

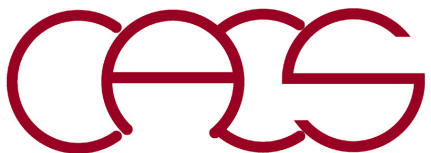
# Molecular Dynamics Simulation: Q & A

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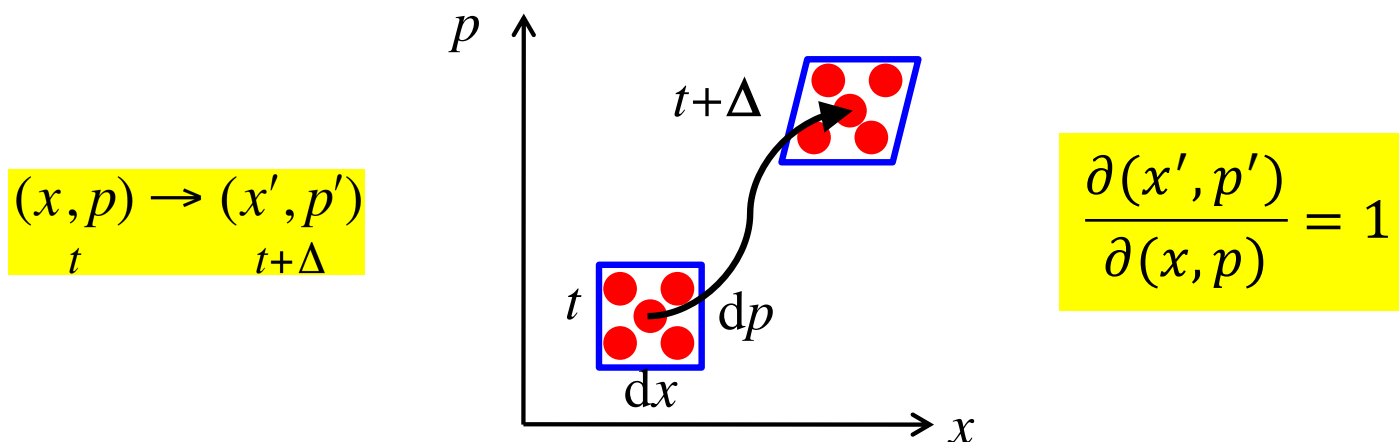
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# Liouville's Theorem

**Q:** Why is it important to preserve the phase-space volume along the molecular-dynamics trajectory?



**A:** Exact phase-space-volume conservation tends to provide long-time stability, though formal analysis of long-time accuracy very hard.

**cf.** Backward error analysis

S. Reich, *SIAM J. Numer. Anal.* **36**, 1549 ('99)

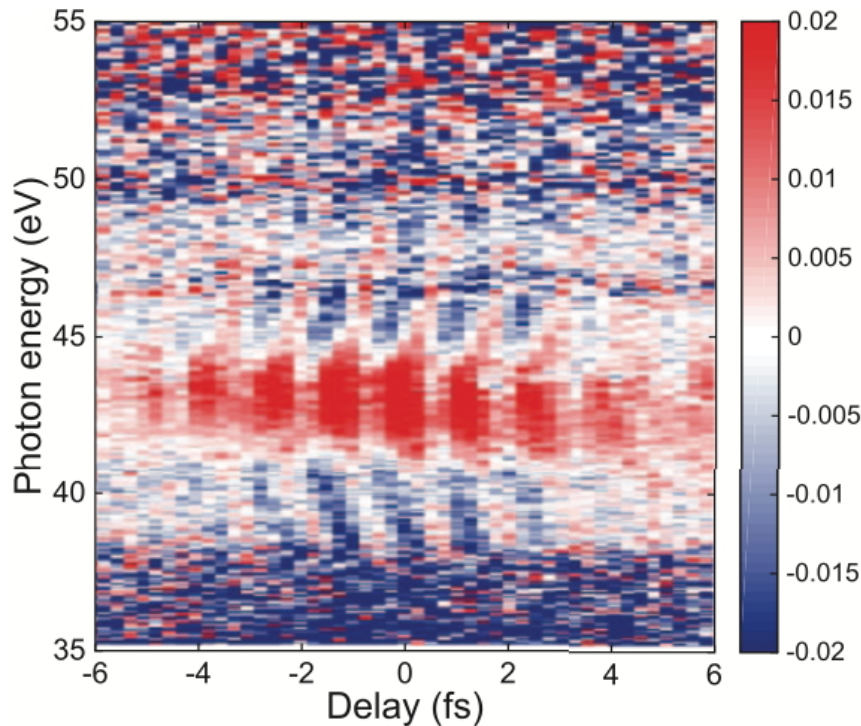
# Velocity Autocorrelation (VAC)

