Fermionic Molecular Dynamics: Ensembles and Fluctuations therein

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Abstract

Fermionic Molecular Dynamics models a system of fermions by means of a trial many-body state composed of an antisymmetrized product of single-particle states which are localized gaussians in coordinate and momentum space. The parameters specifying them are the analogue to the variables in classical molecular dynamics. The time-dependent variational principle yields the equations of motion which are solved for heavy-ion collisions. These calculations show a great variety of phenomena including explosion, sequential fragmentation and multifragmentation. In this contribution we present an approximation for the expectation value of the two-body interaction, define the ensemble of events and show that large fluctuations arise therein.

1 The Fermionic Molecular Dynamics (FMD) Model

The equations of motion in FMD [1] are derived from the time-dependent variational principle of quantum mechanics

$$\delta \int_{t_1}^{t_2} dt \, \langle\, Q \,|\; i\frac{d}{dt} - \underset{\sim}{H} \;|\, Q \,\rangle \;=\; 0 \;, \tag{1}$$

where the trial many-body state $|\, Q \,\rangle = |\, q_1, q_2, \cdots \rangle$ is an antisymmetrized product of single-particle states $|\, q_k \,\rangle$ with a gaussian spatial distribution, spin and isospin.

$$\langle\, \boldsymbol{x} \,|\; q_k \rangle = \exp\left\{ -\frac{(\boldsymbol{x} - \boldsymbol{r}_k)^2}{2a_k} + i\boldsymbol{p}_k \cdot \boldsymbol{x} \right\} \otimes |\, \chi_k \, \phi_k \,\rangle \otimes |\, \xi_k \,\rangle \tag{2}$$

$q_k = \{\boldsymbol{r}_k, \boldsymbol{p}_k, a_k, \chi_k, \phi_k, \xi_k\}, \; k = 1, \cdots, A$ denotes a set of time-dependent parameters containing the mean position, mean momentum, complex width, spin and isospin of the single-particle state with number k. The equations of motion which result from Eq. (1) can be summarized as [1]

$$\sum_{\nu} \mathcal{A}_{\mu\,\nu}\ \dot{q}_{\nu} = -\frac{\partial \mathcal{H}}{\partial q_{\mu}} \qquad \text{with} \qquad \mathcal{H} = \langle\, Q \mid \underset{\sim}{H} \mid Q \,\rangle \quad , \tag{3}$$

$$\langle\, Q \mid \underset{\sim}{T} \mid Q \,\rangle = \sum_{k,l}^{A} \langle\, q_k \mid \underset{\sim}{t} \mid q_l \,\rangle\ O_{lk} \qquad , \qquad \left(O^{-1}\right)_{kl} := \langle\, q_k \mid q_l \,\rangle \tag{4}$$

$$\langle\, Q \mid \underset{\sim}{V} \mid Q \,\rangle = \frac{1}{2} \sum_{k,l,m,n}^{A} \langle\, q_k\ q_l \mid \underset{\sim}{v} \mid q_m\ q_n \,\rangle (O_{mk} O_{nl} - O_{nk} O_{ml}) \quad . \tag{5}$$

For the results presented here we used the Volkov 2 interaction [2]. In order to save computer time we developed the following approximation for the expectation value of the two-body interaction [3]

$$\langle\, Q \mid \underset{\sim}{V} \mid Q \,\rangle \approx \sum_{k<l}^{A} \frac{\langle\, q_k q_l \mid \underset{\sim}{v} \mid q_k q_l \,\rangle - \langle\, q_k q_l \mid \underset{\sim}{v} \mid q_l q_k \,\rangle}{\langle\, q_k q_l \mid q_k q_l \,\rangle} f(c_{kl}) \tag{6}$$

$$f(c_{kl}) = \exp\left\{ -\frac{1}{4}\ c_{kl} \right\} \quad , c_{kl} = \sum_{m \neq k,l}^{A} \left(\frac{\langle q_k | q_m \rangle \langle q_m | q_k \rangle}{\langle q_k | q_k \rangle \langle q_m | q_m \rangle} + \frac{\langle q_l | q_m \rangle \langle q_m | q_l \rangle}{\langle q_l | q_l \rangle \langle q_m | q_m \rangle} \right)$$

