From Quantum Action to Quantum Chaos

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1 Introduction

This article is about the relation between classical mechanics and quantum mechanics. The question is asked: Can quantum mechanics be formulated in such a way that it looks like some sort of classical mechanics? Why do we ask such question in the first place? The answer is interesting from the point of view of interpretation of quantum mechanics. L. de Broglie \cite{1} has pointed out that quantum mechanics has two faces: The particle interpretation and the wave interpretation. Maybe there is a third interpretation, where quantum mechanics has the face of classical mechanics. The answer is interesting also for the purpose of a proper definition, quantitative analysis and understanding of phenomena occuring in quantum physics, the definition of which comes from classical physics. Examples are quantum chaos and quantum instantons. The affirmative answer to the above question has been proposed recently in Refs.\cite{2,3}, stating that quantum transition amplitudes can be expressed in terms of some action, called the quantum action, which has the form of the classical action but has modified parameters.

1.1 Bridges between classical mechanics and quantum mechanics

A general method to build bridges from classical to quantum physics is the path integral. By "bridges" we mean a relation, e.g., involving the quantum action.
transition amplitude and the classical action. In particular, starting from
the path integral, the following "bridges" have been suggested:

(i) *Sum over classical paths.* Let us consider the Q.M. transition amplitude
from \( x_{in}, t_{in} \) to \( x_{fi}, t_{fi} \) given by the path integral. In certain cases this path
integral can be expressed as a sum over classical paths only,
\[
G(x_{fi}, t_{fi}; x_{in}, t_{in}) = \sum_{\{x_{cl}\}} Z \exp \left[ \frac{i}{\hbar} S[x_{cl}]_{x_{in}, t_{in}}^{x_{fi}, t_{fi}} \right],
\]
(1)
where \( S[x_{cl}] \) is the classical action evaluated along the classical trajectory
from \( x_{in}, t_{in} \) to \( x_{fi}, t_{fi} \). This is true, e.g. for the harmonic oscillator. Un-
fortunately, such relation holds only in a few exceptional cases [4].

(ii) *Gutzwiller’s trace formula.* Gutzwiller [5] has established a relation be-
tween the density of states of the quantum system and a sum over classical
periodic orbits (periodic orbit quantisation). The trace formula reads (see
Ref.[6])
\[
\rho(E) = \rho_0(E) - \frac{1}{2\pi\hbar} \text{Im} \sum_p T_p \sum_{n=1}^{\infty} \frac{\exp[i(n\Phi_p(E)/\hbar - \mu_p \tau/2)]}{i \sin[n\lambda_p(E)/2]},
\]
(2)
where \( \rho(E) = Tr[\delta(E - H)] \) denotes the density of states, and \( \rho_0(E) \) is the
average level density. The sum runs over all primitive periodic orbits \( p \),
the index \( n \) denotes repeated traversal of primitive periodic orbits and \( T_p \)
is the traversal time of such an orbit. \( \Phi_p(E) \) is the action of the periodic
orbit \( p \) at energy \( E \) and \( \lambda_p(E) \) denotes a Lyapunov exponent. Here \( \mu_p \) is a
constant characteristic for the orbit \( p \). The trace formula has been applied
successfully in the semi-classical regime (e.g. highly excited states of atom).
Wintgen [7] applied it to the diamagnetic hydrogen system and was able to
extract periodic orbit information from experimental level densities.

