Statistical Properties of Fermionic Molecular Dynamics

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Abstract

Statistical properties of Fermionic Molecular Dynamics are studied. It is shown that, although the centroids of the single–particle wave–packets follow classical trajectories in the case of a harmonic oscillator potential, the equilibrium properties of the system are the quantum mechanical ones. A system of weakly interacting fermions as well as of distinguishable particles is found to be ergodic and the time–averaged occupation probabilities approach the quantum canonical ones of Fermi–Dirac and Boltzmann statistics, respectively.

1 Introduction and summary

Molecular dynamic models are expected to describe multifragmentation of nuclei seen in heavy–ion collisions. These reactions show large fluctuations, for example in the mass distribution, which are beyond an ensemble–averaged mean–field treatment. In this context it is important to understand the statistical properties of molecular dynamic models especially at low temperatures.

There are two aspects of this. One concerns the thermo*static* properties of a molecular dynamic model where the attribute thermostatic refers to the properties of the static canonical statistical operator, which are contained in the partition function $Z(T) = \mathrm{Tr}(\exp\{-\underset{\sim}{H}/T\})$. Once the partition function is calculated within a given model its thermostatic properties can be deduced by standard methods like partial derivatives of $\ln Z(T)$ with respect to temperature T or other parameters contained in the Hamilton operator $\underset{\sim}{H}$. An investigation along this line was performed in refs. [1,2], however, there the quantum features of the many–body trial state were not fully exploited.

In the case of Fermionic Molecular Dynamics (FMD) [3,4] the trace in the

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partition function can be evaluated exactly because the model is based on antisymmetric many–body states which form an overcomplete set covering the whole Hilbert space. Also the states of Antisymmetrized Molecular Dynamics (AMD) [5] provide a representation for the unit operator. As the calculation of the trace does not depend on the representation all thermostatic properties like Fermi–Dirac distribution, specific heat, mean energy as a function of temperature etc. ought to be correct and fully quantal using FMD or AMD trial states.

The issue of this paper is the other and even more important aspect, namely the dynamical behaviour of a molecular dynamic model. A dissipative system which is initially far from equilibrium is expected to equilibrate towards the canonical ensemble. The simulation of such a system within the model provides a crucial test of its thermo*dynamic* behaviour.

The time–evolved FMD state is in general not the exact solution of the Schrödinger equation, so the correct thermo*static* properties do not a priori guarantee correct thermo*dynamic* properties. In other words the question is: does the FMD state as a function of time explore the Hilbert space according to the canonical weight?

Since the parameters of the single–particle wave packets follow classical equations of motion, which are generalized Hamilton equations, one is tempted to infer that the dynamical statistical properties might also be classical. This conjecture, that classical equations of motion always imply classical statistics, is disproven by the following examples, in which we compare time–averaged expectation values of wave–packet molecular dynamics with the equivalent ones of the canonical ensemble at the same excitation energy.

Within Fermionic Molecular Dynamics we study the equilibration of four identical fermions enclosed in a one dimensional harmonic oscillator. The particles interact by a weak repulsive two–body potential which is neccessary to convert the integrable harmonic oscillations into chaotic motion. The important result is that the initial many–body state, which is far from equilibrium, approaches the canonical ensemble with Fermi–Dirac statistics in an ergodic sense. The time–averaged occupation numbers of the harmonic oscillator eigenstates are practically identical with the Fermi–Dirac distribution of the canonical ensemble, provided the canonical ensemble is taken at the time–independent mean excitation energy of the many–body state.

The result does not change when the FMD trial state is replaced by the trial state of Antisymmetrized Molecular Dynamics (AMD). However, AMD also equilibrates if there is no interaction between the particles, which is due to the spurious scattering induced by the time–independent widths of the wave packets.

When distinguishable particles, which are described by a product–state of wave packets, are considered, the molecular dynamic equations for the parameters of the wave packets lead to a Boltzmannn distribution for the occupation numbers of the single–particle eigenstates.

Moreover, also a system of distinguishable particles, where one particle bound in a narrow oscillator is coupled to three particles in a wider oscillator, is ergodic and exhibits the quantum equilibrium properties. All four particles assume the same temperature and therefore share their excitation energy in a ratio given by the quantum canonical ensemble which is not one to three, as it would be for classical particles. Finally, classical thermodynamics is obtained when the many–body state is a product state and the width parameters are not dynamical variables anymore.

A further important result is, that the use of time averages provides us with a tool for establishing relations between well–defined quantities of a molecular dynamic model such as excitation energy and statistical quantities like temperature. This is a first step in investigating excited nuclei and for instance the nuclear liquid–gas phase transition which has been of current experimental interest [6].

2 The Fermionic Molecular Dynamics model

In this section we briefly summarize the basic ideas of Fermionic Molecular Dynamics which have been published in great detail elsewhere [3,4]. FMD is derived from the time–dependent quantum variational principle

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

which for the most general variation of the trial state $\langle\, Q(t) \,|$ leads to the Schrödinger equation. In FMD the trial state is defined by a set of parameters $Q(t) = \{q_\nu(t) | \nu = 1, 2, \ldots\}$. The resulting Euler–Lagrange equations in their most general form can be written as

$$\sum_\nu \mathcal{A}_{\mu\nu}(Q)\; \dot{q}_\nu = -\frac{\partial}{\partial q_\mu} \langle\, Q(t) \,|\, \underset{\sim}{H} \,|\, Q(t) \,\rangle \,, \quad \mathcal{A}_{\mu\nu}(Q) = \frac{\partial^2 \mathcal{L}_0}{\partial \dot{q}_\mu \partial q_\nu} - \frac{\partial^2 \mathcal{L}_0}{\partial \dot{q}_\nu \partial q_\mu} \;, \tag{2}$$

where $\mathcal{L}_0 = \langle\, Q(t) \,|\, i\frac{d}{dt} \,|\, Q(t) \,\rangle$ and $\mathcal{A}_{\mu\nu}(Q)$ is a skew symmetric matrix reflecting the symplectic structure of the equations of motion. The time evolution of the parameters then defines the time dependence of the many–body state $|\, Q(t) \,\rangle$ which has to be used for calculating expectation values.

