# Simulation of Fermionic Evaporative Cooling Using the Direct Simulation Monte Carlo Method

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# Quantum Boltzmann Equation

# Boltzmann Equation

The Boltzmann equation or Boltzmann transport equation (BTE) describes the statistical behaviour of a thermodynamic system not in a state of equilibrium. The general Boltzmann equation is written as:

$$\frac{df}{dt} = (\frac{\partial f}{\partial t})_{force} + (\frac{\partial f}{\partial t})_{diff} + (\frac{\partial f}{\partial t})_{coll} \tag{1}$$

After some calculation, the Boltzmann equation could be written as:

$$\left(\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla_r - \nabla_r V(\mathbf{r}) \cdot \nabla_p\right) f(\mathbf{r}, \mathbf{p}, t) = \mathcal{I}[f] \tag{2}$$

- $\frac{\partial f}{\partial t}$: the time evolution of the distribution function
- $\frac{\mathbf{p}}{m} \cdot \nabla_r f$: the effect of particle transport in position space
- $-\nabla_r V(\mathbf{r}) \cdot \nabla_p f$: the effect of external forces on the change of momentum
- $\mathcal{I}[f]$: the impact of inter-particle collisions on the distribution function

# Discretization of Phase Space Distribution Function

Direct numerical solution of this 6-dimensional phase space distribution is extremely expensive. So we adopt the approximation where $f(\mathbf{r}, \mathbf{p})$ is discretized in phase space points as simulation particles:

$$f(\mathbf{r}, \mathbf{p}) \approx \xi \sum_{k=1}^{N_{\text{sim}}} \delta^3(\mathbf{r} - \mathbf{r}_k)\delta^3(\mathbf{p} - \mathbf{p}_k) \tag{3}$$

Here $\xi = N/N_{sim}$ is the ratio of the actual number of particles $N$ to simulation number of particles $N_{sim}$. Because the number of particles in AMO physics is not very large, so we set $\xi = 1$ in our simulation even though at traditional DSMC $\xi < 1$.

# Molecular Dynamics

# Crossed Optical Dipole Trap (xODT)

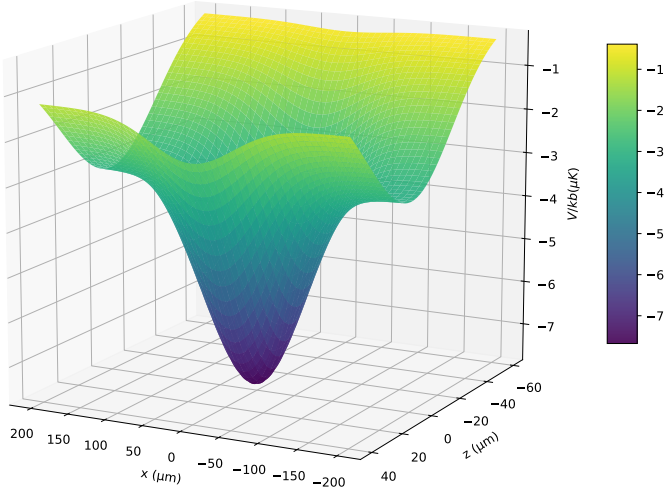


Figure: The xODT potential energy surface $V(\mathbf{r})$, plotted as a function of coordinates $x$ and $z$ along $y = 0$.

# Crossed Optical Dipole Trap (xODT)

xODT is defined as:

$$V_{\mathrm{ODT}}(\mathbf{r}) = -\frac{2\alpha_1 P_1 \exp\left(-\frac{2y^2}{w_{1,y}(x)} - \frac{2z^2}{w_{1,z}(x)}\right)}{\pi w_{1,y}(x) w_{1,z}(x)} - \frac{2\alpha_2 P_2 \exp\left(-\frac{2x^2}{w_{2,x}(y)} - \frac{2z^2}{w_{2,z}(y)}\right)}{\pi w_{2,x}(y) w_{2,z}(y)} \tag{4}$$

Each beam's laser power is denoted by $P_i$ and the molecular polarizability is denoted by $\alpha_i$. $\omega_{\mu,i}(r)$ is represented as:

$$\omega_{\mu,i}(r) = W_{\mu,i}\sqrt{1 + \frac{r^2}{R_{\mu,i}^2}} \tag{5}$$

where $R_{\mu,i} = \pi W_{\mu,i}^2/\lambda$ denoting the Rayleigh length and $W_{\mu,i}$ is the beam width of wavelength $\lambda$.

