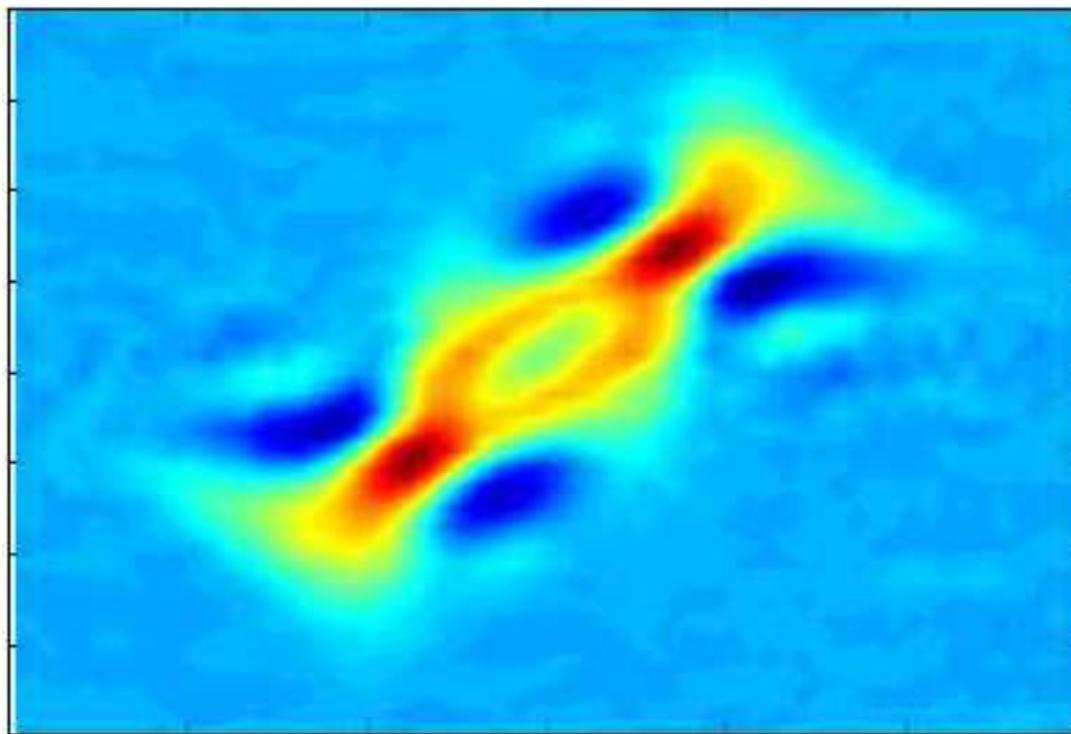


# The Wigner Monte Carlo method for single-body systems



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**MONTE CARLO ALGORITHM FOR SOLVING INTEGRAL  
EQUATIONS WITH POLYNOMIAL NON-LINEARITY.  
PARALLEL IMPLEMENTATION \***

Ivan T. Dimov, Todor V. Gurov

Pliska Stud. Math. Bulgar. **13** (2000), 117-132



Jean Michel Sellier, Mihail Nedjalkov, Ivan Dimov and Siegfried Selberherr

**A benchmark study of the Wigner Monte Carlo method**

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# On the Quantum Correction For Thermodynamic Equilibrium

