EUROPHYSICS LETTERS August 1998

Europhys. Lett., **??** (?), pp. 1-6 (1998)

Thermodynamics of the harmonic oscillator using coherent states

J. Schnack(*)

Universität Osnabrück, Fachbereich Physik
Barbarastr. 7, D-49069 Osnabrück

(received ; accepted)

PACS. 05.30.-d – Quantum statistical mechanics.
PACS. 05.30.Ch – Quantum ensemble theory.
PACS. 02.70.Ns – Molecular dynamics and particle methods.

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. –

Transport models which employ wave packet dynamics are widely used in atomic, solid state and nuclear physics today. Examples range from the description of hydrogen plasmas [1] over the investigation of critical properties of noble gases [2] to simulations of heavy ion collisions in nuclear physics [3, 4, 5]. In all of these models the quantum mechanical time evolution is approximated by the evolution of a (possibly antisymmetrized) product state composed of Gaussian single-particle wave packets (squeezed coherent states [6])

$$\langle\, \vec{x}\,|\,\vec{r},\vec{p},a\,\rangle \quad \propto \quad \exp\left\{-\frac{(\,\vec{x}-\vec{r}\,)^2}{2\,a}+\frac{i}{\hbar}\vec{p}\cdot\vec{x}\right\}\ , \tag{1}$$

where the time dependence of the state is given through the time dependence of the parameters, as there are the mean position $\vec{r}$, the mean momentum $\vec{p}$ and in some cases the complex width a.

Although these models were designed to describe non-equilibrium situations their thermodynamic equilibrium properties are important for two reasons. Firstly, their statistical properties have great influence on final observables like fragment distributions in collisions. Secondly, long time evolutions are used to determine equilibrium behavior and to estimate quantities like the degree of ionization of a plasma [1] or the caloric curve for the nuclear liquid-gas phase

(*) Email: jschnack@uos.de, WWW: http://obelix.physik.uni-osnabrueck.de/~schnack

Typeset using EURO-TEX

transition [7]. The last point is of special interest since approximate quantum evolutions are a possible way to examine thermodynamics properties in cases where the energy spectrum and thus the partition function is not known. In these cases the time-dependent Schrödinger equation cannot be solved, too.

Whereas thermostated time evolutions are on firm grounds in classical mechanics [8, 9, 10, 11] and have been used successfully as well for equilibrium, e.g. to investigate classical spin systems, as for non-equilibrium, e.g. to study glass transitions, in quantum mechanics less attempts were made, some of them are given in refs. [1, 7, 12, 13, 14, 15, 16, 17, 18, 19]. 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 (see for instance [1, 13, 14, 20]): *Since the equations of motion, either approximative ones like in Antisymmetrized Molecular Dynamics (AMD) [5, 17] or Fermionic Molecular Dynamics (FMD) [4, 21] 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 at its best. 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 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 [22] at the University of Washington in summer 1998.

It is the aim of this letter to demonstrate with the algebraicly simple, but 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.

The harmonic oscillator is not a mere example, nowadays it is of special interest for the dynamics of bosonic or fermionic atoms contained in magnetic traps [23, 24, 25] as well as for all systems that show an equidistant level spacing close to the ground state like nuclei or Luttinger liquids.

Thermodynamic mean. –

Given the Hamilton operator $\underset{\sim}{H}$ of the harmonic oscillator

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

coherent states are defined as eigenstates of the destruction operator $\underset{\sim}{a}$

$$\underset{\sim}{a} \ |z\rangle = z \ |z\rangle \ , \quad z = \sqrt{\frac{m\omega}{2\hbar}}\, r + \frac{i}{\sqrt{2m\hbar\omega}}\, p \ . \tag{3}$$

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 [6]

$$\begin{aligned} \underset{\sim}{1}^{(1)} &= \int \frac{\mathrm{d}^2 z}{\pi} \; |\, z \,\rangle\langle\, z \,| \;, \quad \mathrm{d}^2 z = \mathrm{d}\,\mathrm{Re}\,(z)\;\mathrm{d}\,\mathrm{Im}\,(z) \\ &= \int \frac{\mathrm{d}r\,\mathrm{d}p}{(2\pi\hbar)} \; |\, r,\, p \,\rangle\langle\, r,\, p \,| \;. \end{aligned} \tag{4}$$

