# Fermionic Molecular Dynamics for Colliding and Decaying Nuclei

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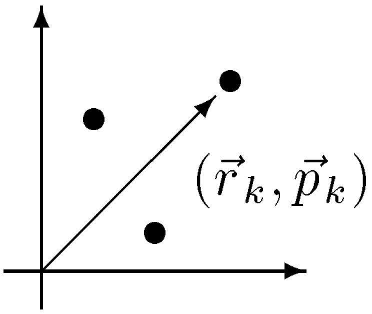
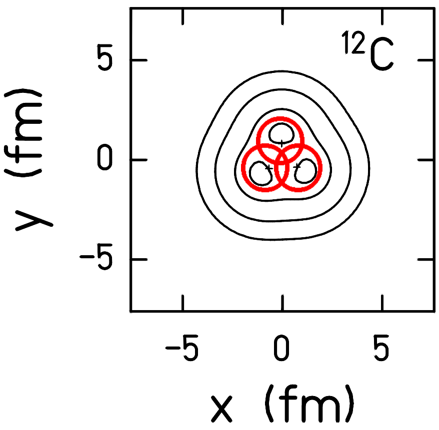
## Classical Molecular Dynamics:




- $\dot{\vec{r}}_k = \frac{\partial H}{\partial \vec{p}_k}$ , $\dot{\vec{p}}_k = -\frac{\partial H}{\partial \vec{r}_k}$
- distinguishable particles
- points in phase space
- BOLTZMANN statistics

## Fermionic Molecular Dynamics (FMD):




- $\sum_\nu \mathcal{A}_{\mu\nu} \dot{q}_\nu = -\frac{\partial \mathcal{H}}{\partial q_\mu}$ ,
  $q_\mu \equiv \{\vec{r}_k, \vec{p}_k, a_k, \chi_k, \phi_k\}$
- indistinguishable particles
- localized wave packets
- FERMI–DIRAC statistics

# Equations of Motion

**Ingredients:**

1. Antisymmetrized Many–Body State

$$|\,Q(t)\,\rangle = \frac{1}{\sqrt{N}}\mathcal{A}\Big(\,|\,q_1(t)\,\rangle \otimes \,|\,q_2(t)\,\rangle \otimes \cdots \otimes \,|\,q_A(t)\,\rangle\Big)$$

$|\,q_k(t)\,\rangle$ parametrized single–particle state

2. Time–Dependent Variational Principle

$$\delta \int_{t_1}^{t_2} dt\,\langle\, Q(t)\,|\, i\frac{d}{dt} \;-\; \underset{\sim}{H}\,|\,Q(t)\,\rangle = 0$$

3. Single–Particle State

$$\langle\,\vec{x}\,|\,q(t)\,\rangle = \exp\left\{-\frac{(\,\vec{x}\,-\vec{r}\,(t)\,)^2}{2\,a(t)} + i\vec{p}\,(t)\cdot\vec{x}\right\} \otimes |\,\chi(t),\phi(t)\,\rangle \otimes |\,\xi\,\rangle$$

$\vec{r}\,(t)$ : mean position, $\vec{p}\,(t)$ : mean momentum,
$a(t)$ : complex width, $\chi(t), \phi(t)$ : spin angles,
$\xi$ : time–independent isospin–3–component

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$$\sum_\nu \mathcal{A}_{\mu\nu}\dot{q}_\nu = -\frac{\partial \mathcal{H}}{\partial q_\mu}$$

$$\mathcal{A}_{\mu\nu} = \frac{\partial^2 \mathcal{L}_0}{\partial \dot{q}_\mu \partial q_\nu} - \frac{\partial^2 \mathcal{L}_0}{\partial \dot{q}_\nu \partial q_\mu}$$

$$\mathcal{H} = \langle\, Q\,|\,\underset{\sim}{H}\,|\,Q\,\rangle$$

$$\mathcal{L}_0 = \langle\, Q\,|\, i\,\tfrac{d}{dt}\;\;|\,Q\,\rangle$$

# Conservation Laws

**1. Generalized Poisson Brackets:**

$\underset{\sim}{B}$ be a time-independent operator.

