

Thermodynamics of the harmonic oscillator using coherent states

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Abstract. – The ongoing discussion whether thermodynamic properties can be extracted from a (possibly approximate) quantum mechanical time evolution using time averages is fed with an instructive example. It is shown for the harmonic oscillator how the Hilbert space or an appropriately defined phase space must be populated in terms of coherent states in order to obtain the quantum result respectively the classical one.

Introduction. –

In thermodynamics it is a convenient method to replace ensemble averages by time averages, because the partition function *e.g.* of the canonical ensemble cannot be evaluated easily. This is especially true in quantum mechanics because the eigenfunctions of the Hamilton operator are unknown for most interacting many-body systems. Therefore, thermostated time evolutions have been used successfully in classical mechanics [1, 2, 3, 4]. In quantum mechanics less attempts were made, some of them are given in refs. [5, 6, 7, 8, 9, 10, 11, 12, 13]. Following these articles one realizes that the matter is still under debate. The questions are twofold. The first concerns the problem whether it is in principle possible to extract thermodynamic properties from a quantum mechanical time evolution. The second question asks in how far a coherent state used as a trial state in an approximate dynamics like a quantum molecular dynamics is able to visit the Hilbert space in time with the correct weight.

Some of the arguments, which doubt a success of time averaging are loosely speaking like: *Since the equations of motion, either approximative ones like AMD [14, 10] or FMD [15, 16] or the Schrödinger equation itself, have a symplectic structure, like Hamilton's equation of motion in classical mechanics, a time averaging should lead to classical statistics. The dynamics does not know about the discrete structure of the energy levels, it is not quantized. One can excite a system, which is described by coherent states, by any small energy, so it does not know about the finite spacing of energy levels. Coherent states are quasi classical states, the dynamics*

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must lead to classical statistics. Or last but not least, the restriction to product states is equivalent to a mean field calculation, the result of time averaging is therefore classical. This ongoing discussion got new momentum during the program INT-98-2 [17] at the University of Washington this summer.

It is the aim of this letter to demonstrate with the instructive example of the harmonic oscillator how the Hilbert space or an appropriately defined phase space must be populated in terms of coherent states in order to obtain the quantum result or the classical one. That means, that one cannot *a priori* say, that a (possibly approximate) quantum mechanical time evolution is not able to reproduce the correct ensemble average nor that the restriction of the trial state to wave packets or products of them impedes correct time averages.

Thermodynamic mean. –

Given the Hamilton operator \tilde{H} of the harmonic oscillator

$$\tilde{H} = \hbar\omega \left(\tilde{a}^\dagger \tilde{a} + \frac{1}{2} \right), \quad (1)$$

coherent states are defined as eigenstates of the destruction operator \tilde{a}

$$\tilde{a} |z\rangle = z |z\rangle, \quad z = \sqrt{\frac{m\omega}{2\hbar}} r + \frac{i}{\sqrt{2m\hbar\omega}} p. \quad (2)$$

Each coherent state is characterized by a complex parameter z which corresponds to a pair of real parameters (r, p) . Coherent states span the Hilbert space, they are over complete and obey the completeness relation [18]

$$\begin{aligned} \mathbf{1}^{(1)} &= \int \frac{d^2z}{\pi} |z\rangle\langle z|, \quad d^2z = d\text{Re}(z) d\text{Im}(z) \\ &= \int \frac{dr dp}{(2\pi\hbar)} |r, p\rangle\langle r, p|. \end{aligned} \quad (3)$$