(iii) The *effective action* has been introduced in quantum field theory in such
a way that it gives an expectation value \( \langle \phi \rangle = \phi_{class} \) which corresponds to
the classical trajectory and which minimizes the potential energy (effective
potential). Thus one can obtain the ground state energy of the quantum
system from its effective potential. The effective action \( \Gamma \) [8, 9] is defined by
\[
\begin{align*}
Z[J] &= e^{-iW[J]} \\
\frac{\partial}{\partial J(x)} W[J] &= -\langle 0 | \phi(x) | 0 \rangle_J \\
\phi_{cl}(x) &= \langle 0 | \phi(x) | 0 \rangle_J \\
\Gamma[\phi_{cl}] &= -W[J] - \int d^4y J(y) \phi_{cl}(y).
\end{align*}
\]
(3)
An effective action has been also considered at finite temperature [10]. Because the effective action has a mathematical structure similar to the classical action, and the quantum effects are taken into account by parameters different from their classical counterparts, the effective action looks like the ideal way to bridge the gap from quantum to classical physics and eventually solve the quantum chaos and quantum instanton problem. However, there is a catch. The effective potential and the effective action in quantum mechanics has been computed using perturbation theory by Canetti et al. [11]. Consider the Lagrangian

\[ L(q, \dot{q}, t) = \frac{m}{2} \dot{q}^2 - V(q) \]

\[ V(q) = \frac{m}{2} \omega^2 q^2 + U(q), \quad (4) \]

and \( U(q) \) is, say, a quartic potential \( U(q) \sim q^4 \). Then the effective action is obtained in doing a loop (\( \hbar \)) expansion

\[ \Gamma[q] = \int dt \left( -V^{eff}(q(t)) + \frac{Z(q(t))}{2} \dot{q}^2(t) + A(q(t)) q^4(t) + B(q(t))(d^2q/dt^2)^2(t) + \cdots \right) \]

\[ V^{eff} = \frac{1}{2} m \omega^2 q^2 + U(q) + \hbar V^{eff}_1(q) + O(\hbar^2) \]

\[ Z(q) = m + \hbar Z_1(q) + O(\hbar^2) \]

\[ A(q) = \hbar A_1(q) + O(\hbar^2) \]

\[ B(q) = \hbar B_1(q) + O(\hbar^2). \quad (5) \]

There are higher loop corrections to the effective potential \( V^{eff} \) as well as to the mass renormalisation \( Z \). The most important property is the occurrence of higher time derivative terms. Actually, there is an infinite series of increasing order. Here comes the problem. When we want to interpret \( \Gamma \) as effective action, the higher time derivatives require more initial/boundary conditions than the classical action. This is a catastrophe. In the following we will present an alternative way to construct an action taking into account quantum corrections.

## 2 Quantum Action

We want to construct a renormalized or quantum action from transition matrix elements, which involve the time evolution. In quantum physics the transition amplitude from \( x_{in}, t_{in} \) to \( x_{fi}, t_{fi} \) is given by

\[ G(x_{fi}, t_{fi}; x_{in}, t_{in}) = \int [dx] \exp \left[ \frac{i}{\hbar} S[x] \right] \bigg|_{x_{in}, t_{in}}^{x_{fi}, t_{fi}} , \quad (6) \]
where $S$ denotes the classical action. In Ref.\cite{2,3} we have proposed the existence of a quantum action which satisfies the following properties:

**Conjecture:** For a given classical action $S = \int dt \frac{m}{2} \dot{x}^2 - V(x)$ there is a quantum action $\tilde{S} = \int dt \frac{\tilde{m}}{2} \dot{\tilde{x}}^2 - \tilde{V}(\tilde{x})$, which allows to express the transition amplitude by

$$G(x_{fi}, t_{fi}; x_{in}, t_{in}) = \tilde{Z} \exp\left[\frac{i}{\hbar} \tilde{S}[\tilde{x}_{cl}]\right]_{x_{in}, t_{in}}.$$  \hspace{1cm} (7)

Here $\tilde{x}_{cl}$ denotes the classical path, such that the action $\tilde{S}(\tilde{x}_{cl})$ is minimal (we exclude the occurrence of conjugate points or caustics). $\tilde{Z}$ denotes the normalisation factor corresponding to $\tilde{S}$. Eq.\text{[7]} is valid with the same action $\tilde{S}$ for all sets of boundary positions $x_{fi}, x_{in}$ for a given time interval $T = t_{fi} - t_{in}$. The parameters of the quantum action depend on the time $T$. The quantum action converges to a non-trivial limit when $T \to \infty$. Any dependence on $x_{fi}, x_{in}$ enters via the trajectory $\tilde{x}_{cl}$. $\tilde{Z}$ depends on the action parameters and $T$, but not on $x_{fi}, x_{in}$.