$$\frac{d}{dt}\,\mathcal{B}(t) = \frac{d}{dt}\,\langle\, Q(t)\,|\,\underset{\sim}{B}\,|\,Q(t)\,\rangle = \sum_{\nu} \dot{q}_\nu\,\frac{\partial}{\partial q_\nu}\,\mathcal{B}$$

$$= \sum_{\mu,\nu} \frac{\partial\,\mathcal{H}}{\partial q_\mu}\,\mathcal{A}^{-1}_{\mu\nu}\,\frac{\partial\,\mathcal{B}}{\partial q_\nu} =: \{\mathcal{H},\mathcal{B}\}$$

**2. Conservation Laws:**

- for time-independent operators $\underset{\sim}{B}$

  $$\frac{d}{dt}\,\mathcal{B}(t) = 0 \ \text{ if } \ \{\mathcal{H},\mathcal{B}\} = \sum_{\mu,\nu} \frac{\partial\,\mathcal{H}}{\partial q_\mu}\,\mathcal{A}^{-1}_{\mu\nu}\,\frac{\partial\,\mathcal{B}}{\partial q_\nu} = 0$$

  obviously for $\underset{\sim}{H}$ since $\mathcal{A}$ and $\mathcal{A}^{-1}$ skew symmetric

- for generators $\underset{\sim}{G}$ which do not map out of the set of trial states and commute with $\underset{\sim}{H}$

  $$\frac{d}{dt}\,\mathcal{G}(t) = \{\mathcal{H},\mathcal{G}\} = \langle\, Q(t)\,|\,i\,[\,\underset{\sim}{H},\underset{\sim}{G}\,]\ \,|\,Q(t)\,\rangle$$

  Relates the choise of the trial state to possible conservation laws, e.g. total momentum conservation is possible if a translated trial state is again a valid trial state.

# Trial State and Expectation Values

**1. Trial State:**

$$\langle\, \vec{x}\, |\, q(t)\, \rangle = \exp\left\{ -\frac{(\,\vec{x}\, - \vec{r}\,(t)\,)^2}{2\,a(t)} + i\vec{p}\,(t)\cdot\vec{x} \right\} \otimes |\,\chi(t), \phi(t)\,\rangle \otimes |\,\xi\,\rangle$$

$\vec{r}\,(t)$ : mean position, $\vec{p}\,(t)$ : mean momentum,
$a(t)$ : complex width, $\chi(t), \phi(t)$ : spin angles,
$\xi$ : time–independent isospin–3–component

$$|\,Q(t)\,\rangle = \frac{1}{\sqrt{N}} \sum_{\pi} \mathrm{sign}(\pi)\, |\,q_{\pi(1)}(t)\,\rangle \otimes |\,q_{\pi(2)}(t)\,\rangle \otimes \cdots \otimes |\,q_{\pi(A)}(t)\,\rangle$$

antisymmetrized many–body state

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**2. Expectation Values:**

$\left(\mathcal{O}^{-1}\right)_{kl} := \langle\, q_k\, |\, q_l\,\rangle$ ; inverse overlapp matrix

$$\langle\, Q\, |\, \underset{\sim}{T}\, |\, Q\,\rangle = \sum_{k,l}^{A} \langle\, q_k\, |\, \underset{\sim}{t}\, |\, q_l\,\rangle\ \mathcal{O}_{lk}$$ kinetic energy

$$\langle\, Q\, |\, \underset{\sim}{V}\, |\, Q\,\rangle = \frac{1}{2} \sum_{k,l,m,n}^{A} \langle q_k q_l |\, \underset{\sim}{v}\, | q_m q_n \rangle \left( \mathcal{O}_{mk}\mathcal{O}_{nl} - \mathcal{O}_{ml}\mathcal{O}_{nk} \right)$$

potential energy

# Ground States in FMD

**Ground State:**

- The ground state is the state $|\, Q \,\rangle$ which is the lowest one in energy.
- $\frac{\partial}{\partial q_\mu} \langle\, Q \,|\, \underset{\sim}{H} \,|\, Q \,\rangle = 0 \quad \forall q_\mu$
- therefore $\dot{q_\mu} = 0 \quad \forall q_\mu$;
  ground state absolutely stationary