The A–fermion trial state $|\,Q(t)\,\rangle$ is given by the antisymmetrized product of single–particle gaussian wave packets

$$|\,Q(t)\,\rangle = \frac{1}{\langle\,\widehat{Q(t)}\,|\,\widehat{Q(t)}\,\rangle^{\frac{1}{2}}}\;\;|\,\widehat{Q(t)}\,\rangle \tag{3}$$
$$|\,\widehat{Q(t)}\,\rangle = \frac{1}{A!}\sum_{all\;\;P}\mathrm{sgn}(P)\;\;|\,q_{P(1)}(t)\,\rangle\otimes\;|\,q_{P(2)}(t)\,\rangle\otimes\cdots\otimes\;|\,q_{P(A)}(t)\,\rangle\;,$$

where each single–particle state is parametrized in terms of the time–dependent mean position $\vec{r}(t)$, mean momentum $\vec{p}(t)$ and the complex width $a(t)$

$$\langle\,\vec{x}\,|\,q(t)\,\rangle = \exp\left\{-\frac{(\,\vec{x}-\vec{b}(t)\,)^2}{2\,a(t)}+i\eta(t)\right\}\otimes\;|\uparrow\uparrow\rangle\;\;,\;\vec{b}=\vec{r}+ia\vec{p}\;. \tag{4}$$

In the notation of (4) the vector $\vec{b}$ is composed of $\vec{r}$, $\vec{p}$ and a. $\eta(t)$ contains the phase and the norm. In general the time dependence of spin and isospin has to be considered, but for this article we assume that all particles are identical fermions, and therefore, they have the same spin and isospin component $|\uparrow\uparrow\rangle$.

Before investigating the statistical properties a few words concerning the FMD equations of motion for systems with a one–body hamiltonian

$$\underset{\sim}{H} = \sum_{l=1}^{A}\underset{\sim}{h}(l) \tag{5}$$

are helpful.

The solution of (2) can be given explicitly for freely moving particles or non–interacting particles in a common harmonic oscillator potential. In both systems it coincides with the exact solution of the Schrödinger equation and the time evolution of the parameters is not influenced by the Pauli principle at all. In the free case one obtains

$$\underset{\sim}{h}(l) = \frac{\underset{\sim}{\vec{k}}^{\,2}(l)}{2m} \quad\Rightarrow\quad \frac{d}{dt}\,\vec{b}_l = 0 \tag{6}$$
$$\frac{d}{dt}\,a_l = \frac{i}{m}\quad. \tag{7}$$

If $\vec{b}_l$ is transformed to $\vec{r}_l$ and $\vec{p}_l$ one gets $\frac{d}{dt}\,\vec{p}_l = 0$ and $\frac{d}{dt}\,\vec{r}_l = \vec{p}_l/m$. Although these are the classical equations for free motion augmented by one for the width, it is also the exact quantum mechanical solution. The centre of each wave packet is moving on the classical trajectory, while the width is spreading.

For fermions in a harmonic oscillator [7]

$$\underset{\sim}{h}(l) = \frac{\vec{\underset{\sim}{k}}^{\,2}(l)}{2m} + \frac{1}{2}\, m\omega^2\, \vec{\underset{\sim}{x}}^{\,2}(l) \quad \Rightarrow \quad \frac{d}{dt}\,\vec{b}_l = -im\omega^2 a_l \vec{b}_l \tag{8}$$

$$\frac{d}{dt}\, a_l = -im\omega^2 a_l^2 + \frac{i}{m} \tag{9}$$

the equations of motion are also the classical ones for $\vec{r}_l$ and $\vec{p}_l$. Replacing the complex $\vec{b}_l$ in eq. (8) yields

$$\frac{d}{dt}\,\vec{r}_l = \frac{\vec{p}_l}{m} \quad \text{and} \quad \frac{d}{dt}\,\vec{p}_l = -m\omega^2 \vec{r}_l \ . \tag{10}$$

In both examples 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 which by construction contains the Pauli principle!

It is also important to note that for these two examples the equations of motion of the parameters are the same, regardless whether the many–body state is antisymmetrized, symmetrized or simply a product state. There are two conditions for that, first, the hamiltonian, which commutes with the antisymmetrization and symmetrization operator, is a one–body operator which acts only on the single–particle states. Second, the single–particle trial state is chosen such that it is a solution of the single–particle Schrödinger equation. If, for example, one would freeze the width degree of freedom, eqs. (6) and (8) or (10) would not hold true any longer for fermions, but they would experience non–existing spurious forces (see also section 3.3).

These two simple examples show that in general it is not possible to conclude classical behaviour just because the equations of motion written in terms of parameters $\vec{r}_l$ and $\vec{p}_l$ are classical equations of motion as has recently been conjectured [2].

