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Phase space approach to real-time quantum evolution: towards non-equilibrium lattice field theory

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Abstract. A strategy of studying non-equilibrium phenomena in lattice field theory is discussed in the framework of Wigner's phase space approach. For a test model, an ensemble of anharmonic oscillators at weak coupling, an analytic non-perturbative solution is found. In this case a quasiclassical approach is shown to be valid for a wide range of parameters.

1. Introduction

Recently there has been considerable progress in the numerical investigation of non-perturbative equilibrium properties of quantum field theories. In lattice approximations, vacuum or thermal expectation values can be computed quite efficiently by standard techniques such as the Metropolis algorithm (Metropolis *et al* 1953) because this problem reduces, with few exceptions, to the evaluation of Euclidean time path integrals of positive measure. Non-equilibrium problems, however, obviously require a real-time approach and cannot be reduced in a similar way to functional integrals of positive measure. No progress comparable to the equilibrium case has therefore been made.

Attempts towards the non-perturbative treatment of non-equilibrium phenomena include the complex Langevin approach. The Langevin simulation is the only method used for equilibrium problems having a chance of being applicable to real-time situations as well. Langevin equations with complex drift terms have been studied by various groups (see, e.g., Klauder and Petersen 1985) and are found to converge towards the corresponding complex measure in some but not all cases. Studies of real-time quantum mechanics (Callaway *et al* 1985, Ilgenfritz and Kripfganz 1986) are encouraging but far from allowing realistic investigations of multi-dimensional problems.

In the present paper we follow a different route. An interesting class of real-time problems is expected to show almost classical behaviour. This should be the case whenever the energy density is large compared to the vacuum energy. A particular problem which has motivated the present analysis has been a classical approach to reheating processes in the early universe (Kripfganz and Ilgenfritz 1985). Classical motion in lattice field theory can be studied by standard techniques and the expected approach to thermal equilibrium, dissipation and reheating has been found. Of course, this approach is justified only if quantum corrections can be estimated and shown to be small.

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Whenever one expects quasiclassical behaviour Wigner's phase space formulation of quantum mechanics (Wigner 1932) should provide a useful and adequate framework, in particular for numerical studies. Recently, this approach has become very popular again but, to our knowledge, has not been applied to the study of non-equilibrium phenomena in lattice field theory. The strategy is in fact quite straightforward and will be briefly reviewed in § 2. We work in the Heisenberg picture. In this case the main problem consists of solving the Heisenberg equation for the Wigner equivalents of the operators whose expectation values are candidates for study. The ensemble average can then be performed by standard Monte Carlo techniques, allowing the numerical evaluation of time-dependent expectation values from first principles. In the quasiclassical expansion the solution of the Heisenberg-Wigner equation is recursively expressed in terms of solutions of the classical equations of motion. The approach is non-perturbative as far as the coupling constants of the theory are concerned.

Already the first quantum corrections to the classical motion do not have a very simple structure and show oscillations increasing with time. Performing the ensemble average might therefore not be totally trivial in practice even when the measure is positive. For this and other reasons it might be desirable to have a simple solvable but non-trivial test model, before embarking on more complicated problems. Such a test model is presented and solved in § 3. The model consists of an ensemble of independent anharmonic oscillators with a weak λq^4 term, but with time t allowed to become of order $1/\lambda$. An analytic solution to the Heisenberg-Wigner equation is found which is correct up to terms of order λ but with terms of order λt summed to all orders. The approach is therefore non-perturbative in λt and $\hbar$. Results are discussed in § 4. The analysis of the test model shows explicitly that for a large range of energy densities quantum effects are irrelevant for the approach to equilibrium. The method will allow to estimate quantum corrections efficiently also for more complicated systems, thereby determining the range of validity of the classical regime.

Similar problems are also under study using the finite element approach to the operator Heisenberg equation (Bender *et al* 1985). Our approach is more limited in scope but also more tractable, and should be superior in all cases where quasiclassical behaviour is anticipated.