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**Potential (Volkov V2 and Coulomb):**

$$V(\vec{x}_{12}) = \left( V_1 \exp\left\{ -\frac{\vec{x}_{12}^2}{r_1^2} \right\} + V_2 \exp\left\{ -\frac{\vec{x}_{12}^2}{r_2^2} \right\} \right) \left( w + m \underset{\sim}{P}^{\vec{r}} \right)$$
$$+ \frac{V_c}{|\vec{x}_{12}|}$$

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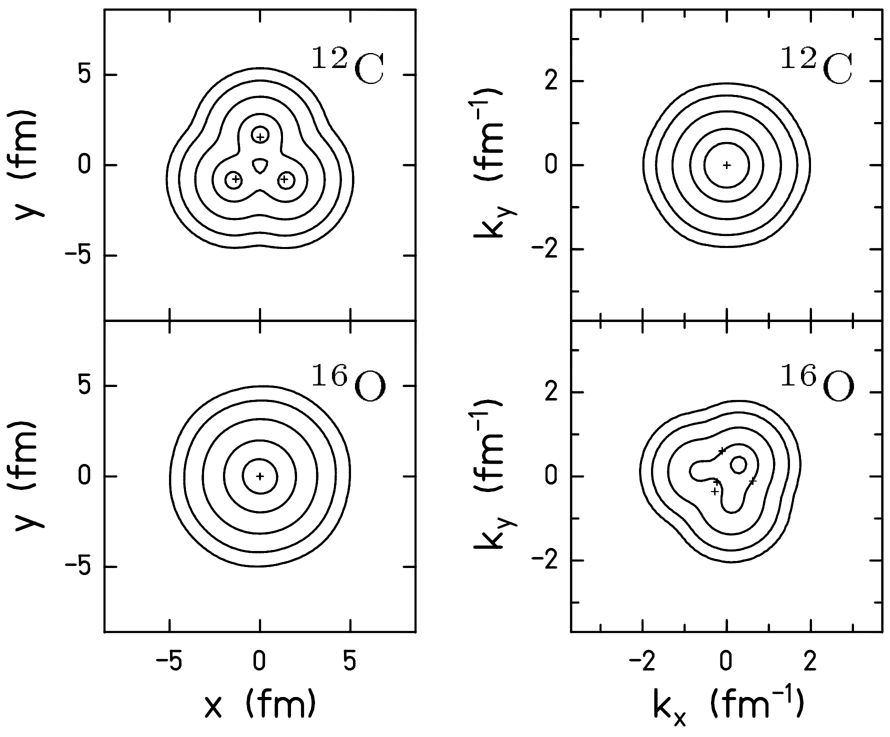

# Effect of the Pauli Principle on Trajectories

**Pauli Principle acts in:**

- $\langle \underset{\sim}{V} \rangle$ via exchange terms
  (additional momentum dependence)

- Matrix $\mathcal{A}_{\mu\nu}$ (metric, virtual forces)