A thermodynamic mean of an observable $\underset{\sim}{B}$ 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 $\underset{\sim}{H}$, it may be a basis like those of coherent states which are characterized by a continuous parameter [21, 26]

$$\begin{aligned} \langle\langle\, \underset{\sim}{B} \,\rangle\rangle &= \frac{1}{Z(\beta)} \int \frac{\mathrm{d}^2 z}{\pi} \; \langle\, z \,|\, \underset{\sim}{B} e^{-\beta \underset{\sim}{H}} \,|\, z \,\rangle \\ &= \frac{1}{Z(\beta)} \int \frac{\mathrm{d}^2 z}{\pi} \; e^{-\frac{1}{2}\,\beta\hbar\omega} \; e^{-|z|^2\left(1-e^{-\beta\hbar\omega}\right)} \; \langle\, e^{-\frac{1}{2}\,\beta\hbar\omega} z \,|\, \underset{\sim}{B} \,|\, e^{-\frac{1}{2}\,\beta\hbar\omega} z \,\rangle \\ &= \frac{1}{Z(\beta)} \int \frac{\mathrm{d}^2 z}{\pi} \; e^{\frac{1}{2}\,\beta\hbar\omega} \; e^{-|z|^2\left(e^{\beta\hbar\omega}-1\right)} \; \langle\, z \,|\, \underset{\sim}{B} \,|\, z \,\rangle \;. \end{aligned} \tag{5}$$

The partition function then reads

$$\begin{aligned} Z(\beta) &= \int \frac{\mathrm{d}^2 z}{\pi} \; \langle\, z \,|\, e^{-\beta \underset{\sim}{H}} \,|\, z \,\rangle \\ &= \int \frac{\mathrm{d}^2 z}{\pi} \; e^{\frac{1}{2}\,\beta\hbar\omega} \; e^{-|z|^2\left(e^{\beta\hbar\omega}-1\right)} \;. \end{aligned} \tag{6}$$

Given the excitation energy

$$\mathcal{H}(z) = \langle\, z \,|\, \underset{\sim}{H} \,|\, z \,\rangle - \frac{1}{2}\,\hbar\omega = \hbar\omega |z|^2 = \frac{p^2}{2m} + \frac{1}{2}\, m\omega^2 r^2 \;, \tag{7}$$

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

$$w_{\mathrm{qm}}(\beta) = e^{-|z|^2\left(e^{\beta\hbar\omega}-1\right)} = e^{-\mathcal{H}(z)\left(e^{\beta\hbar\omega}-1\right)/(\hbar\omega)} \tag{8}$$

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. (5) and (6)

$$\langle\langle\, \underset{\sim}{B} \,\rangle\rangle = \frac{1}{Z(\beta)} \int \frac{\mathrm{d}r\,\mathrm{d}p}{(2\pi\hbar)} \; w_{\mathrm{qm}}(\beta)\; \mathcal{B}(r,p) \tag{9}$$

$$Z(\beta) = \int \frac{\mathrm{d}r\,\mathrm{d}p}{(2\pi\hbar)} \; w_{\mathrm{qm}}(\beta) \;. \tag{10}$$

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

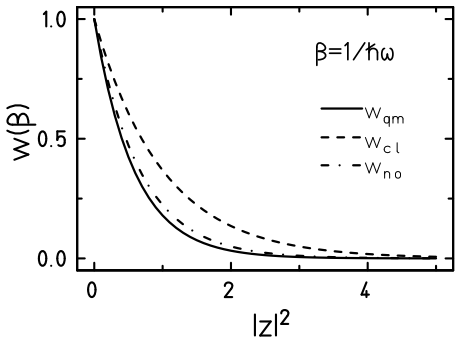

Fig. 1. – Quantum weight (solid line, eq. (8)), classical weight (dashed line, eq. (11)), next order (dashed dotted line, eq. (12)) for the harmonic oscillator potential.

Classical limit. –

The connection to classical mechanics is established either by performing the classical ($\hbar \to 0$) or the high temperature limit ($\beta \to 0$). The exponential in the exponent of $w_{\rm qm}(\beta)$ can be expanded, $\hbar\omega$ drops out and the weight (8) approaches the classical result

$$w_{\rm cl}(\beta) \quad = \quad e^{-\beta \mathcal{H}(z)} \ . \tag{11}$$

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

$$w_{\rm no}(\beta) \quad = \quad e^{-\beta\left(1+\frac{1}{2}\,\beta\hbar\omega\right)\mathcal{H}(z)} \ . \tag{12}$$

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.

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 (9), with the weight $w_{\rm qm}(\beta)$ the statistical properties are quantum mechanically correct.

It is a different question whether a specific approximation of the time-dependent Schrödinger equation or a specific coupling to a thermostat actually results in such a time evolution. In the spirit of Nosé [11] one could for example 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

$$\mathcal{H}(r,p,s,p_s) \quad = \quad \frac{p^2}{2ms^2} + \frac{1}{2}\,m\omega^2 s^2 r^2 + \frac{p_s^2}{2M} + \frac{\hbar\omega}{e^{\beta\hbar\,\omega}-1}\ln(s) \ . \tag{13}$$

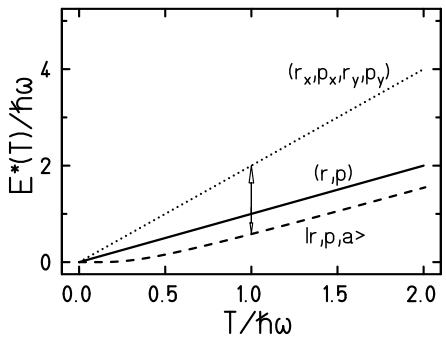

Fig. 2. – Excitation energy for different degrees of freedom. The solid line shows the classical result for a one-dimensional harmonic oscillator, the dotted line the result for two-dimensions; the dashed line displays what happens if the coherent state is replaced by a wave packet with time-dependent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

Another example, which is formulated with the help of a thermostat for a constrained dynamical system, is given in ref. [12].