**Q:** VAC in nonsteady state?

**A:** Present it as a function of two time variables.

$$\langle \vec{v}_i(t) \cdot \vec{v}_i(t') \rangle = vac \left( \underbrace{\tau = t - t', T = \frac{t + t'}{2}} \right)$$

No  $T$  dependence in a steady state

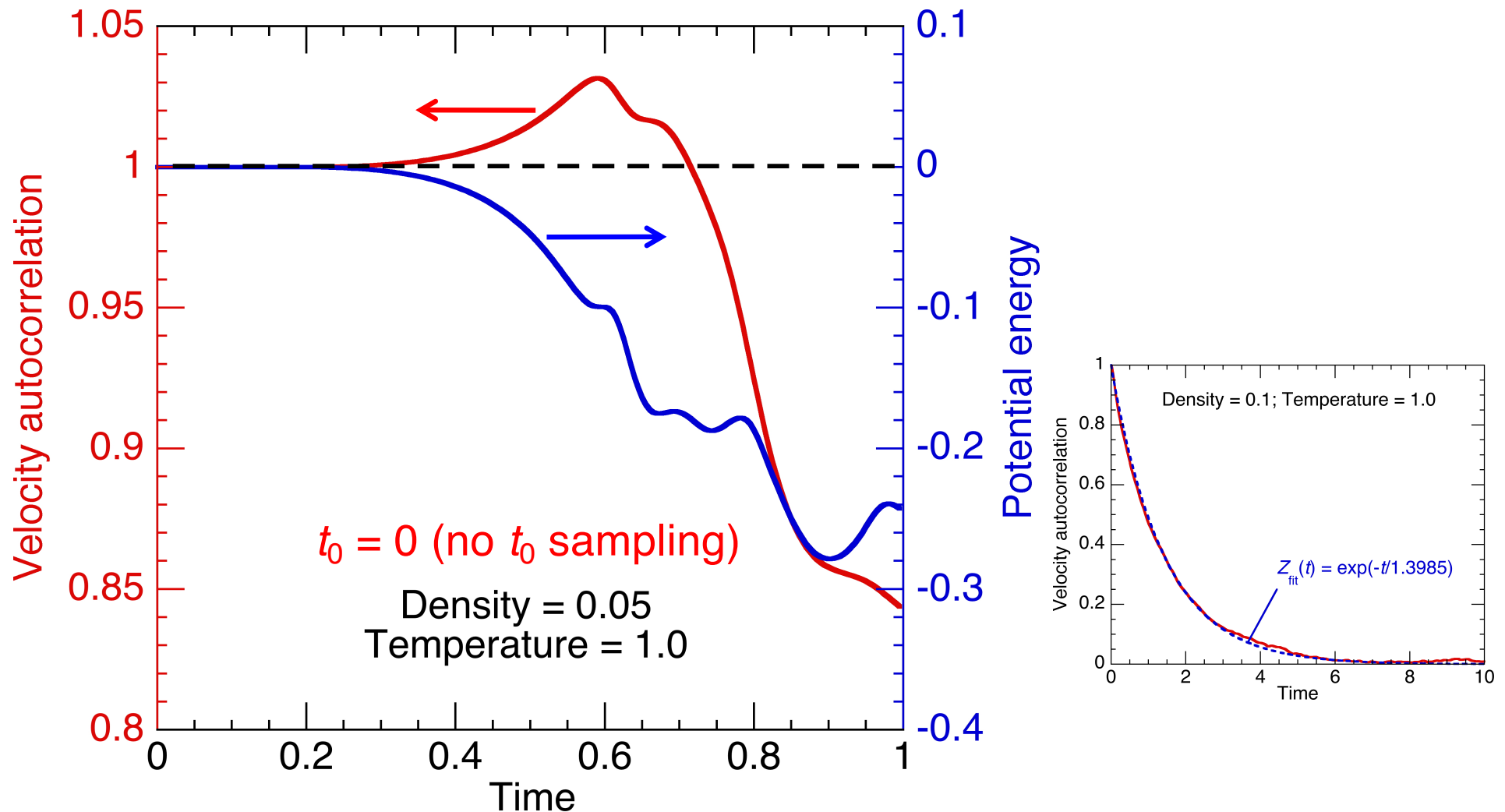


***cf.* Transient photoabsorption spectrum:**  
**Note the atomic-unit energy, 27.2116 eV**  
**=  $h/(0.024 \text{ fs})$ ;  $h$  is Planck's constant**