2. General strategy: quasiclassical approach

The basic problem to be studied is simply to find an efficient algorithm for computing non-perturbatively expectation values

$$\langle A(t)\rangle = \mathrm{Tr}\, A(t)\rho \tag{1}$$

in lattice field theory. Only bosonic theories will be considered here. $A(t)$ is one of the Heisenberg operators

$$A(t) = \exp\left(\frac{\mathrm{i}tH}{\hbar}\right) A(0) \exp\left(-\frac{\mathrm{i}tH}{\hbar}\right) \tag{2}$$

chosen to characterise the time evolution of the system. ρ is the density operator.

In terms of Wigner's distribution functions, (1) is

$$\langle A(t)\rangle = \int \mathrm{d}[q]\,\mathrm{d}[p]\, A_{\mathrm{w}}(\{q\},\{p\},t)\rho_{\mathrm{w}}(\{q\},\{p\}) \tag{3}$$

with the Wigner equivalent of the operator A given by

$$A_w(\{q\},\{p\},t)=\int \mathrm{d}[\tilde{q}]\exp\left(\frac{\mathrm{i}p_j\tilde{q}_j}{\hbar}\right)\langle\{q-\tilde{q}/2\}|A(t)|\{q+\tilde{q}/2\}\rangle \tag{4}$$

and similarly for ρ_w. In the following, we use a single mode notation but the generalisation to many degrees of freedom is straightforward.

Equation (3) expresses the ensemble average of $A(t)$ as phase space integral as in statistical mechanics. In quantum mechanics, however, $\rho_w(q,p)$ need not be positive everywhere, and therefore does not have a strict probability interpretation. $A_w(q,p,t)$ is obtained as a solution of the Wigner equivalent of the Heisenberg equation

$$\frac{\partial A}{\partial t}=\frac{\mathrm{i}}{\hbar}[H,A] \tag{5}$$

which becomes

$$\frac{\partial}{\partial t}A_w(q,p,t)=\frac{2}{\hbar}H_w(q,p)\sin\frac{\hbar\Lambda}{2}A_w(q,p,t) \tag{6}$$

where

$$\Lambda=\frac{\overleftarrow{\partial}}{\partial p}\frac{\vec{\partial}}{\partial q}-\frac{\overleftarrow{\partial}}{\partial q}\frac{\vec{\partial}}{\partial p} \tag{7}$$

is the Poisson bracket operator. These and other useful results are summarised, for example, by Imre *et al* (1967). In the field theory limit (3) becomes a functional integral. In the lattice approximation it can be evaluated by standard Monte Carlo techniques provided one finds efficient algorithms for solving (6).

A formal solution to (6) is of course

$$A_w(q,p,t)=\exp\left(\frac{2t}{\hbar}H_w\sin\frac{\hbar\Lambda}{2}\right)A_w(q,p,0) \tag{8}$$

but it is not very useful for practical purposes. Apart from special cases, where more explicit analytical solutions can be found a quasiclassical approach, i.e. an expansion in $\hbar^2$, suggests itself. The first terms of this expansion have the structure

$$A_w(q,p,t)=A_{cl}(q,p,t)-\frac{\hbar^2}{4!}\int_0^t \mathrm{d}t'\left[H_w(\bar{q},\bar{p})\left(\frac{\overleftarrow{\partial}}{\partial\bar{p}}\frac{\vec{\partial}}{\partial\bar{q}}-\frac{\overleftarrow{\partial}}{\partial\bar{q}}\frac{\vec{\partial}}{\partial\bar{p}}\right)^3\right]A_{cl}(\bar{q},\bar{p},t')+O(\hbar^4) \tag{9}$$

where

$$A_{cl}(q,p,t)=A(q_{cl}(q,p,t),p_{cl}(q,p,t)) \tag{10}$$

and

$$\begin{aligned}\bar{q}&=q_{cl}(q,p,t-t')\\ \bar{p}&=p_{cl}(q,p,t-t').\end{aligned} \tag{11}$$

In this way the quantum solution $A_w(q,p,t)$ is expressed in terms of classical solutions. However, the numerical effort in calculating the $O(\hbar^2)$ or even higher contributions will be considerable due to the need of evaluating derivatives with respect to the initial conditions. A promising method for approaching this problem is a finite element approximation for the time evolution, calculating the required derivatives recursively

from time slice to time slice. Results along these lines will be presented elsewhere. In the following we shall study an instructive example where the quasiclassical expansion can be explicitly summed, through finding the solution to the corresponding partial differential equation (6) analytically.