A thermodynamic mean of an observable \tilde{B} in the canonical ensemble is given by the trace of this operator together with the statistical operator. This trace can be expressed in any basis, it needs not to be the eigenbasis of \tilde{H} , it may be a basis like those of coherent states which are characterized by a continuous parameter [16, 19]

$$\begin{aligned} \langle\langle \tilde{B} \rangle\rangle &= \frac{1}{Z(\beta)} \int \frac{d^2z}{\pi} \langle z | \tilde{B} e^{-\beta\tilde{H}} | z \rangle \\ &= \frac{1}{Z(\beta)} \int \frac{d^2z}{\pi} e^{-\frac{1}{2}\beta\hbar\omega} e^{-|z|^2(1-e^{-\beta\hbar\omega})} \langle e^{-\frac{1}{2}\beta\hbar\omega} z | \tilde{B} | e^{-\frac{1}{2}\beta\hbar\omega} z \rangle \\ &= \frac{1}{Z(\beta)} \int \frac{d^2z}{\pi} e^{\frac{1}{2}\beta\hbar\omega} e^{-|z|^2(e^{\beta\hbar\omega}-1)} \langle z | \tilde{B} | z \rangle. \end{aligned} \quad (4)$$

The partition function then reads

$$\begin{aligned} Z(\beta) &= \int \frac{d^2z}{\pi} \langle z | e^{-\beta\tilde{H}} | z \rangle \\ &= \int \frac{d^2z}{\pi} e^{\frac{1}{2}\beta\hbar\omega} e^{-|z|^2(e^{\beta\hbar\omega}-1)}. \end{aligned} \quad (5)$$

Given the excitation energy

$$\mathcal{H}(z) = \langle z | \tilde{H} | z \rangle - \frac{1}{2} \hbar\omega = \hbar\omega |z|^2 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 r^2, \quad (6)$$

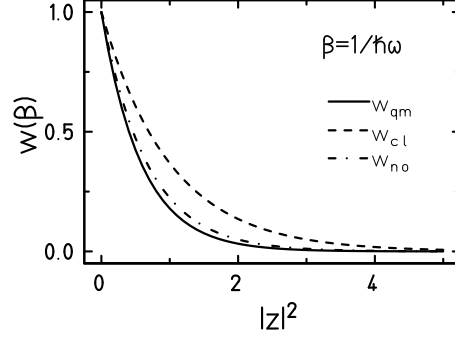


Fig. 1. – Quantum weight (solid line, eq. (7)), classical weight (dashed line, eq. (10)), next order (dashed dotted line, eq. (11)) for the harmonic oscillator potential.

the weight with which a coherent state $|z\rangle = |r, p\rangle$ contributes to a thermodynamic mean is just

$$w_{\text{qm}}(\beta) = e^{-|z|^2(e^{\beta\hbar\omega} - 1)} = e^{-\mathcal{H}(z)(e^{\beta\hbar\omega} - 1)/(\hbar\omega)} \quad (7)$$

where all terms depending only on the zero point energy have been omitted since they cancel with the respective terms in the partition function.

One can now interpret the space of parameters $z = (r, p)$ as a phase space and reformulate eqs. (4) and (5)

$$\langle\langle \tilde{B} \rangle\rangle = \frac{1}{Z(\beta)} \int \frac{dr dp}{(2\pi\hbar)} w_{\text{qm}}(\beta) \mathcal{B}(r, p) \quad (8)$$

$$Z(\beta) = \int \frac{dr dp}{(2\pi\hbar)} w_{\text{qm}}(\beta) . \quad (9)$$

Then $w_{\text{qm}}(\beta)$ is the thermal weight in this phase space and $\mathcal{B}(r, p) = \langle r, p | \tilde{B} | r, p \rangle$ a function of the phase space variables.

Classical limit. –

The connection to classical mechanics is established either by performing the classical ($\hbar \rightarrow 0$) or the high temperature limit ($\beta \rightarrow 0$). The exponential in the exponent of $w_{\text{qm}}(\beta)$ can be expanded, $\hbar\omega$ drops out and the weight (7) approaches the classical result

$$w_{\text{cl}}(\beta) = e^{-\beta\mathcal{H}(z)} . \quad (10)$$

Keeping the next order in the Taylor expansion of the exponential function one gains

$$w_{\text{no}}(\beta) = e^{-\beta(1 + \frac{1}{2}\beta\hbar\omega)\mathcal{H}(z)} . \quad (11)$$

Figure 1 shows all three weights for a specific inverse temperature $\beta = 1/(\hbar\omega)$. One sees that at the same temperature the quantum mechanical distribution is much narrower in $|z|^2 \propto \mathcal{H}(z)$ than the classical one, meaning that the quantum mean excitation energy is less than the classical mean energy.

