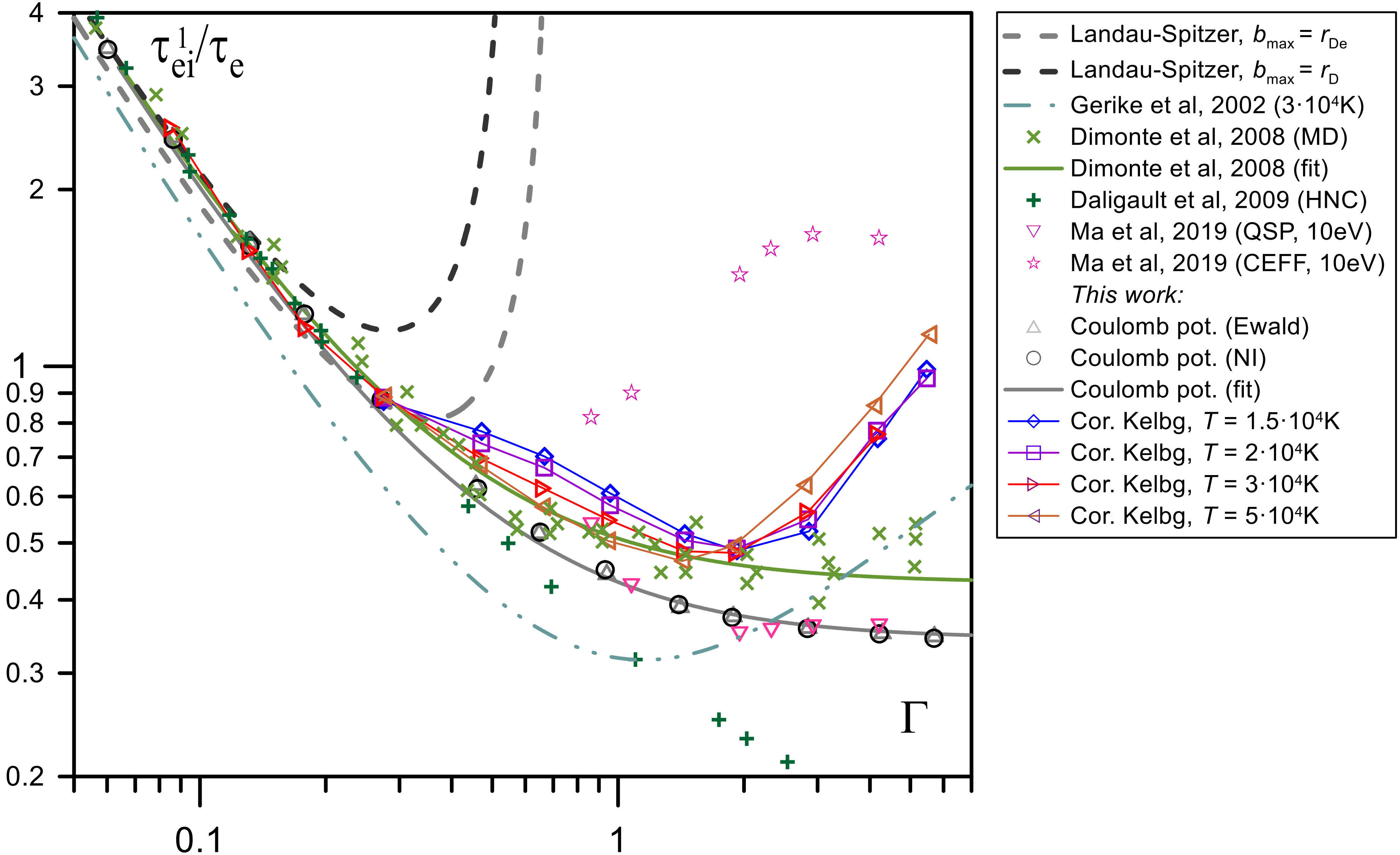

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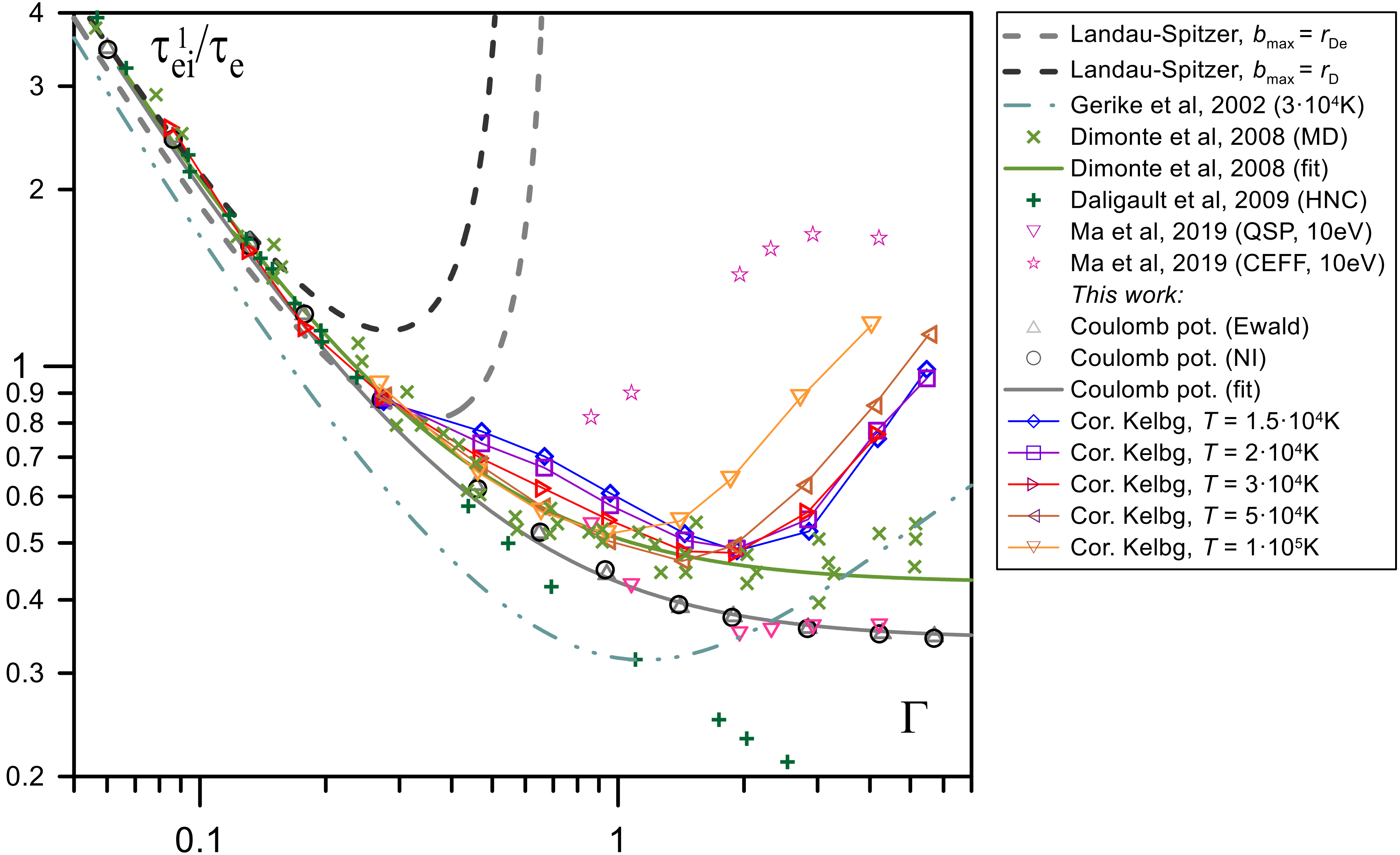

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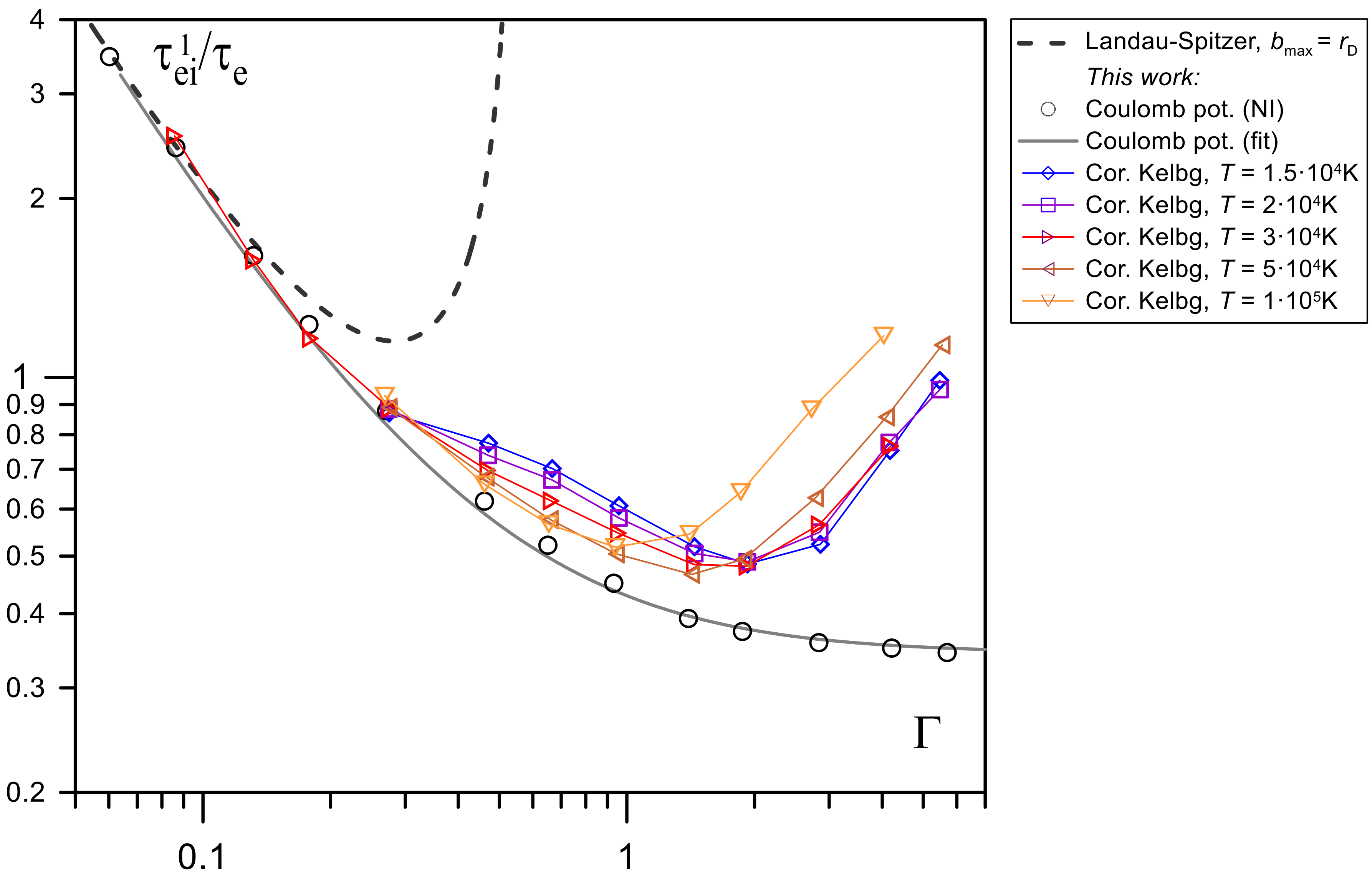