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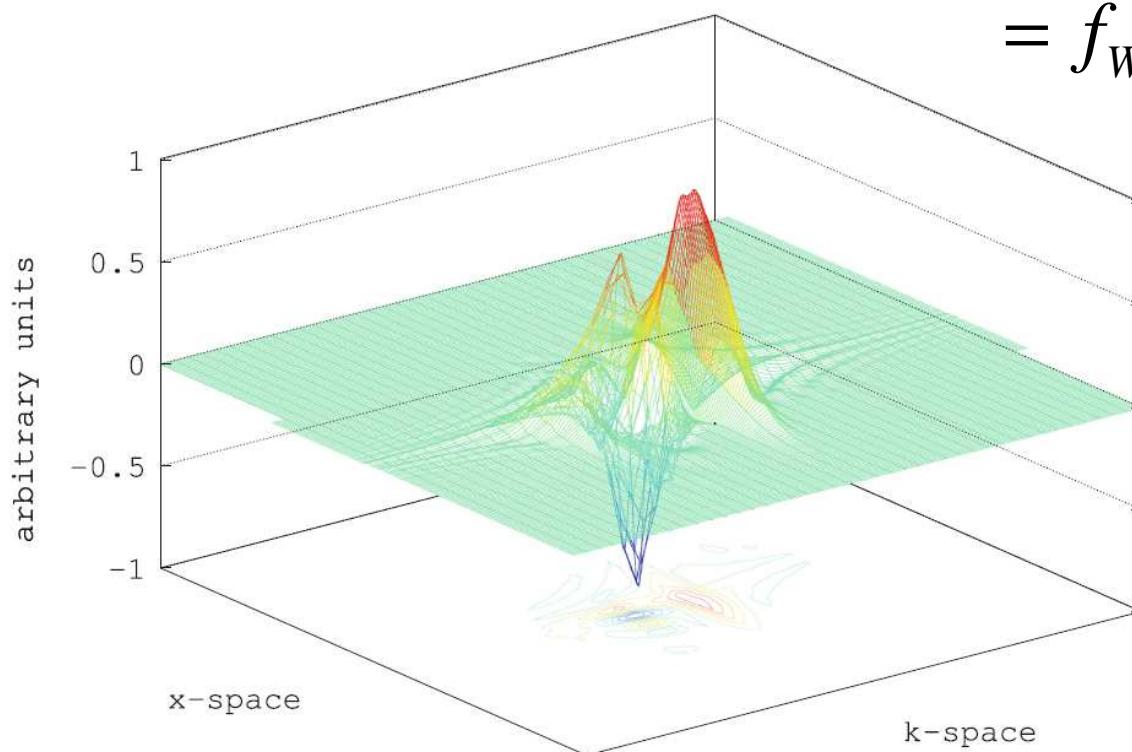
$$\begin{aligned} \frac{\partial f_W}{\partial t} (\mathbf{x}; \mathbf{p}) &= - \frac{\mathbf{p} \cdot \nabla_{\mathbf{x}}}{m} f_W (\mathbf{x}; \mathbf{p}) \\ &+ \int_{-\infty}^{+\infty} d\mathbf{q} f_W (\mathbf{x}; \mathbf{p} + \mathbf{q}) V_W (\mathbf{x}; \mathbf{p}) \end{aligned}$$

# Semi-discrete phase-space

- Discretization of the momentum space

$$\Delta p = \frac{\hbar\pi}{L}$$

$$f_W = f_W(x; p) = \\ = f_W(x; M\Delta p) = f_W(x; M)$$



# Wigner equation in semi-discrete form

- *Reformulation of the single-body Wigner equation in a semi-discrete form.*

$$\frac{\partial f_W(x, M, t)}{\partial t} + \frac{M\Delta p}{m^*} \nabla_{\vec{r}} f_W(x, M, t) =$$

$$= \sum_{n=-\infty}^{+\infty} V_W(x, n) f_W(x, M - n, t)$$

$$V_W(x, n) = \frac{1}{i\hbar} \frac{1}{L} \int_0^{L/2} ds e^{-2sn\Delta p/\hbar} (V(x+s) - V(x-s))$$

# Wigner equation in integral form

- *Reformulation of the semi-discrete Wigner equation as a Fredholm integral equation of 2-nd kind*

$$\begin{aligned} f_W(x, M, t) - e^{-\int_0^t \gamma(x(y)) dy} f_i(x(0), M) &= \\ = \int_0^\infty dt' \sum_{M'= -\infty}^{+\infty} f_W(x(t'), M', t') \Gamma(x', M, M') e^{-\int_{t'}^t \gamma(x(y)) dy} \times \\ \times \theta(t - t') \delta(x' - x(t')) \theta_D(x') \end{aligned}$$