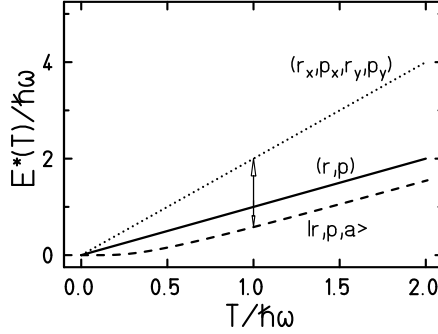


Fig. 2. – Excitation energy for different degrees of freedom. The solid line shows the classical result for a one-dimensional harmonic oscillator, the dotted line the result for two-dimensions; the dashed line displays what happens if the coherent state is replaced by a wave packet with time-dependent width.

Conclusions. –

The purpose of the above exercise is to remind that one can represent quantum mechanics and statistics in a basis which is characterized by a continuous parameter. Although this parameter *does not know anything about the discrete nature of the energy eigenvalues* and moreover leads to the temptation of a classical interpretation, the quantum statistical results are correct, because they do not depend on the chosen representation.

Therefore, if the time evolution of a particle enclosed in a harmonic oscillator and described by a coherent state populates the Hilbert space, or phase space in the sense of (8), with the weight $w_{\text{qm}}(\beta)$ the statistical properties are quantum mechanically correct.

It is a different question whether a specific coupling to a thermostat actually results in such a time evolution. But in the spirit of Nosé [4] one could define a thermostat which works by scaling coordinates and momenta so that the coherent state visits the Hilbert space according to the desired weight. One possible Nosé Hamiltonian would be

$$\mathcal{H}(r, p, s, p_s) = \frac{p^2}{2ms^2} + \frac{1}{2} m\omega^2 s^2 r^2 + \frac{p_s^2}{2M} + \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} \ln(s). \quad (12)$$

Another example, which is formulated with the help of a thermostat for a constrained dynamical system, is given in ref. [5].

Employing a two-body interaction between the thermostat particles and the investigated particle it could be shown numerically in ref. [9] that a coherent state leads to classical statistics, but that the extension of the coherent state towards wave packets with time-dependent width (squeezed coherent states) as used in FMD [16]

$$\langle x | r, p, a \rangle \propto \exp \left\{ -\frac{(x-r)^2}{2a} + \frac{i}{\hbar} px \right\} \quad (13)$$

is sufficient to obtain the quantum result. Having a closer look on the excitation energy

$$\begin{aligned} \mathcal{H}(r, p, a) &= \langle r, p, a | \underline{H} | r, p, a \rangle - \frac{1}{2} \hbar\omega \\ &= \frac{p^2}{2m} + \frac{1}{2} m\omega^2 r^2 + \frac{\hbar}{2} \left(\frac{1}{2m \operatorname{Re}(a)} + m\omega^2 \frac{|a|^2}{2 \operatorname{Re}(a)} \right) - \frac{1}{2} \hbar\omega \end{aligned} \quad (14)$$

which now depends not only on the degrees of freedom r and p , but also on the width parameter a , this might seem counter intuitive compared to classical statistics. As illustrated in fig. 2 in classical statistics additional degrees of freedom, for instance the extension of the one-dimensional oscillator to two dimensions, lead to higher mean energy at the same temperature, whereas the enlarged freedom of the wave function introduced by the non-classical width parameter does the opposite. The wave function is now able to "feel" the underlying density of states which is less than the classical one, therefore, less excitation energy belongs to the same temperature.

In general one must say that whether an approximate quantum dynamics is able to reflect thermal averages does depend on the freedom of the trial state and also on the observables one is interested in. It may very well be that the parameterization of the trial state is rich enough for single-particle observables but not for many-particle observables.

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