3 The ergodic ensemble

Fermionic Molecular Dynamics is a deterministic microscopic transport theory. Given the Hamilton operator and a state $|\, Q(t_0)\,\rangle$ at a certain time t_0 the state $|\, Q(t)\,\rangle$ is known for all time. Expectation values are well–defined in FMD so that one can easily calculate quantities like the excitation energy of a nucleus or the probability of finding the system in a given reference state. But it is not obvious how thermodynamical quantities, such as the temperature, might be extracted from deterministic molecular dynamics with wave packets.

In this section time averaging is compared with a statistical ensemble. If the system is ergodic both are equivalent and statistical properties of molecular dynamics can be evaluated by means of time averaging.

For this the ergodic ensemble is defined by the statistical operator $\underset{\sim}{R}_{\mathrm{erg}}$ as

$$\underset{\sim}{R}_{\mathrm{erg}} := \lim_{t_2\to\infty} \frac{1}{(t_2-t_1)} \int_{t_1}^{t_2} \mathrm{d}t \;\; |\, Q(t)\,\rangle\langle\, Q(t)\,| \;\; . \tag{11}$$

The ergodic mean of an operator $\underset{\sim}{B}$ is given by

$$\overline{\langle\, \underset{\sim}{B}\,\rangle}_{|\,\langle\, \underset{\sim}{H}\,\rangle} := \mathrm{Tr}\left(\underset{\sim}{R}_{\mathrm{erg}}\, \underset{\sim}{B}\right) = \lim_{t_2\to\infty} \frac{1}{(t_2-t_1)} \int_{t_1}^{t_2} \mathrm{d}t\, \langle\, Q(t)\,|\, \underset{\sim}{B}\,|\, Q(t)\,\rangle \;. \tag{12}$$

In general the statistical operator $\underset{\sim}{R}_{\mathrm{erg}}$ is a functional of the initial state $|\, Q(t_1)\,\rangle$, the Hamilton operator $\underset{\sim}{H}$ and the equations of motion. If the ergodic assumption is fulfilled, the statistical operator should only depend on $\langle\, \underset{\sim}{H}\,\rangle$, which is actually a constant of motion. Thus the average in the ergodic ensemble is always perfomed at the same expectation value of the Hamilton operator. In our notation this is denoted by the condition " $\langle\, \underset{\sim}{H}\,\rangle$ " in eq. (12).

3.1 Canonical ensemble of fermions in a harmonic oscillator

With the statistical operator of the canonical ensemble for A fermions in a one–dimensional common harmonic oscillator potential $\underset{\sim}{H}_{\mathrm{HO}}$, given by

$$\underset{\sim}{R}(T) = \frac{1}{Z(T)} \exp\left\{-\frac{\underset{\sim}{H}_{\mathrm{HO}}}{T}\right\} \tag{13}$$

$$\underset{\sim}{H}_{\mathrm{HO}} = \sum_{l=1}^{A} \underset{\sim}{h}(l) \;, \qquad \underset{\sim}{h}(l) = \omega \sum_{n=0}^{\infty} \left(n+\frac{1}{2}\right) \underset{\sim}{c}_n^{+}\, \underset{\sim}{c}_n \;,$$

the statistical mean of an operator $\underset{\sim}{B}$ is calculated as

$$\langle\langle\, \underset{\sim}{B}\,\rangle\rangle_{|\,T} := \mathrm{Tr}\left(\underset{\sim}{R}(T)\, \underset{\sim}{B}\right) \tag{14}$$

$$= \frac{1}{Z(T)} \int \frac{\mathrm{d}r_1\, \mathrm{d}p_1}{2\pi} \cdots \frac{\mathrm{d}r_A\, \mathrm{d}p_A}{2\pi}\, \langle\, \hat{Q}\,|\, \underset{\sim}{B}\, \exp\left\{-\frac{\underset{\sim}{H}_{\mathrm{HO}}}{T}\right\}\, |\, \hat{Q}\,\rangle$$

$$= \frac{1}{Z(T)} \sum_{n_1<\cdots<n_A} \langle\, n_1, \cdots, n_A \,|\, \underset{\sim}{B} \,|\, n_1, \cdots, n_A \,\rangle \, \exp\left\{ -\frac{E(n_1, \cdots, n_A)}{T} \right\} \; .$$

As already mentioned in the introduction the FMD states are a representation of the unit operator [8] and hence can be used to calculate traces. For numerical convenience, however, the mathematically identical third line in eq. (14) is used, where $|\, n_1, \cdots, n_A \,\rangle$ denotes the Slater determinant composed of single–particle oscillator eigenstates $|\, n_1 \,\rangle, \cdots, |\, n_A \,\rangle$ and

$$E(n_1, \cdots, n_A) = \omega \, \sum_{i=1}^{A} \left(n_i + \frac{1}{2} \right) \tag{15}$$

are the eigenenergies of $\underset{\sim}{H}_{\rm HO}$.

In eq. (14) the subscript T indicates that the average is taken at a constant temperature T.

In the following a system of four fermions in a common one–dimensional harmonic oscillator is investigated. The frequency of the oscillator is chosen to be $\omega = 0.04 \mathrm{fm}^{-1}$ in order to get a spacing of 8 MeV between the single–particle states. For the canonical ensemble fig. 1 shows the dependence of the excitation energy on the temperature (l.h.s.) and displays how the lowest eigenstates are occupied in the four–fermion system for five different temperatures (r.h.s.).