One may ask: What is the difference between effective and quantum action? Conceptually, effective action and quantum action look quite similar. However, its technical definition is different and also its physical content. The effective action requires $\langle \phi \rangle = \phi_{cl}$, while the quantum action does not. The effective action corresponds to infinite time and allows to obtain the ground state energy, but the quantum action is defined for arbitrary finite time $T$. In Euclidean formulation, the inverse time corresponds to temperature. Thus the quantum action allows to describe quantum physics at finite temperature including excited states (see below). However, the effective action can be defined also at finite temperature \cite{10}. The effective action can be computed analytically by perturbation theory (loop expansion). However, this series is not convergent. Practically, it can be used only for some small number of loops and small values of the perturbation parameter. The quantum action can be computed non-perturbatively for all values of the coupling parameter. The effective action has the defect of generating higher order time derivatives. The quantum action is postulated to be free of higher time derivative terms. To construct the quantum action being sensitive to excited states, one needs transition matrix elements beyond the vacuum sector. We have chosen to use position states in Q.M. In Q.F.T. this corresponds to Bargman states.
2.1 Construction of quantum action

Suppose the classical action is given by

\[ S = \int_0^T dt \frac{m}{2} \dot{x}^2 - v_4 x^4(t). \]  

Then we make an ansatz for the quantum action

\[ \tilde{S} = \int_0^T dt \frac{\tilde{m}}{2} \dot{x}^2 - \left\{ \tilde{v}_0 + \tilde{v}_1 x(t) + \cdots + \tilde{v}_N x^N(t) \right\}. \]

Then \( \tilde{m}, \tilde{v}_0, \ldots, \tilde{v}_N \) are the renormalized parameters which take into account the quantum corrections. Their values are determined by making a global best fit to a number of transition amplitudes \( G(x_j, T; x_i, 0) \) (which satisfies Eq.7), where \( x_i, x_j \) have been taken from a set of points \( \{x_1, \cdots, x_J\} \) and those points have been chosen to cover some interval \([-a, +a]\). More details are given in Refs.[2, 3].

As an example, the parameters of the quantum action corresponding to the double well potential (action \( S = \int_0^T dt \frac{m}{2} \dot{x}^2 - \{v_0 + v_2 x^2 + v_4 x^4\} \), \( v_0 = \frac{1}{2}, v_2 = -1, v_4 = \frac{1}{2} \)) as function of \( T \) is shown in Fig.[1]. One observes that the parameters of the quantum action vary with the transition time \( T \). For small \( T \) (limit \( T \to 0 \)) the parameters of the quantum action are consistent with those of the classical action. For sufficiently large time \( T \), the parameters of the quantum action tend to converge asymptotically.

2.2 Quantum action at finite temperature

First we make a Wick rotation to imaginary time. The purpose is, first to make the path integral well defined (Wiener measure) allowing to apply Monte Carlo methods for its numerical computation. Secondly, the instanton is defined in imaginary time. One effect of this transformation is that it changes a relative sign between the kinetic term and the potential term of the action. Thus in the following we work with imaginary time (Euclidean) actions and Green’s functions. Let us see how the quantum action is related to finite temperature physics. According to the laws of quantum mechanics and thermodynamic equilibrium, the expectation value of some observable \( O \), like e.g. average energy is given by

\[
< O > = \frac{Tr [O \exp[-\beta H]]}{Tr [\exp[-\beta H]]} = \frac{\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy < x|O|y > < y|\exp[-\beta H]|x >}{\int_{-\infty}^{+\infty} dx < x|\exp[-\beta H]|x >},
\]  

\[ (10) \]
where $\beta$ is related to the temperature $\tau$ by $\beta = 1/(k_B \tau)$. On the other hand the (Euclidean) transition amplitude is given by

$$G(x_{fi}, T; x_{in}, 0) = < x_{fi} | \exp[-HT/\hbar] | x_{in} >$$  \hspace{1cm} (11)