3. A solvable model

We consider an ensemble of independent anharmonic oscillators with Hamiltonian

$$H_w(q,p)=\tfrac{1}{2}p^2+\tfrac{1}{2}m^2q^2+\tfrac{1}{4}\lambda q^4. \tag{12}$$

In this case, the Heisenberg-Wigner equation (6) is explicitly

$$\frac{\partial}{\partial t}A_w=\left(p\frac{\partial}{\partial q}-(m^2q+\lambda q^3)\frac{\partial}{\partial p}+\frac{\hbar^2}{4}\lambda q\frac{\partial^3}{\partial p^3}\right)A_w. \tag{13}$$

Equivalently, it may be written as an integro-differential equation

$$A_w(q,p,t)=A_{cl}(q,p,t)+\hbar^2\int_0^t \mathrm{d}t'\exp[(t-t')\hat{H_1}]\left(\frac{\lambda}{4}q\frac{\partial^3}{\partial p^3}\right)A_w(q,p,t') \tag{14}$$

with

$$\hat{H_1}=p\frac{\partial}{\partial q}-(m^2q+\lambda q^3)\frac{\partial}{\partial p}. \tag{15}$$

The operator $\exp(t\hat{H_1})$ generates the classical motion

$$\exp(t\hat{H_1})f(q,p)=f(q_{cl}(q,p,t),p_{cl}(q,p,t)). \tag{16}$$

Equation (14) may be solved under the following conditions. λ is assumed to be small, with all terms $O(\lambda)$ dropped but terms of order λt kept. Those terms have to be summed to all orders leading to a solution non-perturbative in λt.

First we need the classical solution in this approximation. This is of course a trivial problem leading to

$$\begin{aligned} q_{cl}(t)&=\frac{1}{\sqrt{2m}}[b^+\exp(\mathrm{i}\omega t)+b\exp(-\mathrm{i}\omega t)]+O(\lambda)\\ p_{cl}(t)&=\mathrm{i}\left(\frac{m}{2}\right)^{1/2}[b^+\exp(\mathrm{i}\omega t)-b\exp(-\mathrm{i}\omega t)]+O(\lambda)\end{aligned} \tag{17}$$

with

$$\begin{aligned} &\omega=m+\omega' E \qquad \omega'=\tfrac{3}{4}\lambda/m^3\\ &E=mb^+b+O(\lambda)\end{aligned} \tag{18}$$

and

$$b=\frac{1}{\sqrt{2m}}(mq+\mathrm{i}p) \qquad b^+=b^* \tag{19}$$

b and b^+ (corresponding to annihilation and creation operators in the quantum case) have been introduced here for convenience, because of their simple time translation properties

$$\exp(t\hat{H_1})b=\exp(-\mathrm{i}\omega t)b \qquad \exp(t\hat{H_1})b^+=\exp(\mathrm{i}\omega t)b^+. \tag{20}$$

The approximation (17) is appropriate as long as $\lambda^2 t$ is small, or more precisely

$$\omega'^2 E^2 t \ll m \tag{21}$$

which puts an upper limit on t, i.e. the approximation does not allow us to study the limit $t \to \infty$, λ fixed. Returning to the quantum problem we now have to make a choice which operator A we wish to consider. The simplest choice would be $q(t)$ but the ensemble average $\langle q(t) \rangle$ vanishes identically for symmetric initial distributions. We therefore choose $A(t) = q^2(t)$.

The general structure of the Wigner equivalent of $q^2(t)$ may be easily discovered from the iterative solution to (14). It is

$$(q^2)_w = \frac{1}{m} b^+ b + \frac{1}{m} \mathrm{Re}[b^{+2} g(\tilde{E}, \tilde{t}) \exp(2i\omega t)] + O(\lambda) \tag{22}$$

with

$$\tilde{E} = E/m \qquad \tilde{t} = 2i\omega' m t. \tag{23}$$

Equation (22) results because the factor λ in the kernel of (14) must be compensated by a factor t arising from the t' integral. This can only happen if oscillating factors of the integrand cancel which just occurs for the structure (22)

$$\exp[(t-t')\hat{H_1}] b^{+2} g(\tilde{E}, \tilde{t}') \exp(2i\omega t') = b^{+2} g(\tilde{E}, \tilde{t}') \exp(2i\omega t). \tag{24}$$

