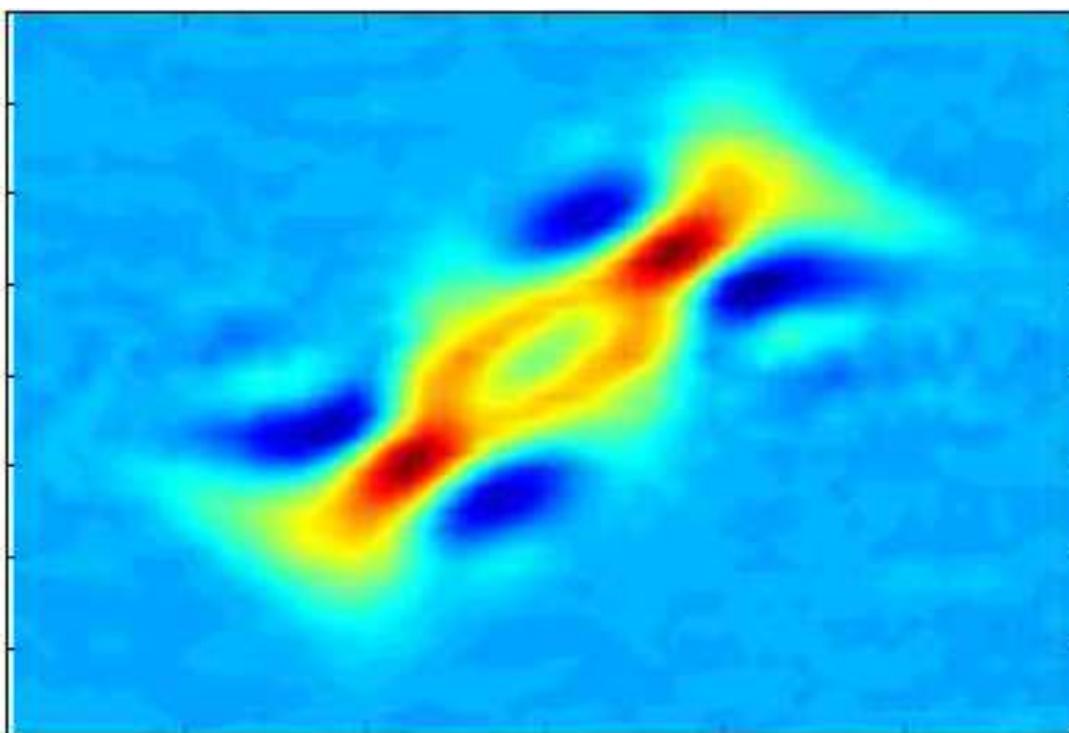
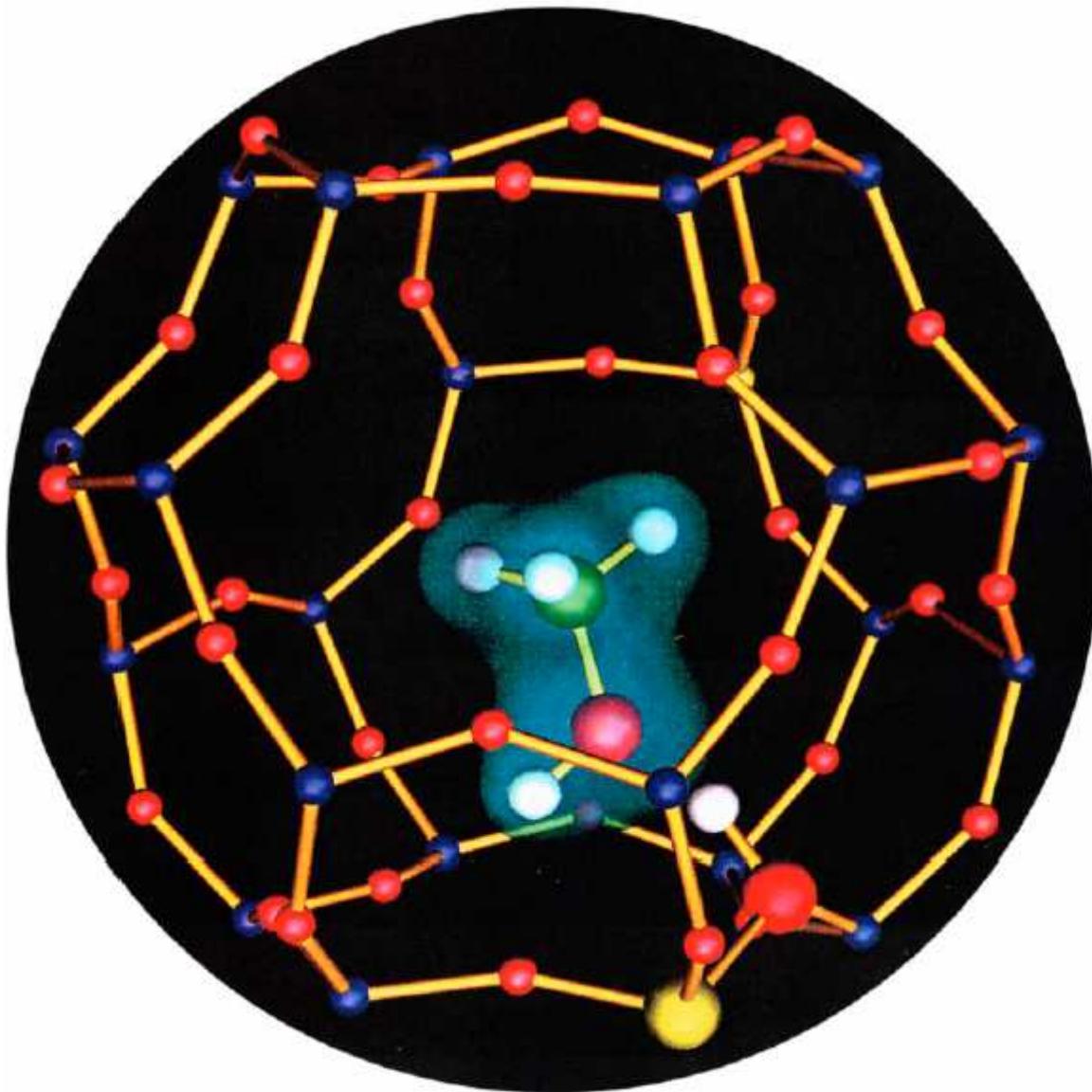