This approximation reduces the computational time by about a factor A. $\mathcal{A}_{\mu\,\nu}(Q)$ is a nontrivial metric given by

$$\mathcal{A}_{\mu\,\nu}(Q) = 2\ \mathrm{Im}\ \langle\, \frac{\partial}{\partial q_{\mu}}\ Q \mid \frac{\partial}{\partial q_{\nu}}\ Q \,\rangle \qquad . \tag{7}$$

The greek indices μ, ν identify both, the number of the wave packet and the particular parameter belonging to this packet.

2 Definition of the ensemble and fluctations therein

Although the hamiltonian is rotationally invariant the ground states are in general not eigenstates of the total spin operator $\underset{\sim}{\boldsymbol{J}}^2$ and $\underset{\sim}{J_z}$ but are deformed in coordinate and momentum space. The breaking of the rotational symmetry is due to the restriction of the many-body trial state to a single Slater determinant. The deformations reflect many-body correlations between the nucleons in the sense that within the manifold a trial state with a special order in the relative positions and momenta of the nucleons is lower in energy than a spherically symmetric configuration. For example in ^{12}C an arrangement in which groups of four wave packets form three α-clusters in a triangle is energetically preferred. This kind of a many-body correlation does not exist in a spherical Slater determinant which contains only correlations due to the Pauli principle. Therefore FMD ground states have to be treated like intrinsically deformed Hartree-Fock states. Ground states with good spin quantum numbers are obtained with help of rotation matrices by projecting the FMD ground states. A $J^\pi = 0^+$ state for instance is constructed by

$$|\, GS; J^\pi = 0^+ \,\rangle = \frac{1}{\sqrt{N}} \int d^3\Omega \;\; |\, Q_{GS}; \mathbf{\Omega} \,\rangle \;, \quad \text{where} \tag{8}$$

$$|\, Q_{GS}; \mathbf{\Omega} \,\rangle := \exp\{-i\mathbf{\Omega} \underset{\sim}{\boldsymbol{J}}\} \;|\, Q_{GS} \,\rangle \tag{9}$$

is the deformed FMD ground state rotated with the three Euler angles $\mathbf{\Omega}$. If the ground state is not a $J^\pi = 0^+$ state the appropriate rotation matrix has to be used.

The initial state of a heavy-ion collision is therefore a coherent superposition of all orientations of the two colliding nuclei. Because of the linearity of the exact time propagator at any time t throughout the collision, the exact many-body state is always the coherent superposition over all initial orientations $\mathbf{\Omega_1}$ and $\mathbf{\Omega_2}$ weighted with the initial time-independent amplitudes. The same holds of course for the finally measured state. In the spirit of a semi-classical approximation the exact solution for a given pair of orientations $\mathbf{\Omega_1}$ and $\mathbf{\Omega_2}$ is replaced by the FMD solution

$$\exp\{-i\underset{\sim}{H}\, t\} \;|\, Q(t=0); \mathbf{\Omega_1}, \mathbf{\Omega_2} \,\rangle \quad \longrightarrow \quad |\, Q(t); \mathbf{\Omega_1}, \mathbf{\Omega_2} \,\rangle \;, \tag{10}$$

where the state vector $|\, Q(t); \mathbf{\Omega_1}, \mathbf{\Omega_2} \,\rangle$ of the two colliding nuclei is evolved in time according to the FMD equations of motion. The semiclassical state $|\, \Psi(t) \,\rangle_{FMD}$ is herewith a coherent superposition of FMD states at time t which had the initial orientations $\mathbf{\Omega_1}$ and $\mathbf{\Omega_2}$.

In fig. 1 four initial orientations are selected and evolved in time. While the superposition of all orientations at $t = 0$ represents the initial state with the spherical ground states, the same superposition of the right hand column is the final semiclassical many-body state. The collisions are for the same impact parameter $b = 1$ fm and the same beam energy $E_{LAB} = 28.7$ AMeV but differ in the initial orientations $\mathbf{\Omega_1}$ and $\mathbf{\Omega_2}$ of the two ^{12}C. Due to the nonlinear equations of motion the final results at 300 fm/c are quite different. The first and the third case end up with two excited ^{12}C while the second and fourth result in multifragmentation into ^{8}Be and ^{4}He.