From (14), $g(\tilde{E}, \tilde{t})$ is found to satisfy the equation

$$\frac{\partial g}{\partial \tilde{t}} = -\frac{\hbar^2}{8}\left[6\tilde{t} - \tilde{t}^2\tilde{E} - 2\tilde{t}\tilde{E}\frac{\partial}{\partial \tilde{E}} + 6\frac{\partial}{\partial \tilde{E}} - \tilde{E}\frac{\partial^2}{\partial \tilde{E}^2}\right] g \tag{25}$$

with initial condition $g(\tilde{E}, 0) = 1$ independent of E. In this way the problem has been reduced from a third-order partial differential equation of three variables to one of second order and two variables.

Perhaps surprisingly, (25) is solved exactly by the ansatz

$$g(\tilde{E}, \tilde{t}) = \rho(\tilde{t}) \exp(\tilde{E}\varphi(\tilde{t})) \tag{26}$$

leading to the ordinary differential equations

$$\frac{\mathrm{d}}{\mathrm{d}\tilde{t}}\varphi = -\tfrac{1}{8}\hbar^2[-\tilde{t}^2 - 2\tilde{t}\varphi - \varphi^2] \qquad \varphi(0) = 0 \tag{27}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}\tilde{t}}\rho = -\frac{\hbar^2}{8}[6\tilde{t} + 6\varphi]\rho \qquad \rho(0) = 1. \tag{28}$$

They can also be solved by the obvious substitution $y = \phi - \tilde{t}$. The result is

$$y(\tilde{t}) = \frac{\sqrt{8}}{\hbar}\tan\frac{\hbar\tilde{t}}{\sqrt{8}} - \tilde{t} \tag{29}$$

$$\rho(\tilde{t}) = \exp\left(6\log\cos\frac{\hbar\tilde{t}}{\sqrt{8}}\right). \tag{30}$$

The final result for $(q^2)_w$ is now easily obtained:

$$(q^2)_w = \frac{1}{m} b^+ b + \frac{1}{m}\exp\left(6\log\cosh\frac{2\hbar\omega' m t}{\sqrt{8}}\right) \times \mathrm{Re}\left[b^{+2}\exp(2imt)\exp\left(i\sqrt{8}\frac{E}{\hbar m}\tanh\frac{2\hbar\omega' m t}{\sqrt{8}}\right)\right]. \tag{31}$$

4. Discussion

In the same way explicit solutions for other operators can be obtained as well. With the solution for $A_w(q, p, t)$ available one can now study ensemble averages, according to (3). We shall discuss a simple example for the $t=0$ density operator, namely the Gibbs ensemble of harmonic oscillators at inverse temperature β and frequency $\bar{m}$. The corresponding Wigner function is given by

$$\rho_w(q, p) = \mathcal{N}^{-1} \exp[-\tilde{\beta}(\tfrac{1}{2}p^2 + \tfrac{1}{2}\bar{m}^2 q^2)] \tag{32}$$

with

$$\tilde{\beta} = \frac{2}{\hbar\bar{m}} \tanh \frac{\hbar\bar{m}\beta}{2} \tag{33}$$

and

$$\mathcal{N} = \cosh \frac{\hbar\bar{m}\beta}{2}. \tag{34}$$

At $t=0$ the Hamiltonian (12) is switched on. In general, the determination of the initial Wigner distribution is by itself a non-trivial problem. In the case of (32) the ensemble average can be trivially performed leading, for example, to

$$\begin{aligned}\langle q^2(t)\rangle = {} & \frac{1}{\tilde{\beta}m^2}\frac{1+\Gamma}{2} + \frac{\Gamma-1}{2m^2\tilde{\beta}} \exp\left(6 \log\cosh \frac{2\hbar\omega' m t}{\sqrt{8}}\right) \\ & \times \operatorname{Re}\left[\exp(2\mathrm{i}mt)\left(1 - \frac{\mathrm{i}\sqrt{8}}{\hbar\tilde{\beta}m}\tanh\frac{2\hbar\omega' m t}{\sqrt{8}}\right)^{-3/2}\right. \\ & \left. \times\left(1 - \Gamma\frac{\mathrm{i}\sqrt{8}}{\hbar\tilde{\beta}m}\tanh\frac{2\hbar\omega' m t}{\sqrt{8}}\right)^{-3/2}\right]\end{aligned} \tag{35}$$