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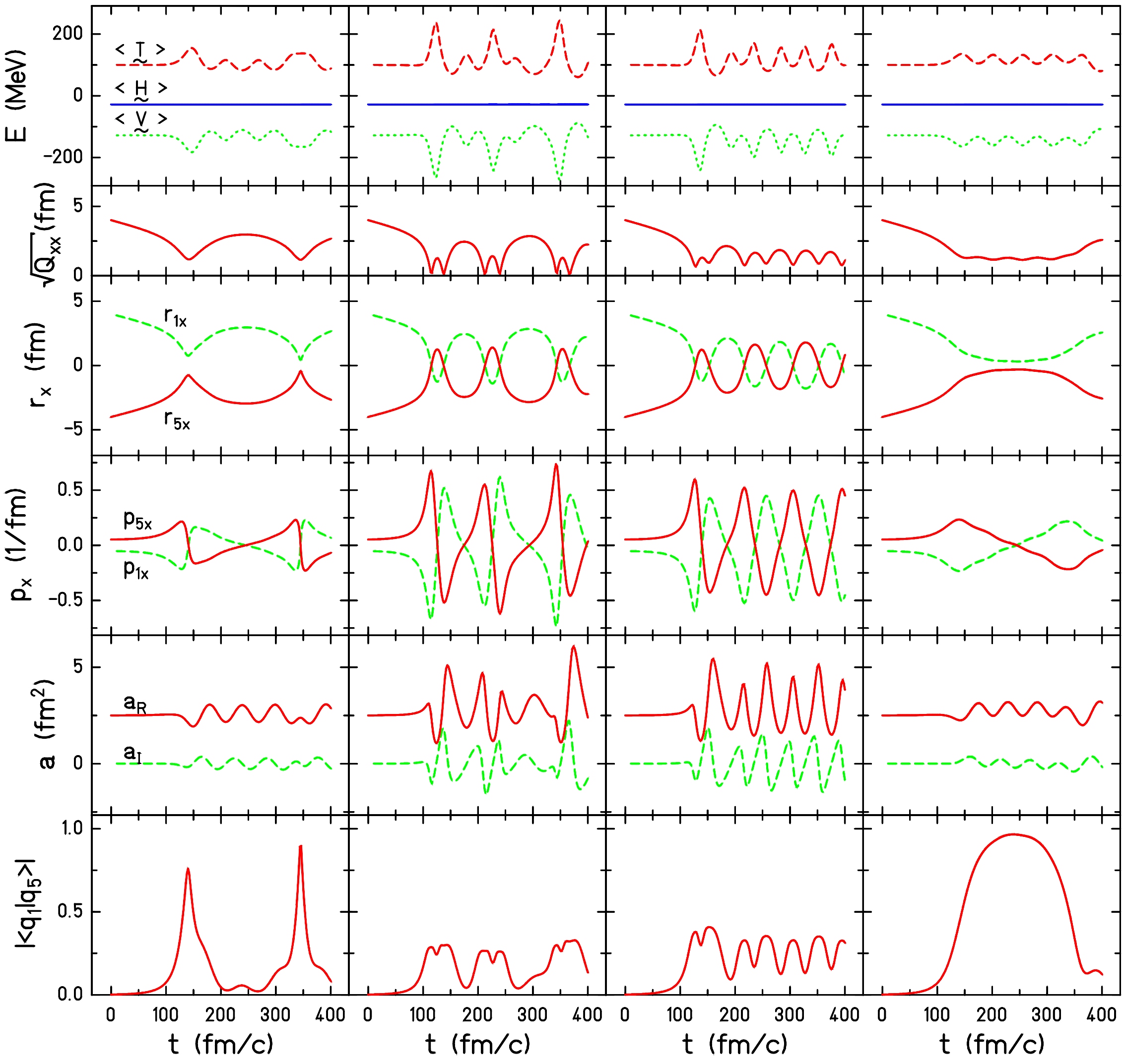
$^4$**He–**$^4$**He–collisions:**



# Role of the Dynamical Width Parameter

**Important Degree of Freedom for Evaporation and Fragmentation:**

- A packet with fixed width carries always $\approx 10$ MeV zero–point energy.
- A packet with time–dependent width "pays binding with zero–point energy", i.e., it spreads in coordinate space ( little overlapp) and shrinks in momentum space (less zero–point energy).