Thus from the definition of the quantum action, Eq.(7), one obtains

$$< O > = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy < x | O | y > \exp[-\tilde{S}_\beta(x,y)] \int_{-\infty}^{+\infty} dx \exp[-\tilde{S}_\beta(x,0)]$$  \hspace{1cm} (12)

if we identify

$$\beta = \frac{1}{k_B \tau} = T/\hbar.$$  \hspace{1cm} (13)

As a result, the quantum action $\tilde{S}_\beta$ computed from transition time $T$, describes equilibrium thermodynamics at $\beta = T/\hbar$, i.e. temperature $\tau = 1/(k_B \beta)$.

In the case of the double well potential we have found that parameters of the quantum action vary as function of $T$ (Fig.[1]). Translating this behavior into temperature, it means that the parameters of the quantum action are temperature dependent (or $\beta$-dependent). In particular, we can interpret the behavior for small $T$ as follows. $T = 0$ means temperature $\tau = \infty$. The quantum action at infinite temperature coincides with the classical action. On the other hand, the limit $T \to \infty$ corresponds to temperature $\tau \to 0$. The quantum behavior is dominated by the ground state (Feynman-Kac formula).

3 Quantum Instantons

Quantum mechanics, which describes physics at atomic length scales can not be understood by the laws of classical physics valid at macroscopic length scales. Examples are: Heisenberg’s uncertainty principle, quantum tunneling, Schrödinger’s cat paradox, entangled states, Einstein-Rosen-Podolski paradox, quantum cryptology, quantum computing etc. On the other hand, in modern physics there are notions which have proven to be quite useful and which have their origin in classical physics. For example consider instantons. Instantons play a role in quantum chromodynamics (QCD), the standard model of strong interactions. They may be important for the mechanism of confinement of quarks. Presumably they play an important role in nuclear matter at high temperature and density, where a phase transition from the hadronic phase to the quark-gluon plasma has been predicted.
Even a richer phase structure may exist \[12\]. Furthermore, in the inflationary scenario of the early universe, instantons are important. For a review see Ref.\[13\]. During inflation, quantum fluctuations of the primordial field expand exponentially and eventually end up as a classical field. The fluctuations are of the size of the horizon \[14\]. The classical fluctuations eventually lead to galaxy formation \[15\].

In quantum physics, an instanton solution is conventionally defined as the saddle point approximation of the (Euclidean) path integral. However, there is a problem with the proper definition of instantons in quantum physics: Let us consider a 1-D system in quantum mechanics with a particle of mass \(m\) moving in a potential \(V(x) = A(x^2 - a^2)^2\). This potential has two minima at \(x = \pm a\). The instanton \(x_{\text{inst}}(t)\) is the solution of the classical equation of motion in imaginary time, with boundary conditions such that the particle starts at \(x(t = -\infty) = -a\), \(\dot{x}(t = -\infty) = 0\) and arrives at \(x(t = +\infty) = +a\), \(\dot{x}(t = +\infty) = 0\). The problem again is that quantum mechanics does not allow to specify both, position and momentum with zero uncertainty.

In Ref.\[3\] we have suggested to define a quantum instanton solution via the quantum action. This means to compute non-perturbatively the quantum action \(\tilde{S}\) (in imaginary time) and analyze if the corresponding quantum potential \(\tilde{V}\) has multiple degenerate minima (degenerate vacua). Then the quantum instanton is defined as the classical solution \(\tilde{x}_{\text{class}}\) between those minima (there is no problem with boundary conditions). Such quantum instanton solutions have been computed in quantum mechanics for the 1-D double well potential in Ref.\[3\]. The quantum instantons were found to be "softer" than the classical instantons (potential minima were closer and the potential barrier was lower).