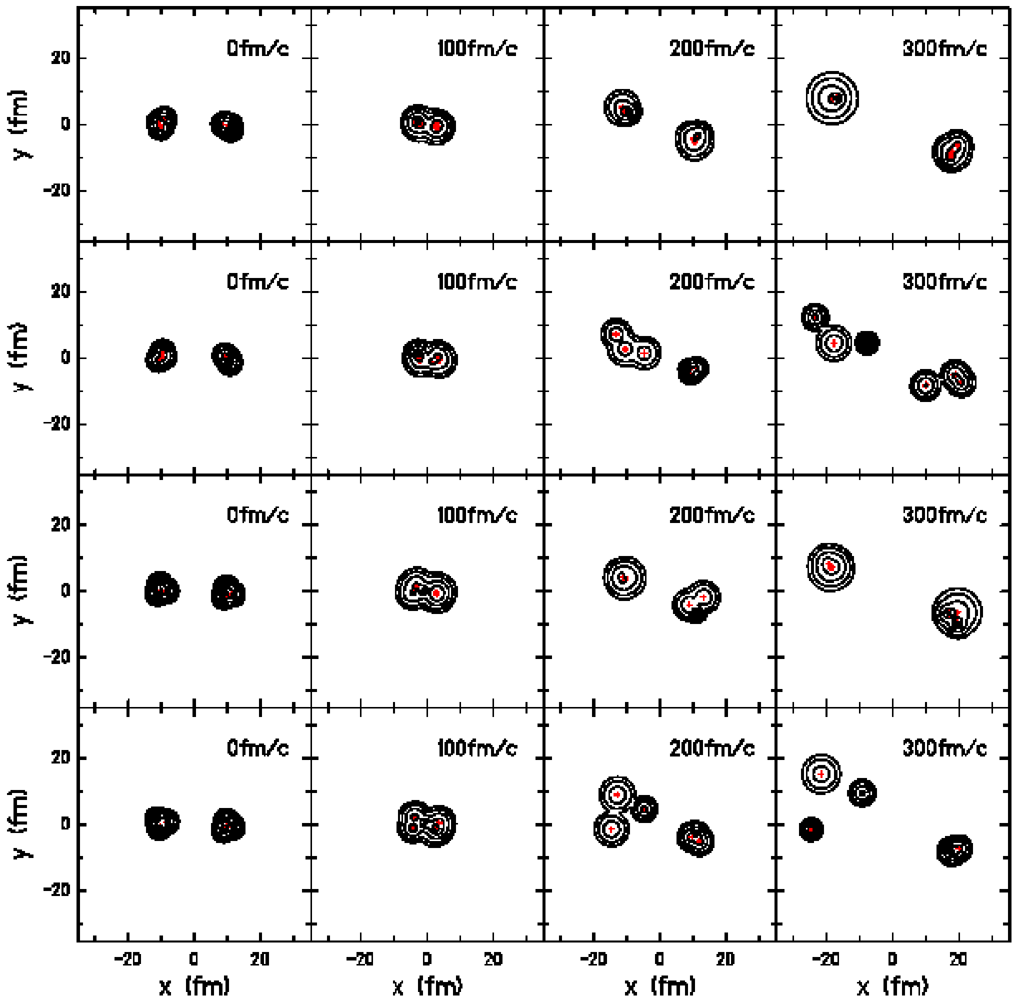

Fig. 1: Densities in coordinate space, integrated over z-direction, for four collisions of ^{12}C and ^{12}C at $E_{LAB} = 28.7$ AMeV and $b = 1$ fm which differ only in the initial orientations of the two nuclei.