# The Change of xODT with Time

During evaporative cooling, the trap depth which promotes the loss of energetic molecules should be lowered by reducing the trap power.

$$P_i(t) = P_i(0) - \Delta P_i \left( \frac{1 - e^{-t/\tau}}{1 - e^{-t_d/\tau}} \right) \tag{6}$$

where $\Delta P_i$ is the change in laser power of beam $i$, $t_d$ denotes the characteristic decay time and $\tau$ denotes the forced evaporation time.

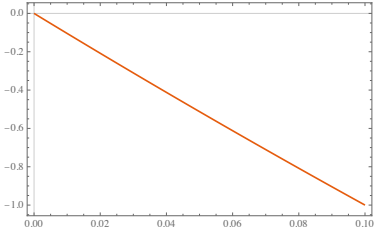


Figure: Small $t_d/\tau$

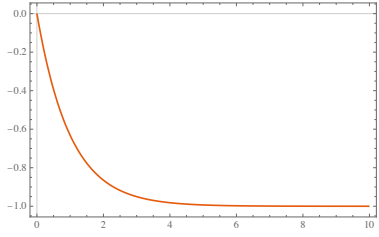


Figure: Large $t_d/\tau$

# Lennard-Jones (LJ) potential

For intermolecular forces, we employ the Lennard-Jones potential to model the interactions between two molecules. LJ potential is defined as:

$$V_{\mathrm{LJ}}(r) = 4\epsilon \left[ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \tag{7}$$

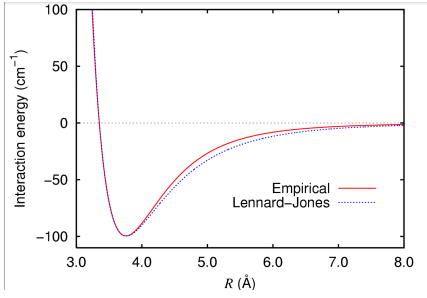


Figure: The interaction energy as a function of interatomic distance $R$. The red solid line represents an empirical potential, while the blue dotted line represents the Lennard Jones potential $V_{LJ}$.

# Velocity Verlet Algorithm

To update the velocities and displacements of particles, we apply the Velocity Verlet symplectic algorithm. This algorithm is advantageous due to its stability and ability to conserve energy over long simulation periods.

$$v_k(t + \frac{\Delta t}{2}) = v_k(t) + F_k(r_k)\frac{\Delta t}{2m} \tag{8a}$$

$$r'_k = r_k(t) + v_k(t + \frac{\Delta t}{2})\Delta t \tag{8b}$$

$$r_k(t + \Delta t) = r'_k \tag{8c}$$

$$v_k(t + \Delta t) = v_k(t + \frac{\Delta t}{2}) + F_k(r'_k)\frac{\Delta t}{2m} \tag{8d}$$

# Direct Simulation Monte Carlo

# Key Strategies

The DSMC method was proposed by Graeme Bird at 1970. DSMC is a numerical method for modeling **rarefied gas** flows. The DSMC method has been applied to the solution of flows ranging from estimation of the Space Shuttle re-entry aerodynamics to the modeling of microelectromechanical systems.