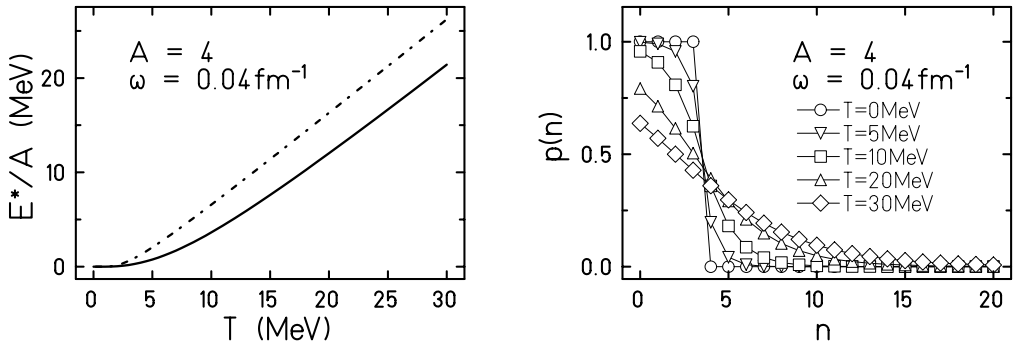

Fig. 1: A system of four fermions in a common oscillator described by the canonical ensemble. L.h.s.: Excitation energy as a function of temperature (solid line). The dashed–dotted line shows the result for a product state (Boltzmann statistics). R.h.s.: Occupation numbers $p(n)$ of the oscillator eigenstates for five temperatures (eq. (16)). The lines are drawn as a guide for the eye.

The mean occupation probabilities are given by

$$p(n) = \langle\langle \; \underset{\sim}{c}{}^{+}_{n} \, \underset{\sim}{c}_{n} \; \rangle\rangle_{|_T} \quad , \tag{16}$$

where $\underset{\sim}{c}^+_n$ denotes the creation operator of a fermion in the oscillator eigenstate $|\, n \,\rangle$.

3.2 Ergodic ensemble of fermions in a harmonic oscillator

In this section the averages of the occupation numbers in the ergodic ensemble are evaluated and compared with those of the canonical ensemble discussed in the previous section. As pointed out in section 2, in Fermionic Molecular Dynamics the time evolution of gaussian wave packets in a common oscillator is exact, and thus the occupation probabilities of the eigenstates of the Hamilton operator do not change in time. In order to equilibrate the system a repulsive short–range interaction $\underset{\sim}{V}_I$ is introduced.

$$\underset{\sim}{H} = \underset{\sim}{H}_{\rm HO} + \underset{\sim}{V}_{\rm I} \tag{17}$$

$$\underset{\sim}{V}_{\rm I} = \sum_{k<l} V_0 \exp\left\{ -\frac{(\underset{\sim}{x}_k - \underset{\sim}{x}_l)^2}{r_0^2} \right\} \;; \quad V_0 = (10^4 \ldots 10^5)\omega \;, \;\; r_0 = \frac{0.01}{\sqrt{m\omega}}$$

The strength of the interaction is chosen such that the resulting matrix elements of $\underset{\sim}{V}_{\rm I}$ are small compared to the level spacing ω and the excitation energy E^*. The contribution of $\langle\, \underset{\sim}{V}_{\rm I} \,\rangle$ to the total energy is of the order of $0.1 \ldots 1.0$ MeV.

The initial state is prepared in the following way. Three wave packets with a width of $a = 1/m\omega$ are put close to the origin at $x = (-d, 0, d)$ — with $d = 0.5/\sqrt{m\omega}$ — whereas the fourth packet with the same width is pulled away from the centre in order to obtain the desired energy. As the mean momenta are all zero, the excitation is initially only in potential energy which has to be converted into thermal energy by means of the small interaction $\underset{\sim}{V}_{\rm I}$.

The initial system, which is far from equilibrium, is evolved over about 2000 periods of the harmonic oscillator ($2\pi/\omega = 157$ fm/c). The equilibration time is rather large as we are using a very weak interaction in order not to introduce correlations which would destroy the ideal gas picture implied in the canonical ensemble (13) of non–interacting particles. The time averaging of the occupation numbers (18) starts at time $t_1 = 10000$ fm/c in order to allow a first equilibration.

$$\overline{\langle\, \underset{\sim}{c}^+_n \underset{\sim}{c}_n \,\rangle}\Big|_{\langle\, \underset{\sim}{H} \,\rangle} = \lim_{t_2 \to \infty} \frac{1}{(t_2 - t_1)} \int_{t_1}^{t_2} {\rm d}t \, \langle\, Q(t) \,|\, \underset{\sim}{c}^+_n \underset{\sim}{c}_n \,|\, Q(t) \,\rangle \tag{18}$$

Figure 2 gives an impression of how the occupation numbers evolve in time.