Concerning approximations of the time-dependent Schrödinger equation it could be shown numerically that distinguishable particles contained in a common harmonic oscillator field and interacting via a short-ranged two-body force which are described by coherent states approach classical statistics on time-average [16], but that the extension of the coherent state towards wave packets with time-dependent width (squeezed coherent states) as used in FMD [21]

$$\langle\, x \,|\, r, p, a \,\rangle \quad \propto \quad \exp\left\{ -\frac{(\,x - r\,)^2}{2\,a} + \frac{i}{\hbar} p x \right\} \tag{14}$$

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

$$\begin{aligned} \mathcal{H}(r,p,a) &= \langle\, r,p,a \,|\, \underset{\sim}{H} \,|\, r,p,a \,\rangle - \frac{1}{2}\,\hbar\omega \\ &= \frac{p^2}{2m} + \frac{1}{2}\,m\omega^2 r^2 + \frac{\hbar}{2}\left(\frac{1}{2m\,\mathrm{Re}\,(a)} + m\omega^2 \frac{|a|^2}{2\,\mathrm{Re}\,(a)} \right) - \frac{1}{2}\,\hbar\omega \end{aligned} \tag{15}$$

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.

***

I would like to thank the National Institute for Nuclear Theory at the University of Washington for the warm hospitality during the program INT–98–2 where a part of this work was done and I would like to thank the Deutsche Forschungsgemeinschaft (DFG) for financial support of this visit. I am thankful for stimulating discussions to G. Bertsch, A. Bulgac, P. Borrmann, H. Feldmeier, P.G. Reinhard, R. Roth, H. Schanz and E. Suraud and to K. Bärwinkel and T. Neff for carefully reading the manuscript.

REFERENCES

[1] W. Ebeling, B. Militzer, *Phys. Lett.*, **A226** (1997) 298.
[2] A. Ohnishi, J. Randrup, *Phys. Rev.*, **A55** (1997) R3315.
[3] J. Aichelin, H. Stöcker, *Phys. Lett.*, **B176** (1986) 14.
[4] H. Feldmeier, *Nucl. Phys.*, **A515** (1990) 147.
[5] A. Ono, H. Horiuchi, Toshiki Maruyama, A. Ohnishi, *Phys. Rev. Lett.*, **68** (1992) 2898.
[6] J.R. Klauder, B.-S. Skagerstam, *Coherent States*, (World Scientific Publishing Co. Pte. Ltd., Singapore) 1985.
[7] J. Schnack, H. Feldmeier, *Phys. Lett.*, **B409** (1997) 6.
[8] S. Nosé, *J. Chem. Phys.*, **81** (1984) 511.
[9] W.G. Hoover, *Phys. Rev.*, **A31** (1985) 1685.
[10] D. Kusnezov, A. Bulgac, W. Bauer, *Ann. of Phys.*, **204** (1990) 155.
[11] S. Nosé, *Prog. of Theor. Phys. Suppl.*, **103** (191) 1.
[12] D. Kusnezov, *Phys. Lett.*, **A184** (1993) 50.
[13] A. Ohnishi, J. Randrup, *Nucl. Phys.*, **A565** (1993) 474.
[14] D. Klakow, C. Toepffer, P.-G.Reinhard, *Phys. Lett.*, **A192** (1994) 55.
[15] P. Blaise, P. Durand, O. Henri-Rousseau, *Physica*, **A209** (1994) 51.
[16] J.Schnack, H. Feldmeier, *Nucl. Phys.*, **A601** (1996) 181.
[17] A. Ono, H. Horiuchi, *Phys. Rev.*, **C53** (1996) 2341.
[18] A. Ohnishi, J. Randrup, *Phys. Lett.*, **B394** (1997) 260.
[19] J. Schnack, *Physica*, **A259** (1998) 49.
[20] D. Klakow, C. Toepffer, P.-G.Reinhard, *J. Chem. Phys.*, **101** (1994) 1.
[21] H. Feldmeier, J. Schnack, *Prog. Part. Nucl. Phys.*, **39** (1997) 393.
[22] http://www.phys.washington.edu/∼bulgac/int_98.html
[23] M.H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman, E.A. Cornell, *Science*, **269** (1995) 198.
[24] K.B. Davis, M.-O. Mewes, M.R. Andrews, N.J. van Druten, D.S. Durfee, D.M. Kurn, W. Ketterle, *Phys. Rev. Lett.*, **75** (1995) 3969.
[25] C.C. Bradley, C.A. Sackett, R.G. Hulet, *Phys. Rev. Lett.*, **78** (1997) 985.
[26] J. Schnack, *dissertation*, (TH Darmstadt) 1996.