Come back Boltzmann equation:

$$\left(\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla_r - \nabla_r V(\mathbf{r}) \cdot \nabla_p\right) f(\mathbf{r}, \mathbf{p}, t) = \mathcal{I}[f] \tag{9}$$

- Free-stream kinetics (Velocity Verlet algorithm)
- Collision term

# Octree Algorithm

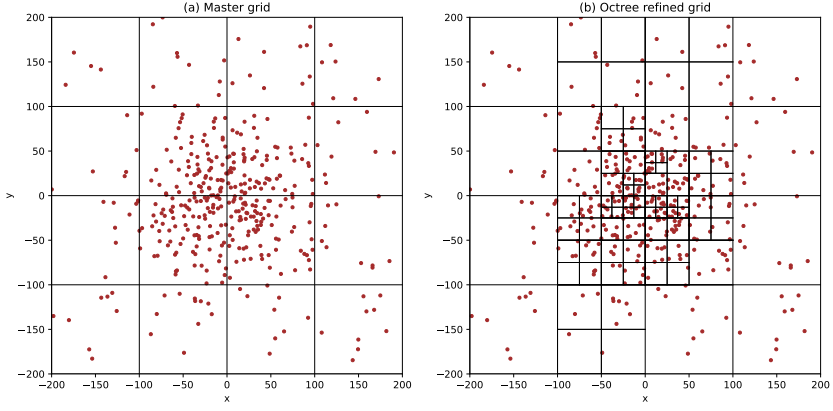


Figure: 2-d visualisation of the octree algorithm refinement (b) applied to the master grid (a), projected in 2-dimensions. In this figure, there are initially 16 master grid cells with $N = 400$, and $N_{max}^{cell} = 10$, with Gaussian distributed points in arbitrary units.

# Collision Occurrences Step

In collision occurrences step, a collision proceeds between test particles $i$ and $j$, with probability:

$$P_{ij} \approx \xi \frac{\delta t}{m \Delta V_{\text{cell}}} |\mathbf{p}_{ij}| \sigma(\mathbf{p}_{ij}) \tag{10}$$

where $\mathbf{p}_{ij} = \mathbf{p}_i - \mathbf{p}j$ and here we set collision cross section $\sigma(\mathbf{p}_{ij}) = \pi\sigma^2$ where $\sigma$ is the scale parameter in Lennard-Jones potential.

To simulate **two body loss** which against the system into Fermi degeneracy, the cross section could be written as:

$$\sigma(ij) = \sigma_{eff} + \sigma_{loss} \tag{11}$$

Here $\sigma_{eff}$ denotes elastic cross section and $\sigma_{loss}$ denotes inelastic cross section. When we use $\sigma_{loss}$ in collision section, two particles are moved from the xODT trap, as we have observed in experiments about the phenomenon of two body loss.

# Pauli Blocking Factor

Quantum statistics or Pauli blocking factor require an additional **accept reject step**, where the sampled post collision momenta are only accepted with probability

$$P'_{ij} = (1 - h^3 f'_i)(1 - h^3 f'_j) \tag{12}$$

otherwise, no collision is said to have occurred.

$$f(\mathbf{r}, \mathbf{p}) \approx \xi \sum_{k=1}^{N_{\text{sim}}} \delta^3(\mathbf{r} - \mathbf{r}_k)\delta^3(\mathbf{p} - \mathbf{p}_k) \tag{13}$$

# Gaussian Convolution Kernel

We change the $\delta$-function to Gaussian convolution kernel. These kernels are taken to have spatial width $\vartheta_\nu$ along axis $\nu$ and momentum width $\vartheta_p$. So the discretization noise could be smoothed out while the distribution function remains physically consistent.

$$\vartheta_\nu = \sqrt{\left(\frac{\hbar}{m\omega_\nu}\right)^{1/2}\left(R_\nu \frac{T}{T_F}\right)} \tag{14a}$$

$$\vartheta_p = \sqrt{(m\hbar\overline{\omega})^{1/2}\left(p_F \frac{T}{T_F}\right)} \tag{14b}$$

$$\delta^3(\mathbf{r}-\mathbf{r}_k) \to c_r(\mathbf{r}-\mathbf{r}_k) \equiv \prod_{\nu=1}^{3} \frac{e^{-(r-r_k)^2/\vartheta_\nu^2}}{\sqrt{\pi\vartheta_\nu^2}} \tag{15a}$$

$$\delta^3(\mathbf{p}-\mathbf{p}_k) \to c_p(\mathbf{p}-\mathbf{p}_k) \equiv \prod_{\nu=1}^{3} \frac{e^{-(p-p_k)^2/\vartheta_{p_\nu}^2}}{\sqrt{\pi\vartheta_{p_\nu}^2}} \tag{15b}$$