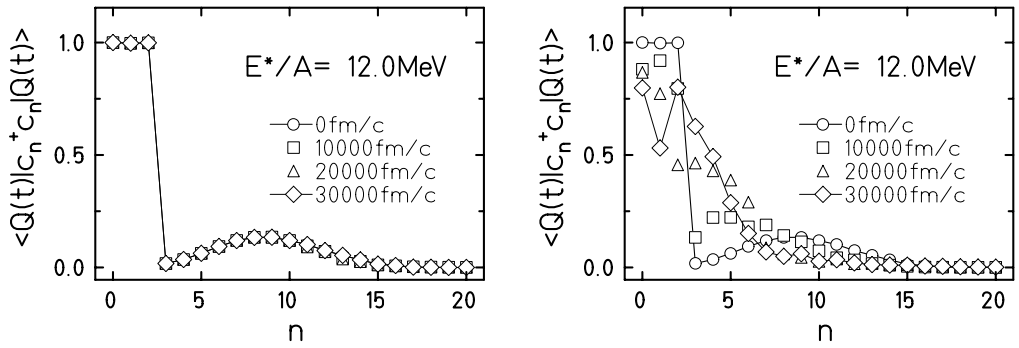

Fig. 2: Time evolution of the occupation probabilities $\langle\, Q(t)\,|\ \underset{\sim}{c}_n^{+}\underset{\sim}{c}_n\ |\,Q(t)\,\rangle$ for four fermions in a common harmonic oscillator potential without (l.h.s.) and with two–body interaction (r.h.s.). The distributions at $t = 0$ and $t = 30000$fm/c are connected by a solid line.

The part to the left shows the time evolution without interaction which is just a unitary transformation in the one–body space. Thus the occupation numbers do not change in time although the wave packets are swinging. This has been expected since the $\underset{\sim}{c}_n^{+}$ create eigenstates of the hamiltonian $\underset{\sim}{H}_{\rm HO}$. It also serves as an accuracy test of the integrating routine. The part to the right displays the evolution with interaction at three later times. The occupation probabilities are reshuffled due to the interaction and they fluctuate in time. In fig. 3 (l.h.s.) the chaotic time dependence of $\langle\, Q(t)\,|\ \underset{\sim}{c}_n^{+}\underset{\sim}{c}_n\ |\,Q(t)\,\rangle$ for $n = 0, 3$ and 6 is depicted.

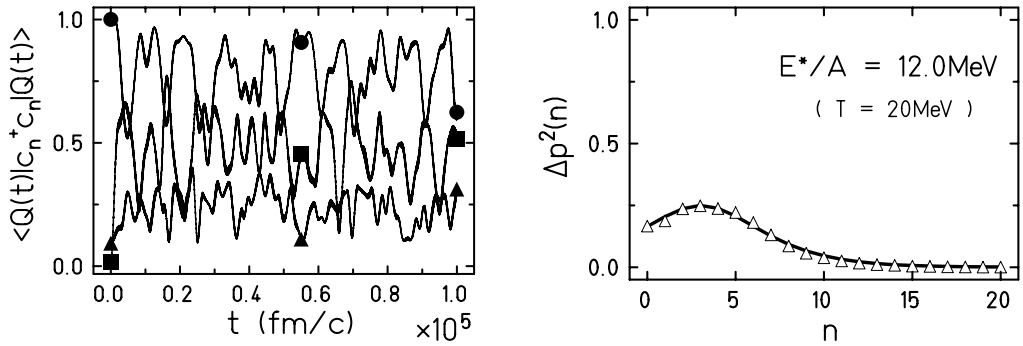

Fig. 3: L.h.s.: Occupation probabilities $\langle\, Q(t)\,|\ \underset{\sim}{c}_n^{+}\underset{\sim}{c}_n\ |\,Q(t)\,\rangle$ versus time — $n = 0$: circles, $n = 3$: boxes, $n = 6$: triangles.
R.h.s.: Variance of the fluctuations $\Delta p^2(n)$ calculated in the canonical ensemble (solid line) and in the ergodic ensemble (circles).

The result of time averaging is seen in fig. 4 (symbols) for four different initial displacements which are correspond to four different excitation energies

of the fermion system. To each case we assign a canonical ensemble which has the same mean energy. The solid lines in fig. 4 show the corresponding distributions of occupation probabilities for these canonical ensembles. Their temperatures T are also quoted in the figure. It is surprising to see that there is almost no difference between the ergodic and the canonical ensemble:

$$\overline{\langle\, \underset{\sim}{c}^{+}_n \underset{\sim}{c}_n \,\rangle}_{|\,\langle\, \underset{\sim}{H} \,\rangle} \;\approx\; \langle\langle\, \underset{\sim}{c}^{+}_n \underset{\sim}{c}_n \,\rangle\rangle_{|T} \qquad \forall\, n\;, \tag{19}$$

provided both have the same excitation energy

$$E^* = \overline{\langle\, \underset{\sim}{H}_{\rm HO} - E_0 \,\rangle}_{|\,\langle\, \underset{\sim}{H} \,\rangle} \;=\; \langle\langle\, \underset{\sim}{H}_{\rm HO} - E_0 \,\rangle\rangle_{|T} \;, \quad E_0 = 8\,\omega\;. \tag{20}$$

The relation between E^* and T is given by eq. (14) and displayed in fig. 1.