M. Lucchini *et al.*, *Science* **353**, 916 ('16)

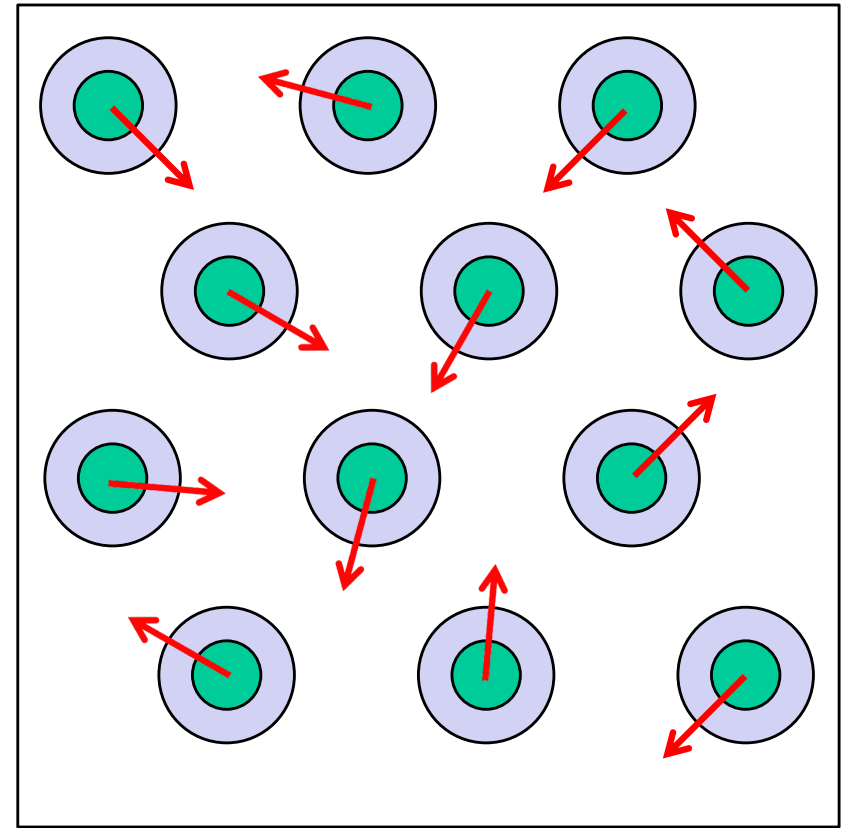