# Simulation Results

# MD & DSMC

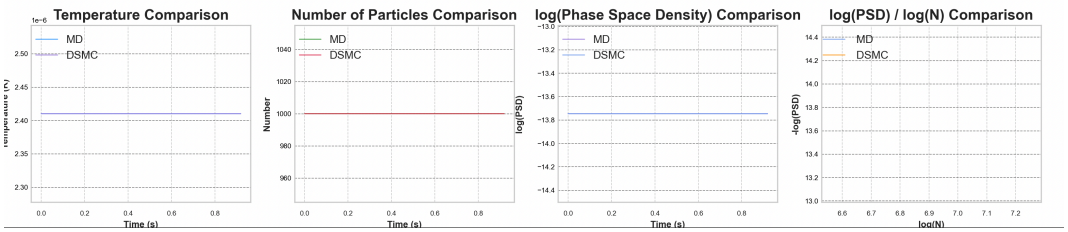


Figure: In a Periodic Boundary Conditions (PBC) box and no trap.

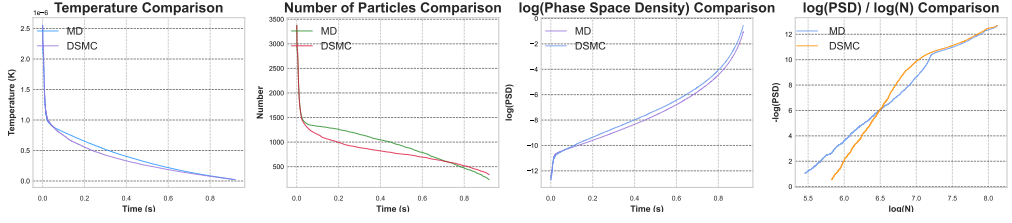


Figure: Use cutoff scheme and xODT.

# DSMC

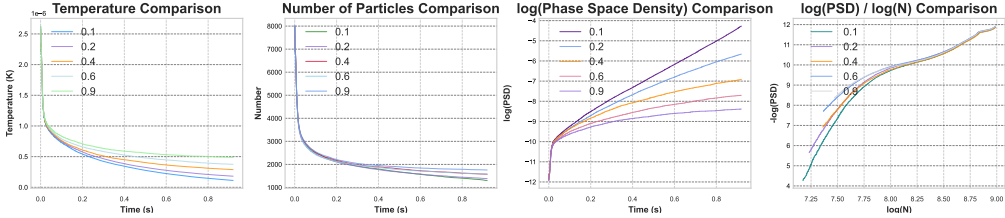


Figure: Change the ratio of final trap depth and initial trap depth.

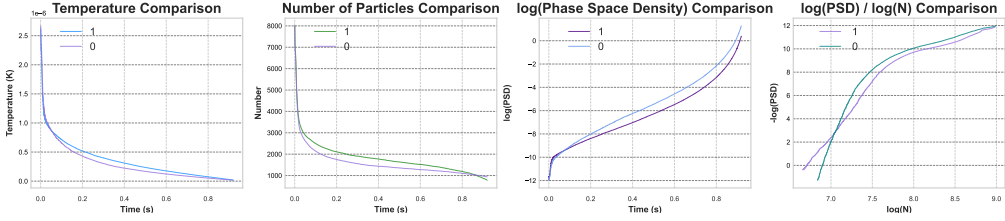


Figure: Pauli blocking factor effect.

# DSMC

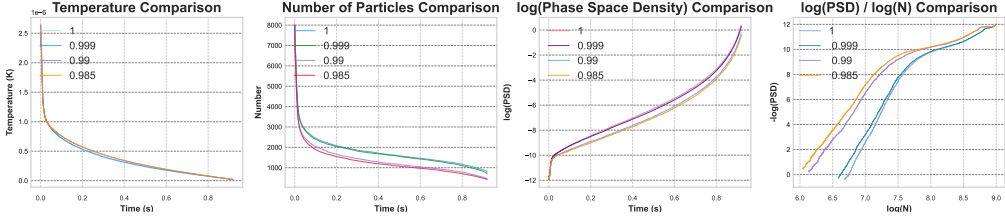


Figure: Change the ratio of elastic cross section and total cross section.