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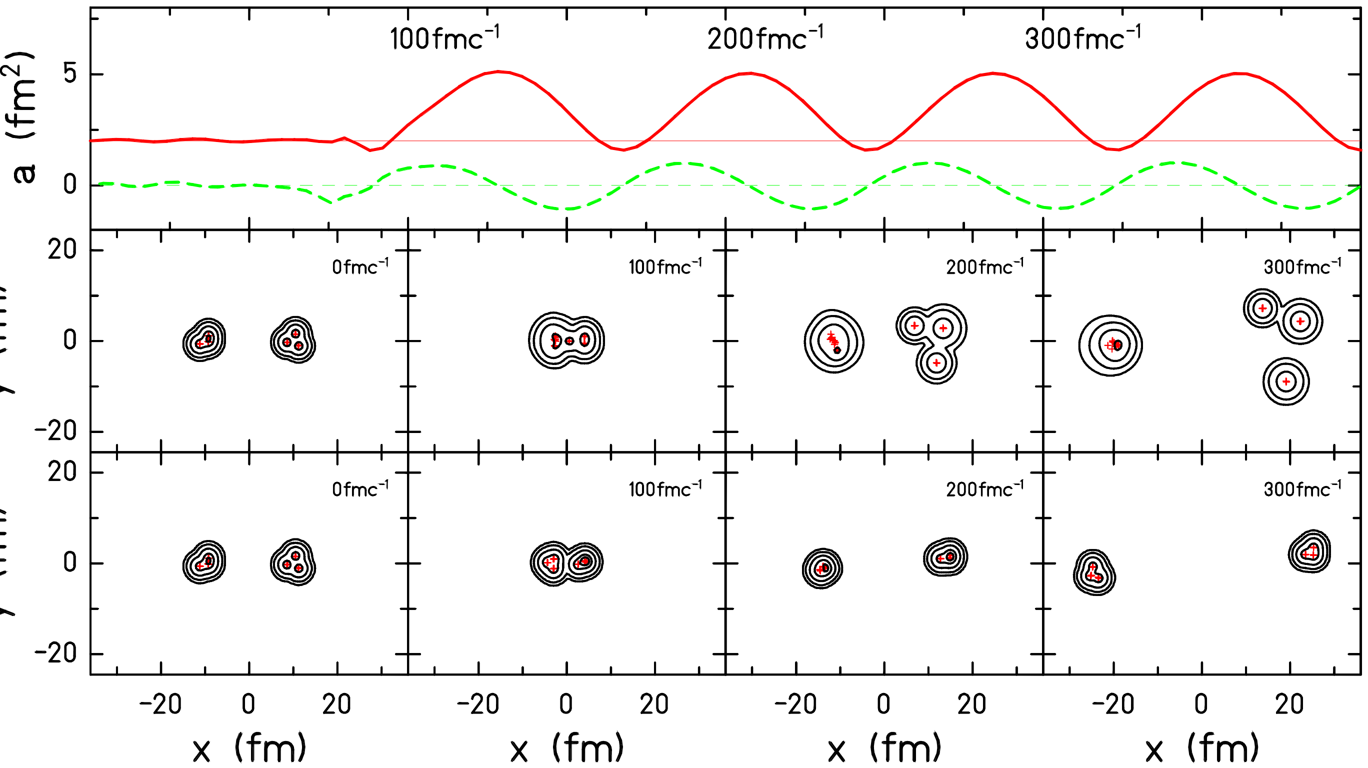
**$^{12}$C–$^{12}$C–Collisions(Dynamical & Fixed Width):**



# Event Ensemble

**Definition of the Event Ensemble:**

- FMD ground states have to be treated like intrinsically deformed Hartree–Fock states.
- The event ensemble consists of all orientations of the two initial ground states: $|\,Q\,;\vec{\Omega}_1,\vec{\Omega}_2\,\rangle$ .
  The same holds for the impact parameter.
- Within the ensemble large fluctuations arise.