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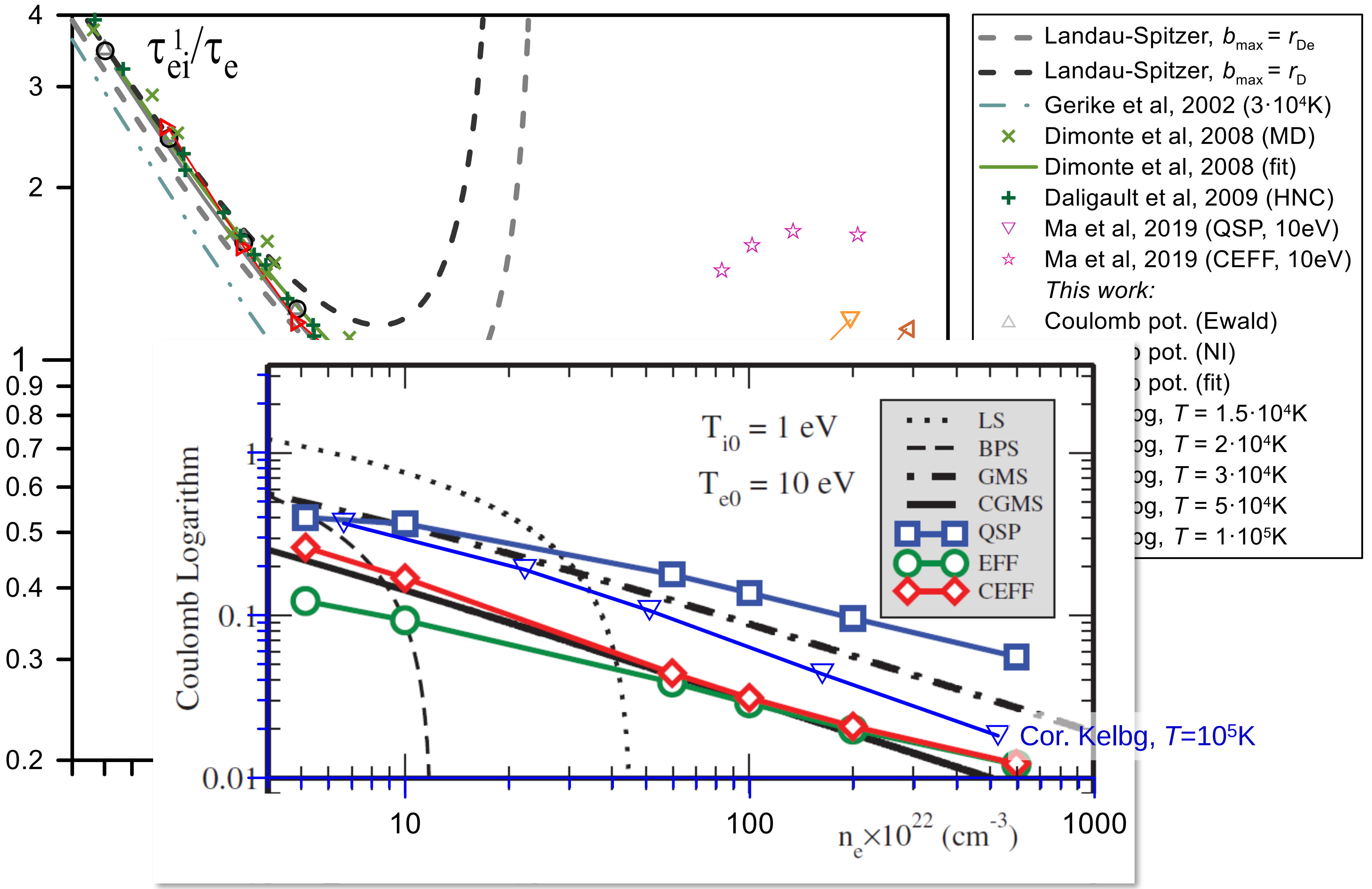

Q. Ma, J. Dai, D. Kang, M. Murillo, Y. Hou, Z. Zhao, J. Yuan // Phys. Rev. Lett. 2019. V. 122, no. 1. P. 015001.

Conclusions

- **Classical molecular dynamics simulations are used for studying electron-ion temperature relaxation in nonideal plasmas**
- **The accuracy of simulation results is improved due to better statistical averaging and studying dependencies on the number of particles and mass ratios**
- **Simulation results are obtained for two interaction models: the corrected Kelbg and the pure Coulomb for like charges**
- **The results for $\Gamma > 0.3$ are not in good agreement with existing theoretical models and WPMD simulations; more WPMD and WPMD-DFT simulations are to be done**