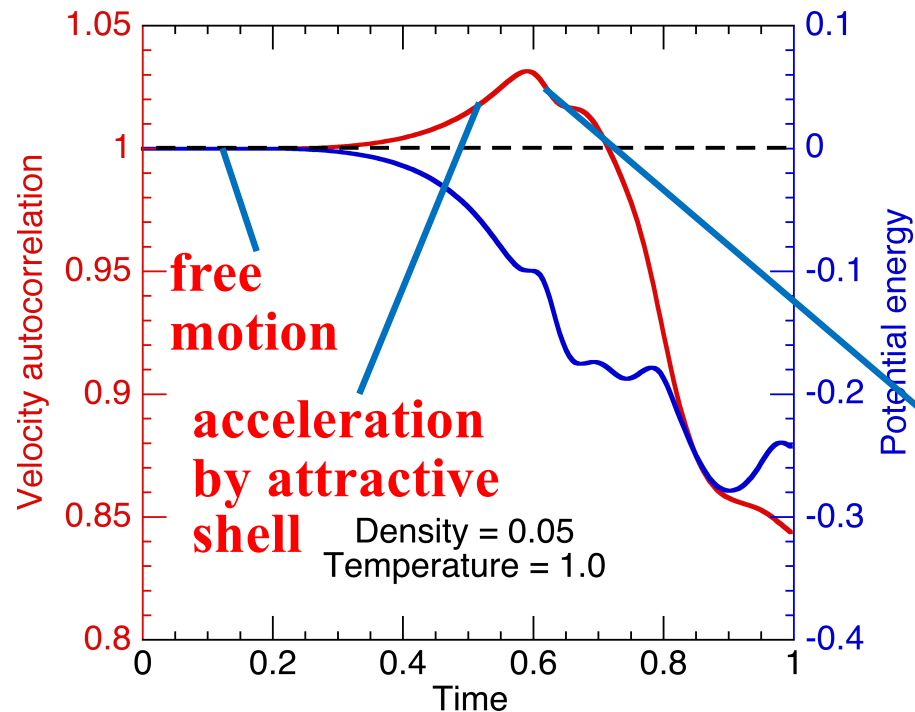
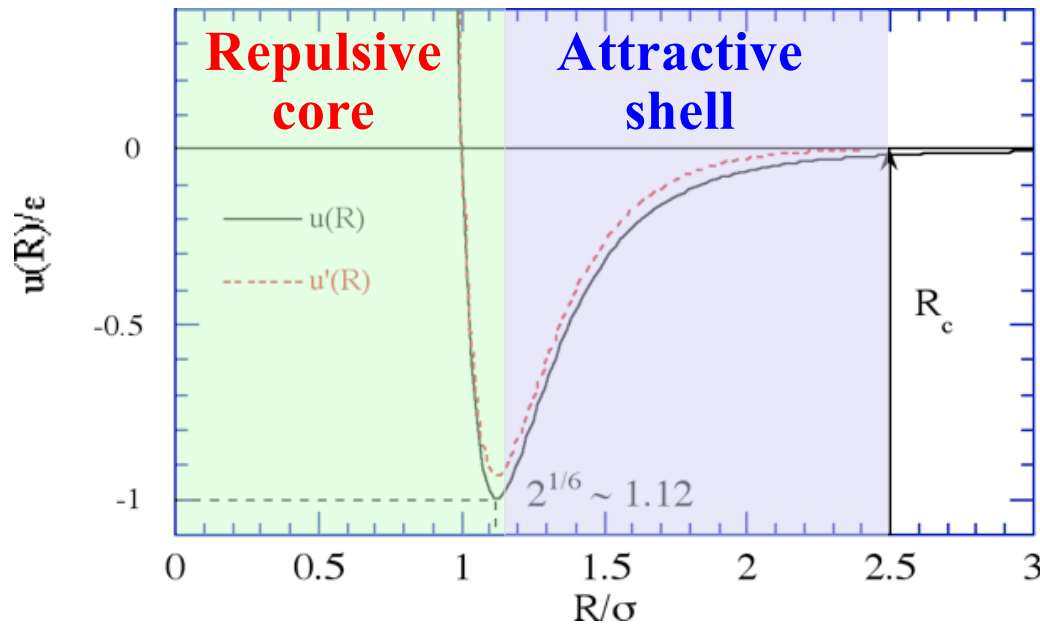
# Velocity Autocorrelation > 1?