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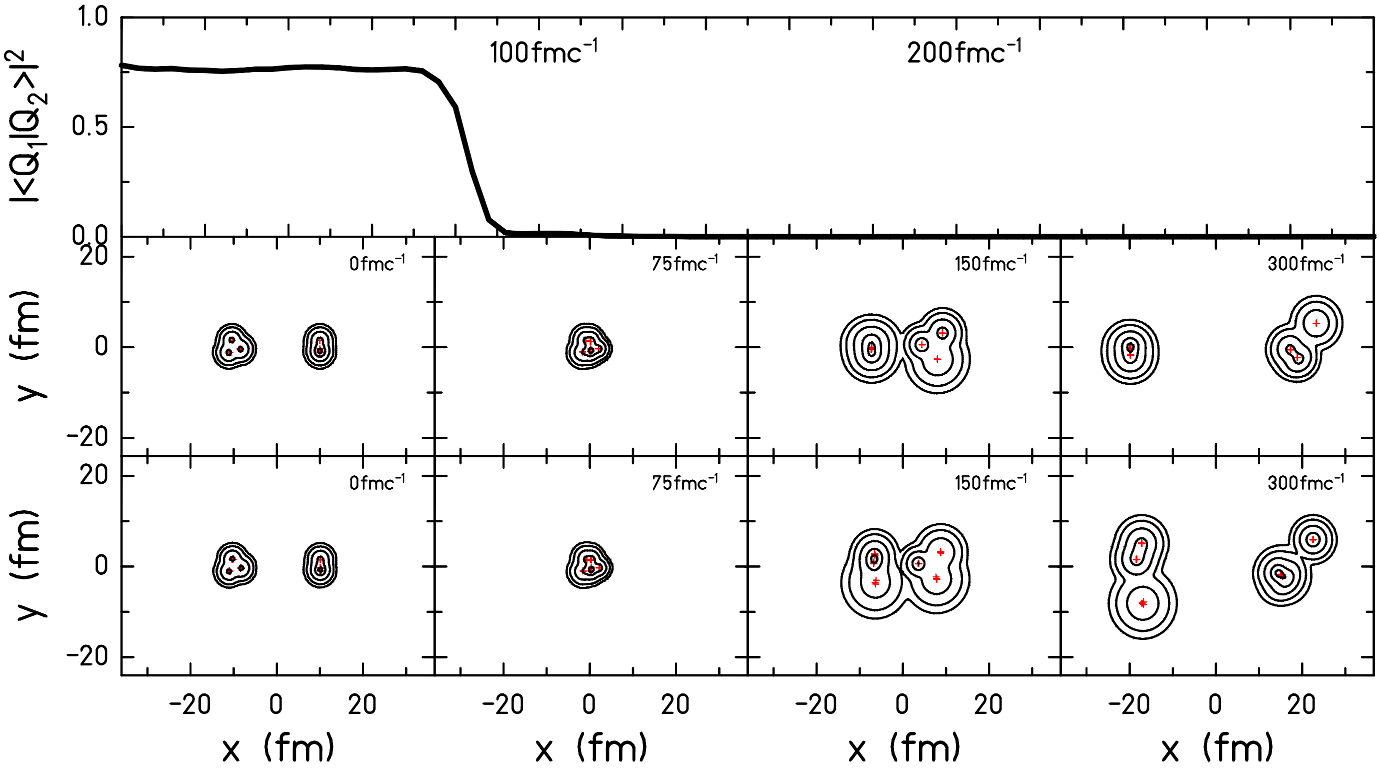
**Overlapp of Two $^{12}$C–$^{12}$C–Collisions:**



# Statistical Properties of FMD – 1

**The Ergodic ensemble:**

The statistical operator $\underset{\sim}{R}_{\text{erg}}$:

$$\underset{\sim}{R}_{\text{erg}} \quad := \quad \lim_{t_2 \to \infty} \frac{1}{(t_2 - t_1)} \int_{t_1}^{t_2} \mathrm{d}t \ |\, Q(t)\,\rangle\langle\, Q(t)\,|$$