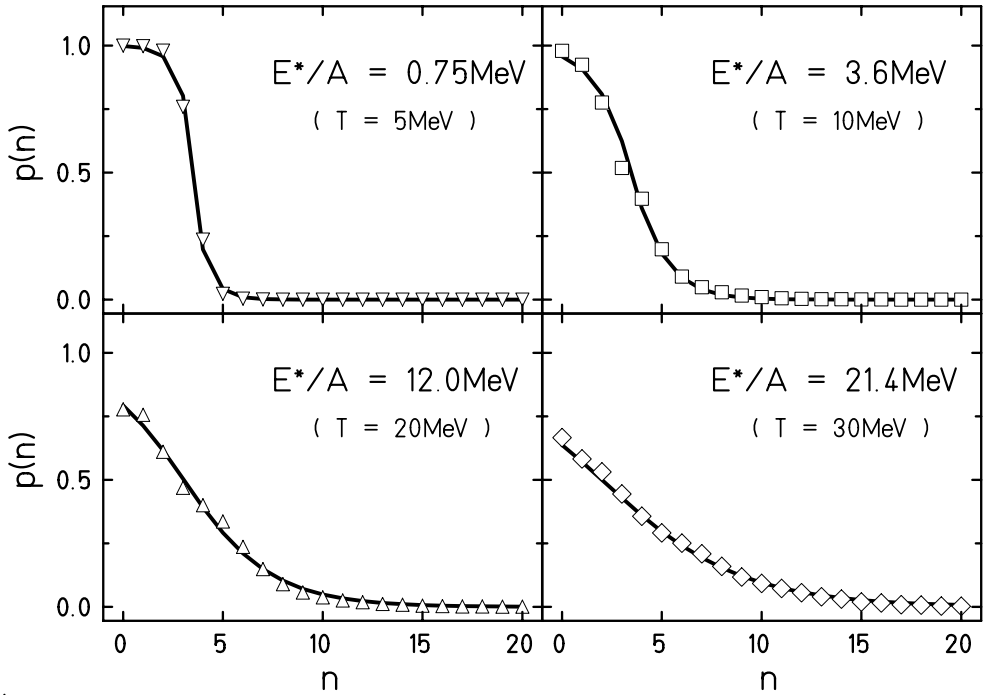

Fig. 4: Occupation numbers calculated in the ergodic ensemble (symbols, eq. (18)) compared with those calculated in the canonical ensemble (solid line, eq. (16)).

This result is not trivial because, firstly, the system is very small, consisting of only four particles, and secondly, the equations of motion are approximated by FMD. The one–to–one correspondence between the occupation probabilities of the ergodic ensemble and the ones of the canonical ensemble, which has the same mean energy $\langle\, \underset{\sim}{H} \,\rangle$ as the pure state, is an impressive demonstration

that the system is ergodic and that the FMD many–body trajectory covers the phase space according to Fermi–Dirac statistics.

Not only the one–body distributions of the two ensembles coincide, but also the variances of the fluctuations $\Delta p^2(n)$,

$$\Delta p^2(n) := \langle\langle\ (\underset{\sim}{c}_n^+ \underset{\sim}{c}_n)^2\ \rangle\rangle_{|T}\ - \langle\langle\ \underset{\sim}{c}_n^+ \underset{\sim}{c}_n\ \rangle\rangle_{|T}^2\ , \tag{21}$$

as is demonstrated in fig. 3 (r.h.s.). The ergodic mean converges to the result of the canonical ensemble which is $\Delta p^2(n) = p(n)(1-p(n))$.

3.3 Describing the system with AMD trial states

The trial states of Antisymmetrized Molecular Dynamics (AMD) [5] differ from those of FMD only in the time–independent width and spin parameters. As explained already in the introduction both FMD and AMD trial states span the whole Hilbert space and thus have the same thermostatic properties. The thermodynamic properties of AMD will however also depend on the fluctuating collision term, which is an important part of AMD.

The following investigations focus on the role of the fixed width parameters only. Since the width parameters are not allowed to evolve in time the AMD trial state differs from the exact solution in the case of non–interacting fermions. For the common harmonic oscillator it agrees with the exact solution only if all width parameters are $a_l = (m\omega)^{-1}$, because then da_l/dt is zero anyhow (see (9)). If the width has a different value spurious scattering occurs.

The left hand part of fig. 5 displays for the very same system as in the previous section the result of the time–evolution without interaction. If the widths are chosen to be $a_l = (m\omega)^{-1}$ (circles), then the time evolution is just a unitary transformation in the one–body space and the occupation probabilities are stationary. But if the widths are taken as $a_l = 1.2(m\omega)^{-1}$, different from FMD or the exact solution, the evolution is not a unitary transformation in the one–body space any longer and the occupation probabilities are reshuffled. The spurious scattering equilibrates this system even without interaction. The right hand part of fig. 5 shows the mean occupation probabilities in the ergodic ensemble (triangles). One sees that the AMD trial state equilibrates towards the canonical ensemble. The sole reason is antisymmetrization as can be seen in the following section.

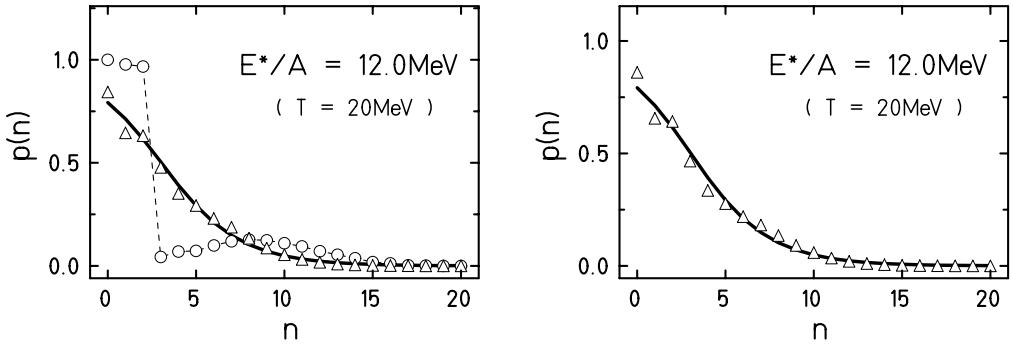

Fig. 5: Occupation probabilities calculated in the ergodic ensemble using AMD trial states (symbols, eq. (18)) compared to those calculated in the canonical ensemble (solid line, eq. (16)). L.h.s.: Without interaction ($\underset{\sim}{V}_{\rm I} = 0$), circles: $a_l = (m\omega)^{-1}$, triangles: $a_l = 1.2(m\omega)^{-1}$. R.h.s.: With interaction $\underset{\sim}{V}_{\rm I}$, $a_l = 1.2(m\omega)^{-1}$.