# *Liouville-Neumann series*

- Fredholm equation of second kind

$$f(t) = \phi(t) - \lambda \int_a^b K(t, s) \phi(s) ds$$

- Solution

$$\phi(x) = \sum_{n=0}^{+\infty} \lambda^n \phi_n(x)$$

$$\phi_0(x) = f(x)$$

$$\phi_n(x) = \int K_n(x, z) f(z) dz$$

$$K_n(x, z) = \iiint \dots \int K(x, y_1) K(y_1, y_2) \dots K(y_{n-1}, z) dy_1 dy_2 \dots dy_{n-1}$$

# Mean value of a function

- *Thus, a macroscopic variable can be expressed in terms of the following series*

$$\langle A \rangle(\tau) = \int_0^\infty dt \int dx \sum_{M=-\infty}^{+\infty} f_W(x, M, t) A(x, M) \delta(t - \tau) = \sum_{i=0}^{+\infty} \langle A \rangle_i$$

# Mean value of a function

- *The first few terms read*

$$\langle A \rangle_0(\tau) = \int dx' \sum_{M'=-\infty}^{+\infty} f_i(x_i, M') e^{-\int_0^\tau \gamma(x_i(y)) dy} A(x_i(\tau), M')$$

$$\langle A \rangle_1(\tau) = \int_0^\infty dt' \int dx_i \sum_{M'=-\infty}^{+\infty} f_i(x_i, M') e^{-\int_0^{t'} \gamma(x_i(y)) dy} \theta_D(x_1) \cdot$$

$$\cdot \int_{t'}^\infty dt \sum_{M=-\infty}^{+\infty} \Gamma(x_1, M, M') e^{-\int_{t'}^t \gamma(x_1(y)) dy} A(x_1(t), M, t) \delta(t - \tau)$$

# Physical interpretation

- *Physical interpretation of the terms  $\langle A \rangle_0$ .*

$$\langle A \rangle_0(\tau) = \int dx' \sum_{M'=-\infty}^{+\infty} f_i(x_i, M') e^{-\int_0^\tau \gamma(x_i(y)) dy} A(x_i(\tau), M')$$

# Physical interpretation of

$$\langle A \rangle_0 + \langle A \rangle_1 + \langle A \rangle_2$$

$$\begin{aligned}
\sum_{s=0}^2 \langle A \rangle_s &= \int_0^\tau dt' \int dx_i \sum_{M'=-\infty}^{+\infty} f_i(x_i, M') e^{-\int_0^{t'} \gamma(x_i(y)) dy} \times \\
&[A(x_1(t), M, t) \delta(t' - \tau) + \int_{t'}^\tau dt_1 \sum_{M=-\infty}^{+\infty} \Gamma(x_1, M_1, M') e^{-\int_{t'}^{t_1} \gamma(x_1(y)) dy} \times \\
&[A(x_2(t), M, t) \delta(t_1 - \tau) + \int_{t_1}^\tau dt_2 \sum_{M=-\infty}^{+\infty} \Gamma(x_2, M_2, M) e^{-\int_{t_1}^{t_2} \gamma(x_2(y)) dy} A(x_3(t), M_2, t) \delta(t_2 - \tau)]]
\end{aligned}$$

*The iteration expansion of  $\langle A \rangle$  branches.*

*Interpretation: creation of two new particle (+,-)*

$$\frac{\Gamma(x, M, M')}{\gamma(x)} = \frac{V_W^+(x, M - M')}{\gamma(x)} - \frac{V_W^+(x, M' - M)}{\gamma(x)} + \delta_{M, M'}$$

# Monte Carlo method

- Consider  $\gamma(x) = \sum_{M=-\infty}^{+\infty} V_w^+(x, M) = \sum_{M=-\infty}^{+\infty} V_w^-(x, M)$  as a particle generation rate.
- The Wigner potential generates two particles, one positive and one negative, and the sign carries the quantum information.