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The ergodic mean of an operator $\underset{\sim}{B}$:

$$\overline{\langle\, \underset{\sim}{B} \,\rangle}\Big|_{\langle\, \underset{\sim}{H} \,\rangle} \quad := \quad \mathrm{Tr}\,(\underset{\sim}{R}_{\text{erg}}\ \underset{\sim}{B})$$

$$= \quad \lim_{t_2 \to \infty} \frac{1}{(t_2 - t_1)} \int_{t_1}^{t_2} \mathrm{d}t \ \langle\, Q(t)\,|\, \underset{\sim}{B} \,|\, Q(t)\,\rangle$$

- Time–averaging instead of ensemble–averaging.
- If the ergodic assumption is fulfilled, the statistical operator should only depend on $\langle\, \underset{\sim}{H} \,\rangle$ , but not on $|\, Q(t_1)\,\rangle$, $\underset{\sim}{H}$ or the equations of motion.
- Since $\langle\, \underset{\sim}{H} \,\rangle$ is a constant of motion, the average in the ergodic ensemble is always perfomed at the same expectation value of the Hamilton operator.

# Statistical Properties of FMD – 2

**Equations of Motion for Wave Packets in a Common Harmonic Oscillator Potential:**

Single-Particle Wave Packet:

$$\langle\, \vec{x} \,|\, q_l(t)\,\rangle = \exp\left\{ -\frac{(\,\vec{x} - \vec{b}_l(t)\,)^2}{2\,a_l(t)} \right\} \;,\; \vec{b}_l = \vec{r}_l + i a_l\, \vec{p}_l$$

Hamilton Operator:

$$\underset{\sim}{H} = \sum_{l=1}^{A} \underset{\sim}{h}(l) \;, \quad \underset{\sim}{h}(l) = \frac{\underset{\sim}{\vec{k}}^2(l)}{2m} + \frac{1}{2}\, m\omega^2\, \underset{\sim}{\vec{x}}^2(l)$$

Equations of Motion:

$$\Rightarrow \left\{ \begin{array}{l} \dfrac{d}{dt}\,\vec{b}_l = -im\omega^2 a_l \vec{b}_l \quad \left( \Rightarrow \dot{\vec{r}}_l = \frac{\vec{p}_l}{m} \;,\; \dot{\vec{p}}_l = -m\omega^2 \vec{r}_l \right) \\ \dfrac{d}{dt}\, a_l = -im\omega^2 a_l^2 + \frac{i}{m} \end{array} \right.$$

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- The parameters $\vec{r}_l$ and $\vec{p}_l$ follow the classical trajectories. Nevertheless, the parametrized trial state is the exact solution of the Schrödinger equation.

- Since $\underset{\sim}{H}$ is a one–body operator, the equations of motion of the parameters are the same, regardless whether the many–body state is antisymmetrized, symmetrized or simply a product state.

# Statistical Properties of FMD – 3

**The Canonical Ensemble of Fermions in a Common Harmonic Oscillator Potential:**

The statistical operator $\underset{\sim}{R}(T)$:

$$\underset{\sim}{R}(T) \quad = \quad \frac{1}{Z(T)} \exp\left\{-\frac{\underset{\sim}{H}}{T}\right\}$$

The ensemble mean of an operator $\underset{\sim}{B}$:

$$\begin{aligned} \langle\langle\, \underset{\sim}{B} \,\rangle\rangle\Big|_T \quad &:= \quad \mathrm{Tr}\,(\underset{\sim}{R}(T)\; \underset{\sim}{B}) \\ &= \quad \frac{1}{Z(T)} \sum_{n_1,\dots,n_A=0}^{\infty} {}_a\langle\, n_1,\dots,n_A \,|\, \underset{\sim}{B} \,|\, n_1,\dots,n_A \,\rangle_a \\ &\qquad \times \exp\left\{-\frac{1}{T}\, E(n_1,\dots,n_A)\right\} \end{aligned}$$