The ab-initio Wigner Monte Carlo method



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W. Kohn: Electronic structure of matter (Nobel Lecture)

The many-body Wigner Monte Carlo method for time-dependent ab-initio quantum simulations

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The many-body Wigner equation

$$\frac{\partial f_W}{\partial t}(\mathbf{x}; \mathbf{p}; t) + \sum_{k=1}^n \frac{\mathbf{p}_k}{m_k} \cdot \nabla_{\mathbf{x}_k} f_W = \int d\mathbf{p} f_W(\mathbf{x}; \mathbf{p}; t) V_W(\mathbf{x}; \mathbf{p}; t)$$

$$V_W(\mathbf{x}; \mathbf{p}; t) = \frac{i}{\pi^{dn} \hbar^{dn+1}} \int d\mathbf{x}' e^{-(\frac{2i}{\hbar}) \sum_{k=1}^n \mathbf{x}'_k \cdot \mathbf{p}_k} \times \\ \times \left[V\left(\mathbf{x} + \frac{\mathbf{x}'}{2}; t\right) - V\left(\mathbf{x} - \frac{\mathbf{x}'}{2}; t\right) \right]$$

$$\int d\mathbf{x}' = \int d\mathbf{x}'_1 \int d\mathbf{x}'_2 \dots \int d\mathbf{x}'_n$$

$$\int d\mathbf{p} = \int d\mathbf{p}_1 \int d\mathbf{p}_2 \dots \int d\mathbf{p}_n$$