The figure also shows that the final individual FMD channels have practically no overlap anymore, i.e.

$$\langle\, Q(t\to\infty); \mathbf{\Omega_1}, \mathbf{\Omega_2} \,|\, Q(t\to\infty); \mathbf{\Omega_1'}, \mathbf{\Omega_2'} \,\rangle \propto \delta_{\Omega_1\Omega_1'}\ \delta_{\Omega_2\Omega_2'}\ . \tag{11}$$

It turns out [3] that in the nonlinear FMD time-evolution the many-body overlap drops rapidly to zero when the two nuclei touch. The last two rows compare two initial conditions which differ only slightly in a rotation of the left-hand nucleus by 30^0. Nevertheless the final states are quite different.

This implies that for the expectation value of an arbitrary operator $\underset{\sim}{B}$ the coherent summation can be replaced by an incoherent average over the weighted initial orientations which defines the ensemble average denoted by $\langle\langle \cdot \rangle\rangle$

$$\langle\langle\, \underset{\sim}{B}\, \rangle\rangle := \left(\frac{1}{8\pi^2}\right)^2 \int d^3\Omega_1 d^3\Omega_2 \langle\, Q; \mathbf{\Omega_1}, \mathbf{\Omega_2} \,|\, \underset{\sim}{B} \,|\, Q; \mathbf{\Omega_1}, \mathbf{\Omega_2} \,\rangle \ . \tag{12}$$

Therefore $|\, Q(t); \mathbf{\Omega_1}, \mathbf{\Omega_2} \,\rangle$ can be regarded as a member of an ensemble.

This is different from classical molecular dynamics or QMD [4] where random initial positions and random initial momenta of the particles often constitute the ensemble. Since FMD has stationary ground states with the parameters given by the requirement of minimal total energy, the relative positions and momenta between the wave packets cannot be chosen at random. The ensemble in FMD consists of all orientations of the two deformed initial ground states, in accordance with the quantal picture discussed above.

Actually, the ensemble consists also of the different possibilities to choose an impact parameter. As in all other models for inelastic heavy-ion collisions we have tacitly supposed that the assumption (12) of incoherence in the final state applies also to the initial coherent superposition of impact parameters or angular momenta which one needs to set up an incoming plane wave in the relative motion of the centers of masses. The averaging over the initial orientations has to be understood in the same way as the averaging over the initial positions of the nuclei.

If one superimposes the different columns of the FMD results shown in fig. 1 one obtains the ensemble averaged one-body density $\langle\langle\, \underset{\sim}{\rho}(\boldsymbol{x})\, \rangle\rangle$ according to eq. (12). It is obvious that for fragmentation reactions mean-field theories like BUU [5] which are based on the ensemble averaged one-body phase-space distribution can make sense only in the initial stage of the collision up to the time when the system expands and decays into clusters. The final $\langle\langle\, \underset{\sim}{\rho}(\boldsymbol{x})\, \rangle\rangle$ is a highly diluted density smeared over a large area without any resemblance of the outcoming clusters. In the expansion phase of a fragmentation reaction many-body correlations which are not contained in a one-body density govern the dynamics.

It is evident that the amount of fluctuation will depend on the size of the deformation in the initial state. This effect has already been seen experimentally in low energy fusion reactions [6], where the different orientations of the intrinsic deformation lead to fluctuations of the fusion barrier.

The example of fig. 1 and many others [3] show that FMD is capable of producing large fluctuations in the final channels. They originate from quantal fluctuations in the orientation of the intrinsically deformed initial ground state.

3 Summary

Fermionic Molecular Dynamics sets an example how to treat the Pauli principle in trajectory calculations. The model is quantal in the sense that it cannot violate the uncertainty principle as it works with wave packets. The model by construction must also obey the Pauli principle because the many-body trial state is always antisymmetric with respect to particle exchange. These two fundamental properties guarantee that FMD has the correct treatment of Fermi motion and shell model properties. On the other hand, in the limit of narrow non-overlapping wave packets, the FMD equations reduce to Newton's equations of motion for classical particles.

Although FMD has deterministic equations of motion it exhibits large fluctuations in the final channels when averaging over the orientations of the intrinsic states in the initial ground state. These orientations define the event ensemble for a given energy and impact parameter. Within an ensemble one sees multifragmentation, sequential fragmentation, explosion and sequential decay.

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