with

$$\Gamma = m^2/\bar{m}^2. \tag{36}$$

The solution (35) is non-perturbative in $\hbar$ as well as λt, with a simple singularity structure determined by the two branch cuts. The non-perturbative regime starts with

$$\frac{\sqrt{8}}{\hbar\tilde{\beta}m}\tan\frac{2\hbar\omega' m t}{\sqrt{8}} \gtrless 1 \text{ or } 1/\Gamma \text{ respectively} \tag{37}$$

and shows damped oscillations caused by the non-linear λq^4 contribution. The essential feature is that at sufficiently large energy density (i.e. $\tilde{\beta} \ll 1$) the non-perturbative behaviour of the classical contribution sets in already for $\omega' t$ small ($\omega' t \sim \tilde{\beta}$). In this time range quantum corrections are still small, as is obvious from (35), and can be treated perturbatively. This is precisely the situation where the quasiclassical approach outlined in § 2 becomes appropriate.

A numerical example is shown in figure 1, with parameters $m=1$, $\Gamma=0.5$, $\tilde{\beta}=0.25$, $\omega'=0.05$. Quantum effects are impressively unimportant in the transient region. A similar observation has already been made at strong coupling (Ilgenfritz and Kripfganz 1985) but in this case only a very short time interval could have been studied.

The very large time behaviour may in fact be very different for the classical and quantum systems, respectively, with quasi-periodicity expected in the quantum case. This cannot be studied here because condition (21) restricts the allowed time range.

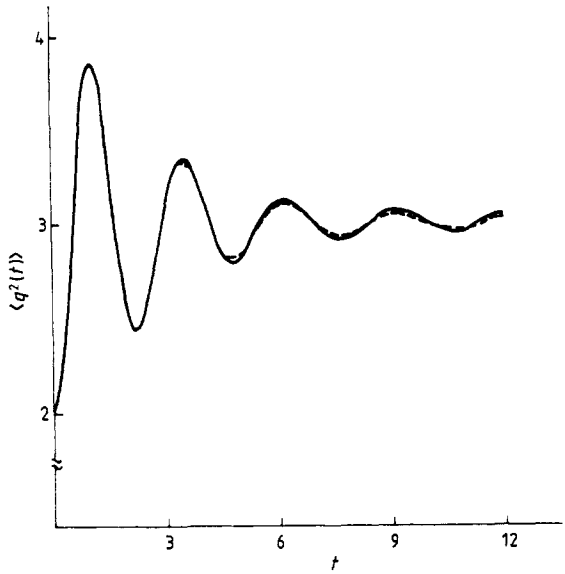

Figure 1. Evolution of the ensemble average of $q^2(t)$ for a set of parameters described in the text. The quantum solution is given by the full curve and the classical one by the broken curve.

In many cases this would be of no practical importance as long as the time dependence becomes already sufficiently weak in the quasiclassical region.

For more complicated systems the solution of the Heisenberg-Wigner equation will have to be generated numerically, and also the ensemble average has to be done by Monte Carlo methods. One might question whether in such cases the numerical accuracy could be achieved to see small differences between quantum and classical behaviour like the one in figure 1. This is not such a severe problem, however, because the correction term is calculated separately. For the example of figure 1 we have checked that a sample of about 1000 trajectories is sufficient to reproduce the correction term in good quality.

The method is not expected to work very well near the ground state and in particular if tunnelling phenomena are relevant. Still, there remains a large class of interesting problems, where considerable progress could be expected. One such problem is quantum chaos, in particular the role of quantum contributions near the stochastic transition of simple non-integrable systems. Dissipative phenomena in scalar $(1+1)$-dimensional lattice field theory are currently under study.

We should also emphasise that the approach outlined in this paper should be very useful not only for non-equilibrium problems but as well for non-perturbative studies of multi-time correlation functions in equilibrium.

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