It would be interesting to see how the collision term influences the dynamical statistical properties of AMD. As the Pauli–blocking prescription is consistent with the AMD state we expect again a Fermi–Dirac distribution.

3.4 Canonical and ergodic ensemble for distinguishable particles

In this section it is shown that time averaging results in quantum Boltzmann statistics if the fermions are replaced by distinguishable particles. For this end the antisymmetrized many–body state is replaced by a product state of gaussian wave packets. The resulting equations of motion differ from the FMD case in the skew–symmetric matrix $\mathcal{A}_{\mu\nu}(\mathcal{Q})$ (given in eq. (2)) which does not couple the generalized velocities of different particles any longer.

For product states the ergodic ensemble is again investigated at different energies and compared with the canonical ensembles with the same mean energies. The appropriate relation between temperatures and excitation energies in the canonical ensemble for distinguishable particles

$$E^* = \langle\langle\, \underset{\sim}{H}_{\rm HO} - E_0 \,\rangle\rangle_{|T} = 4\,\frac{\omega}{2}\left[\coth\left(\frac{\omega}{2\,T}\right) - 1\right], \quad E_0 = 2\,\omega \tag{22}$$

is shown by the dashed–dotted line in fig. 1.

Since distinguishable particles are not affected by the Pauli principle, the occupation numbers for the many–body ground state look quite different. For

instance for zero temperature all particles occupy the eigenstate $|0\rangle$ of the harmonic oscillator (fig. 6, l.h.s.).

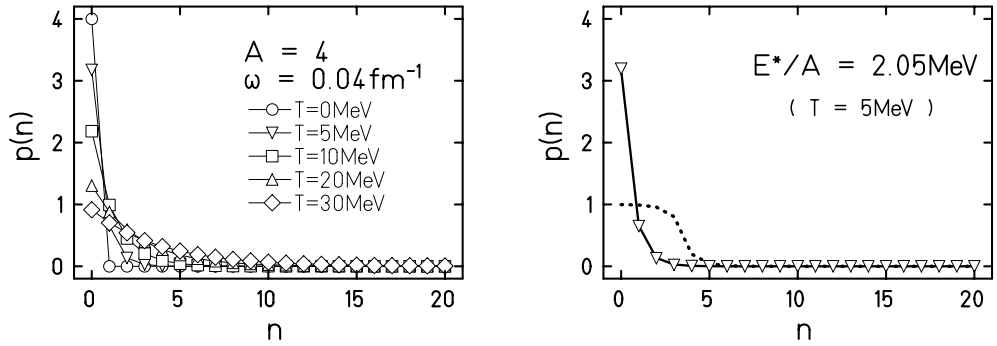

Fig. 6: Occupation probabilities for a product state (Boltzmann statistics). L.h.s.: Occupation probabilities $p(n)$ of the oscillator eigenstates for five temperatures for the canonical ensemble. R.h.s: Occupation probabilities calculated in the ergodic ensemble (symbols) compared with those calculated in the canonical ensemble (solid line) for an excitation energy of $E^* = 2.05$ AMeV which corresponds to a temperature $T = 5$ MeV in the canonical ensemble. The dotted line shows the result for Fermi–Dirac statistics at the same temperature.

The initial single–particle states of the interacting system are the analogue to the fermion case. Again the time evolution of the system exhibits ergodic behaviour for all excitation energies. As an example fig. 6 (r.h.s.) is showing the case of $E^*/A = 2.05$ MeV ($T = 5$ MeV) after a time averaging of about 2000 periods. The ergodic ensemble (triangles) and the Boltzmann canonical ensemble (solid line) are the same within the size of the symbols. The result for Fermi–Dirac statistics with the same temperature is included to demonstrate the difference (dotted line).

This result shows that equations of motion which are not influenced by the Pauli principle anymore still lead to the quantum mechanical occupation probabilities, namely the quantum Boltzmann distribution. The only difference to "true classical" equations is the presence of the width parameters as dynamical variables. Only if they are removed from the equations of motion the statistical behaviour of the ergodic ensemble is that of classical statistics. This will be demonstrated in the following section.

3.5 Equilibration within two different oscillators

After removing antisymmetrization the remaining quantum property is the fact that the Hamilton operator has only discrete energies with a level spacing of ω. Therefore, the specific heat at low temperatures is smaller for larger ω

(see eq. (22)). In order to investigate the quantum effect of discrete eigenvalues and to emphasize further that classical equations of motion do not necessarily imply classical statistics we discuss a system of distinguishable particles where a particle bound in a narrow oscillator is coupled to three particles in a wider oscillator [9] (see fig. 7 l.h.s.). The Hamilton operator of the system is given by

$$\underset{\sim}{H} = \sum_{l=1}^{4} \underset{\sim}{h}(l) + \underset{\sim}{V}_{\rm I} \ , \qquad \underset{\sim}{h}(l) = \frac{\underset{\sim}{k}^{\,2}(l)}{2\,m} + \frac{1}{2}\, m\omega_l^2\, \underset{\sim}{x}^{\,2}(l) \tag{23}$$

$$\frac{\omega_1}{e} = \omega_2 = \omega_3 = \omega_4 \ ,$$

with ω_2, ω_3 and ω_4 being an irrational fraction of ω_1, we choose $e = 2.71828\ldots$.