The discretized many-body Wigner equation

$$\frac{\partial f_W}{\partial t}(\mathbf{x}; \mathbf{M}; t) + \sum_{k=1}^n \frac{\mathbf{M}_k \Delta \mathbf{p}}{m_k} \cdot \nabla_{\mathbf{x}_k} f_W = \sum_{\mathbf{M}=-\infty}^{+\infty} f_W(\mathbf{x}; \mathbf{M}; t) V_W(\mathbf{x}; \mathbf{M}; t)$$

$$V_W(\mathbf{x}; \mathbf{M}; t) = \frac{i}{\pi^{dn} \hbar^{dn+1}} \int d\mathbf{x}' e^{-(\frac{2i}{\hbar}) \sum_{k=1}^n \mathbf{x}'_k \cdot \mathbf{M}_k \Delta \mathbf{p}} \times \\ \times \left[V\left(\mathbf{x} + \frac{\mathbf{x}'}{2}; t\right) - V\left(\mathbf{x} - \frac{\mathbf{x}'}{2}; t\right) \right]$$

$$\sum_{\mathbf{M}=-\infty}^{+\infty} = \sum_{\mathbf{M}_1=-\infty}^{+\infty} \sum_{\mathbf{M}_2=-\infty}^{+\infty} \cdots \sum_{\mathbf{M}_n=-\infty}^{+\infty}$$

Fredholm equation of second kind

$$f_W(\mathbf{x}; \mathbf{M}; t) - e^{-\int_0^t \gamma(\mathbf{x}(y)) dy} f_i(\mathbf{x}(0); \mathbf{M})$$

$$= \int_0^\infty dt' \sum_{\mathbf{M}'=-\infty}^{+\infty} \int d\mathbf{x}' f_W(\mathbf{x}'; \mathbf{M}'; t') \Gamma(\mathbf{x}'; \mathbf{M}; \mathbf{M}')$$

$$e^{-\int_{t'}^t \gamma(\mathbf{x}(y)) dy} \theta(t - t') \delta(\mathbf{x}' - \mathbf{x}(t')) \theta_D(\mathbf{x}')$$

$$\langle A \rangle(\tau) = \int dt \int d\mathbf{x} \sum_{\mathbf{M}=-\infty}^{\infty} f_W(\mathbf{x}; \mathbf{M}; t) A(\mathbf{x}; \mathbf{M}) \delta(t - \tau)$$

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 (+,-)

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

Quantum 2-body system

$$\begin{aligned} & \frac{\partial f_W}{\partial t}(x_1, x_2; p_1, p_2; t) + \frac{p_1}{m} \frac{\partial f_W}{\partial x_1} + \frac{p_2}{m} \frac{\partial f_W}{\partial x_2} \\ &= \int dp'_1 \int dp'_2 f_W(x_1, x_2; p_1 + p'_1, p_2 + p'_2; t) V_W(x_1, x_2; p'_1, p'_2) \end{aligned}$$

$$\begin{aligned} V_W(x_1, x_2; p_1, p_2) &= \frac{i}{\pi^2 \hbar^3} \int dx'_1 \int dx'_2 e^{-(\frac{2i}{\hbar})(x'_1 p_1 + x'_2 p_2)} \\ &\times [V(x_1 + x'_1, x_2 + x'_2) - V(x_1 - x'_1, x_2 - x'_2)] \end{aligned}$$

Initial Conditions

$$f_W^0(x_1, x_2; p_1, p_2) = N e^{-(\frac{x_1 - x_1^0}{\sigma})^2} e^{-(\frac{x_2 - x_2^0}{\sigma})^2} e^{-(p_1 - p_1^0)^2 \sigma^2} e^{-(p_2 - p_2^0)^2 \sigma^2}$$

$$\begin{aligned} f_W^0(x_1, x_2; p_1, p_2) &= N_1 e^{-(\frac{x_1 - x_1^0}{\sigma})^2} e^{-(p_1 - p_1^0)^2 \sigma^2} \\ &\quad + N_2 e^{-(\frac{x_2 - x_2^0}{\sigma})^2} e^{-(p_2 - p_2^0)^2 \sigma^2} \\ &\quad + N_{12} e^{-(x_1 - x_1^0)^2 \sigma_e^2} e^{-(x_2 - x_2^0)^2 \sigma_e^2} \\ &\quad \times e^{-\frac{|p_1 - p_1^0|}{2\sigma_e}} e^{-\frac{|x_2 - x_2^0|}{2\sigma_e}} \\ &\quad \times 2 \sin\left(\frac{p_1 - p_1^0}{\sigma_e}\right) \\ &\quad \times 2 \sin\left(\frac{p_2 - p_2^0}{\sigma_e}\right), \end{aligned}$$