- Yes, in a gas phase just when starting from an FCC lattice



- Why? Hint = time variation of the potential energy

# Finite-Range Lennard-Jones Potential



# Why Taylor Expansion?

$$\frac{d}{dt} \Gamma = \hat{L} \Gamma$$

$$\Downarrow \exp(\hat{L}t) \equiv \sum_{n=0}^{\infty} \frac{1}{n!} (\hat{L}t)^n$$

$$\Gamma(t) = \exp(\hat{L}t) \Gamma(0)$$

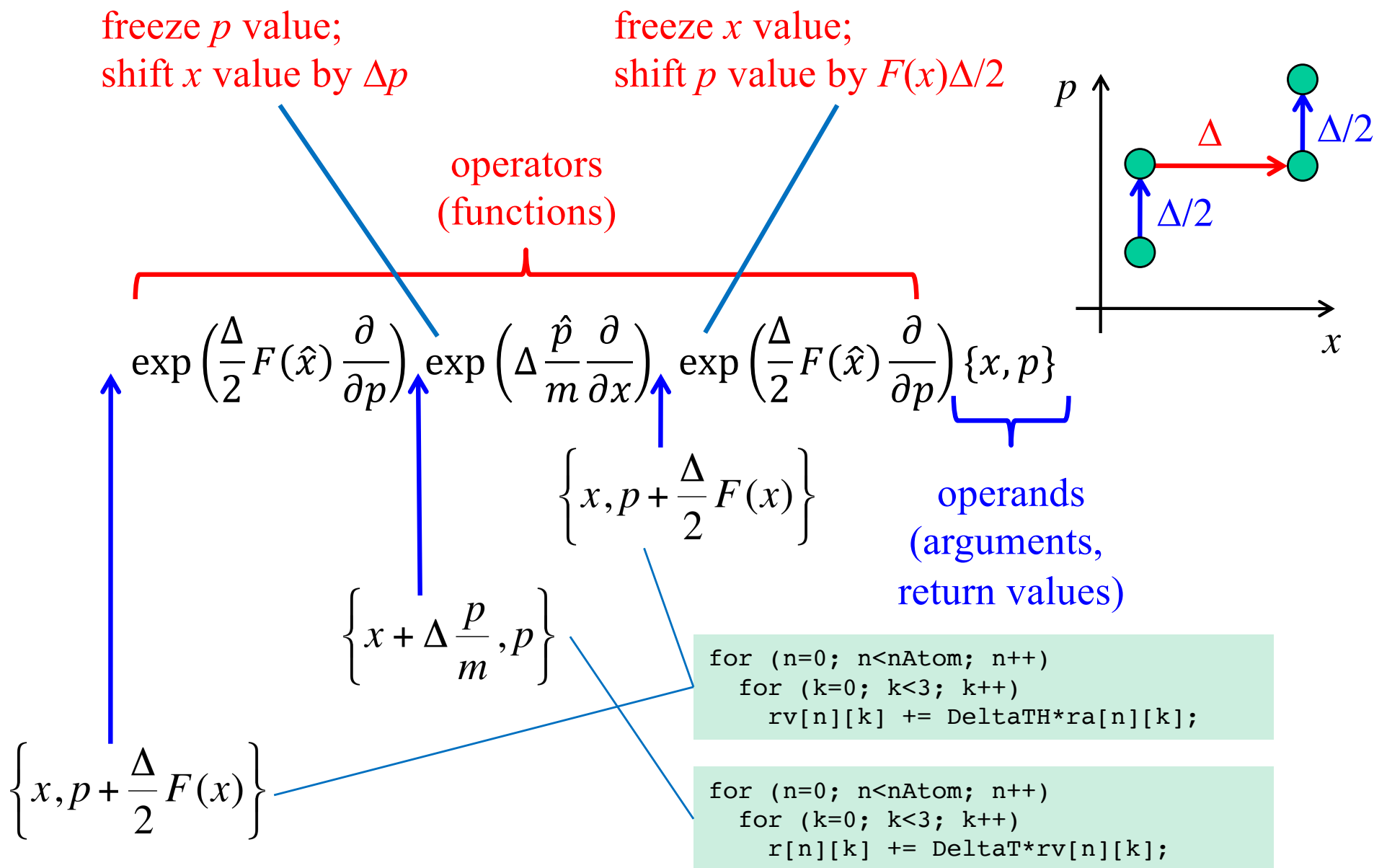
**A:** Exponentiation of a differential operator is “defined” through Taylor expansion, in which the power of the operator is operationally well defined as successive applications of the operator

$$\left( t \left( F(x) \frac{\partial}{\partial p} + \frac{p}{m} \frac{\partial}{\partial x} \right) \right)^3 f(x, p) =$$
$$t \left( F(x) \frac{\partial}{\partial p} + \frac{p}{m} \frac{\partial}{\partial x} \right) \left\{ t \left( F(x) \frac{\partial}{\partial p} + \frac{p}{m} \frac{\partial}{\partial x} \right) \left[ t \left( F(x) \frac{\partial}{\partial p} + \frac{p}{m} \frac{\partial}{\partial x} \right) f(x, p) \right] \right\}$$

**But, it is very hard to obtain a closed form**

$$\{?, ?\} = \exp \left[ t \left( F(x) \frac{\partial}{\partial p} + \frac{p}{m} \frac{\partial}{\partial x} \right) \right] \{x, p\}$$

# Velocity Verlet Time Propagator?



**It's shift operation!**

# Explicit Form of Mapping?