If the system exhibits quantum statistical properties, the ratio of the excitation energy of particle one in the first oscillator to the excitation energy of the three particles in the second oscillator should agree with the value given by the canonical ensemble of quantum Boltzmann statistics. This ratio differs from the result of classical statistics, where it is 1 to 3 for all excitation energies, because the classical specific heat does not depend on temperature.

The mean excitation energy of one particle bound in a harmonic oscillator potential of frequency ω_l is

$$\langle\langle\ \underset{\sim}{h}(l)\ \rangle\rangle_{|\,T} \ = \frac{\omega_l}{2}\,\coth\left(\frac{\omega_l}{2\,T}\right) \ . \tag{24}$$

Thus, for equal temperatures the excitation energies in the narrow and the wide oscillator are, respectively,

$$E_1^* = \frac{\omega_1}{2}\,\left[\coth\left(\frac{\omega_1}{2\,T}\right) - 1\right] \quad \text{and} \quad E_2^* = 3\,\frac{\omega_2}{2}\,\left[\coth\left(\frac{\omega_2}{2\,T}\right) - 1\right] \ . \tag{25}$$

Figure 7 (r.h.s.) displays these excitation energies (thick lines) as a function of the sum of both. The result of time averaging is depicted by solid triangles which are lying close to the thick lines.

The system needs very long for equilibration since the forces, $-\frac{\partial}{\partial q_\mu}\langle\, Q \,|\, \underset{\sim}{V}_{\rm I} \,|\, Q\,\rangle$, are calculated from the expectation value of the interaction. Even if $\underset{\sim}{V}_{\rm I}$ is of short range, the averaging over the wave packets leads to an effective range, which is of the order of the size of the packets. Thus, at the low excitation energies considered here, the radial dependence of the interaction is rather smooth. In order to avoid correlations among the three particles in the wider potential the strength cannot be chosen to be too strong. On the other hand

a weak interaction cannot easily promote the particle in the narrow potential to the high lying first excited state. Therefore time averaging has to be performed over more than 30000 periods of the wider oscillator starting after 30000 periods in which the system equilibrates.

This system does not equilibrate so readily as the previous cases, nevertheless, from the r.h.s. of fig. 7 it is evident that the excitation energies in the ergodic ensemble are much closer to the quantum result (thick lines) than to the classical one (thin lines). This is surprising because there is only one difference to classical mechanics, namely the width degrees of freedom.

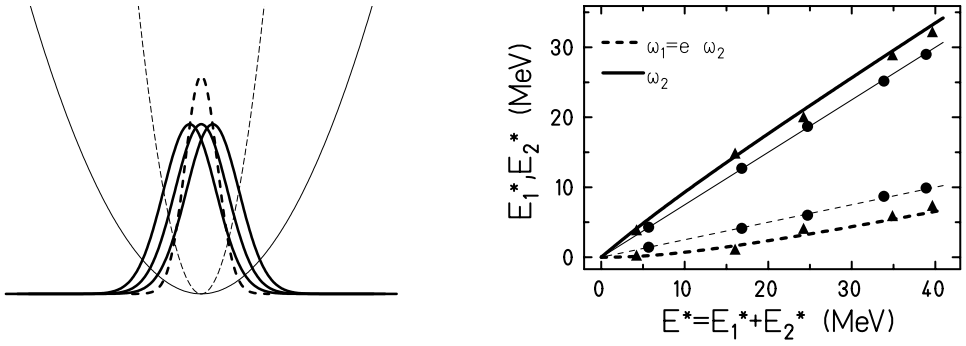

Fig. 7: A system of four distinguishable particles in two different oscillator potentials. L.h.s.: One particle is bound in a narrow oscillator (ω_1, dashed lines), three other particles in a wider oscillator (ω_2, solid lines). R.h.s.: Mean excitation energy of oscillator 1 and 2 versus the sum of both excitation energies. The result of the canonical ensemble is depicted by thick lines and the result of the classical canonical ensemble by thin lines. Solid triangles represent the results of the ergodic ensemble, solid circles the results of the ergodic ensemble, but now using fixed witdth parameters.

To render this study complete the width degrees of freedom are frozen at their respective ground state values and the classical equations of motion are solved with the two–body interaction given in eq. (17), but the operators $\underset{\sim}{x}_k$ being replaced by the classical variables r_k. Now the time averaging yields the classical result as can be seen in fig. 7, where the excitation energies of the ergodic ensemble (circles) coincide with the classical ones.

The result of this subsection is that in the quantum, as well as in the classical case, both subsystems in the two different oscillator potentials approach the same temperature. The only difference between the classical equations and the quantum ones is that the latter ones contain the complex width parameters as additional degrees of freedom. Their presence seems to be sufficient for the system to know about the discrete spectrum of $\underset{\sim}{H}_{\rm HO}$ and to populate the Hilbert space properly.

This subsection was added in order to see under which conditions molecular

dynamics with wave packets finally becomes a system with purely classical statistical properties. As the main purpose was to demonstrate that FMD leads to Fermi–Dirac statistics we kept this subsection rather short, although it is deserving a more extensive discussion.

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