Q & A

# Phase Space Distribution Function

The Boltzmann equation or Boltzmann transport equation (BTE) describes the statistical behaviour of a thermodynamic system not in a state of equilibrium; it was devised by Ludwig Boltzmann in 1872.

The many body system could be described by a 6 dimensional phase space distribution function $f(\mathbf{r}, \mathbf{p}, t)$, which is defined as:

$$\int d^3r\, d^3p\, f(\mathbf{r}, \mathbf{p}, t) = N \tag{16}$$

# Harmonic Trap

In other way, this Gaussion trap $V_{ODT}$ could be seen as harmonic around the trap minima:

$$V_{\text{harm}}(r) = \frac{1}{2} m \sum_{\nu} \omega_{\nu}^2 r_{\nu}^2, \tag{17}$$

where $\omega_\nu$ are the harmonic trap frequencies along coordinate axis $\nu$.

$$A_x = \frac{\alpha_1 P_1 \lambda_1^2 \left(W_{1,y}^4 + W_{1,z}^4\right)}{\pi^3 W_{1,y}^5 W_{1,z}^5} + \frac{4\alpha_2 P_2}{\pi W_{2,x}^3 W_{2,z}} \tag{18a}$$

$$A_y = \frac{4\alpha_1 P_1}{\pi W_{1,y}^3 W_{1,z}} + \frac{\alpha_2 P_2 \lambda_2^2 \left(W_{2,x}^4 + W_{2,z}^4\right)}{\pi^3 W_{2,x}^5 W_{2,z}^5} \tag{18b}$$

$$A_z = \frac{4\alpha_1 P_1}{\pi W_{1,y}^3 W_{1,z}} + \frac{4\alpha_2 P_2}{\pi W_{2,x}^3 W_{2,z}} \tag{18c}$$

The harmonic trap frequencies are defined as:

$$\omega_\nu^2 = \frac{2A_\nu}{m} \tag{19}$$

# Pauli Blocking

When temperature is lower than the Fermi temperature $T_F$, the Pauli blocking must be included into collision term, then the collision term could be written as:

$$\mathcal{I}[f] = \int \frac{d^3p_1}{m} |\mathbf{p}-\mathbf{p}_1| \int d\Omega' \frac{d\sigma}{d\Omega'} \times [f'f'_1(1-h^3f)(1-h^3f_1) - ff_1(1-h^3f')(1-h^3f'_1)] \quad (20)$$

$$k_B T_F = E_F = \hbar\bar{\omega}(6N)^{1/3} \quad (21)$$

# Position Space Cutoff Scheme

A position space cutoff scheme is used to effectively simulate the evaporative cooling following a lowering of the trap depth. A particle is taken as evaporated from this xODT trap if it goes past a position which is 6 times the thermal width of the initial cloud $\sqrt{k_B T_0 / m\omega_\nu^2(0)}$ from the trap minimum:

$$|r_\nu - r_{\nu,\min}| > 6\sqrt{\frac{k_B T_0}{m\omega_\nu^2(0)}} \tag{22}$$

where $T_0$ denotes the initial equilibrium temperature setting at beginning during simulation, $r_{\nu,\min}$ denotes the position of the trap minimum along axis $\nu$ and it was set to be 0 in our simulation.

# Evaporative Cooling Theory

In evaporative cooling theory, $\log_{10}\rho_{\mathrm{PSD}}/\log_{10}N$ describes the forced evaporation trajectory where $\rho_{PSD}$ is the phase space density and $N$ is the particle number of this system. So we could extract an evaporation efficiency through a linear fit of its decrease:

$$\mathcal{E}_{\mathrm{evap}} = -\frac{\partial \log_{10}\rho_{\mathrm{PSD}}}{\partial \log_{10} N} \tag{23}$$

$$\rho_{PSD} = \langle n\rangle \lambda_{th}^3, \quad \lambda_{th} = h/\sqrt{2\pi m k_B T} \tag{24}$$