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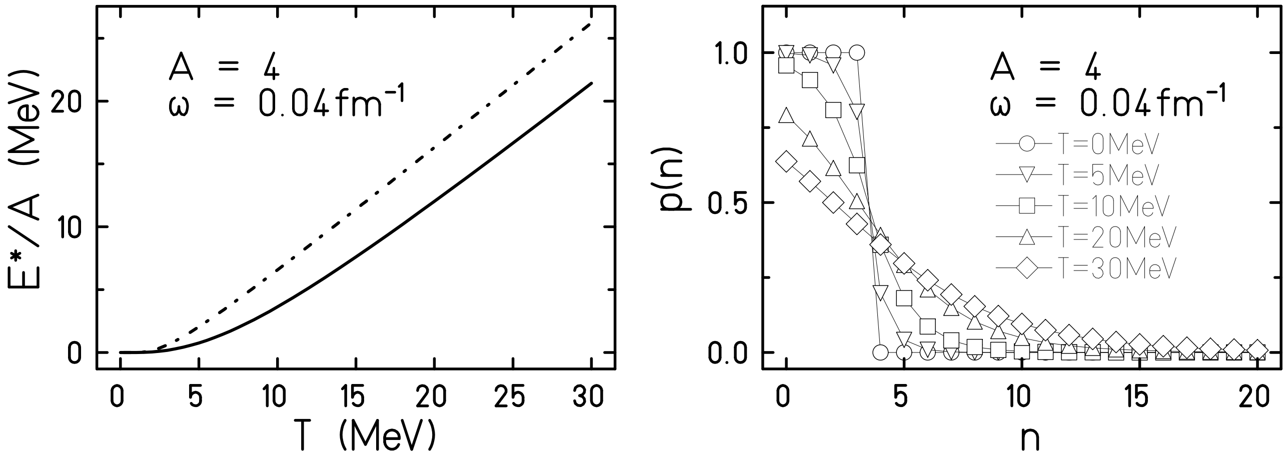
- $|\, n_1, \dots, n_A \,\rangle_a$ denotes the Slater determinant composed of single–particle oscillator eigenstates $|\, n_1 \,\rangle, \dots, |\, n_A \,\rangle$.
- $E(n_1, \dots, n_A)$ is the eigenenergy belonging to $|\, n_1, \dots, n_A \,\rangle_a$.

# Statistical Properties of FMD – 4

**Excitation Energy and Occupation Probabilities in the Canonical Ensemble:**




$$E^* = \langle\langle \underset{\sim}{H} - E_0 \rangle\rangle \Big|_T \quad , \quad E_0 = 8\,\omega \; .$$

$$p(n) = \langle\langle \underset{\sim}{c}_n^+ \underset{\sim}{c}_n \rangle\rangle \Big|_T \quad , \quad \underset{\sim}{c}_n^+ \,|\,0\,\rangle = \,|\,n\,\rangle$$

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- Now compare the canonical ensemble and the ergodic ensemble at the same excitation energy $E^*$, which is related to a temperature in the canonical ensemble.

$$\langle\langle \underset{\sim}{H} - E_0 \rangle\rangle \Big|_T = \overline{\langle\, \underset{\sim}{H} - E_0 \,\rangle} \Big|_{\langle \underset{\sim}{H} \rangle}$$

# Statistical Properties of FMD – 5

## Occupation Numbers in the Ergodic Ensemble:

- In order to equilibrate the system a repulsive short–range interaction $\underset{\sim}{V}_I$ is introduced, which is small compared to the level spacing of the oscillator. Time–averaging is done over about 2000 periods.
- Numerically there is no difference between the ergodic and the canonical ensemble, provided both have the same excitation energy. This equivalence attributes a temperature to the pure many–body state $\mid Q(t)\,\rangle$.
- The FMD many–body trajectory covers the phase space according to Fermi–Dirac statistics.

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