4 Quantum Chaos

Classical deterministic chaos has been observed in a huge number of phenomena in macroscopic i.e. classical physics. But chaotic phenomena were also found in systems ruled by quantum mechanics. For example, the hydrogen atom in a strong magnetic field shows strong irregularities in its spectrum \[16\]. Irregular patterns have been found in the wave functions of the quantum mechanical model of the stadium billiard \[17\]. Billiard like boundary conditions have been realized experimentally in mesoscopic quantum systems, like quantum dots and quantum corrals, formed by atoms in semi-conductors \[18\].

So what is the problem with chaos in quantum physics? It has to do with...
its proper definition. The underlying reason is due to the dynamical group of time evolution. In classical mechanics time evolution of a system can be viewed as an infinite sequence of infinitesimal canonical transformations. The corresponding dynamical group is the symplectic group. In quantum mechanics, a system governed by a time independent Hamiltonian, follows the time evolution of the unitary group. This difference has simple but drastic consequences: In classical physics, chaos is characterized, e.g. by Lyapunov exponents or Poincaré sections. This is based on identifying trajectories in phase space (position and conjugate momentum). In quantum mechanics, Heisenberg’s uncertainty relation $\Delta x \Delta p \geq \hbar/2$ does not allow to specify a point in phase space with zero error! Consequently, the apparatus of classical chaos theory can not be simply taken over to quantum physics.

Due to this problem, workers in quantum chaos have tried to characterize such systems in different ways, alternative to those of classical chaos. One successful route has been to characterize the spectral density of quantum system with chaotic classical counterpart by Poisson versus Wigner distributions. There is a conjecture by Bohigas et al. [13], which says that the signature of a classical chaotic system is a the spectral density following a Wigner distribution.

### 4.1 Quantum chaos in 2 dimensions

As the problem with a proper definition of quantum chaos has the same root as the problem with quantum instantons, we suggest also to apply the same strategy of solution, i.e. define quantum chaos via the quantum action. Then the quantum action $\tilde{S}$ incorporates the effects of quantum physics, but has mathematically the structure of a classical action. The apparatus of classical chaos theory, like Lyapunov exponents, Poincaré sections etc. can be applied to the quantum action $\tilde{S}$.

As is well known 1-dimensional conservative systems with a time-independent Hamiltonian are integrable and do not produce classical chaos. An interesting candidate to consider is the K-system, corresponding to the potential $V = x^2y^2$. This describes a 2-D Hamiltonian system, being almost globally chaotic, having small islands of stability [20]. However, from the numerical point of view more convenient, but also showing classical chaos, is the following related system, investigated by Pullem and Edmonds [21]. It is defined by the classical action

$$S = \int_0^T dt \frac{1}{2} m (\dot{x}^2 + \dot{y}^2) - (v_{2+2}(x^2 + y^2) + v_{22}x^2y^2).$$

(14)
As parameters of the classical action we use $m = 1$, $v_{2+2} = 0.5$, $v_{22} = 0.05$ and the convention $\hbar = k_B = 1$. The Poincaré sections corresponding to energies $E = 10, 20, 50$ are shown in Figs.[2a,3a,4a].

For the corresponding quantum action, we make the following ansatz, which is compatible with time-reversal symmetry, parity conservation and symmetry under exchange $x \leftrightarrow y$,

$$
\tilde{S} = \int_0^T dt \left( \frac{1}{2} \tilde{m}_{2+2}(\dot{x}^2 + \dot{y}^2) + \frac{1}{2} \tilde{m}_{11}\dot{x}\dot{y} \right)
- \left\{ \tilde{v}_0 + \tilde{v}_{11}xy + \tilde{v}_{2+2}(x^2 + y^2) + \tilde{v}_{22}x^2y^2 + \tilde{v}_{1+3}(xy^3 + x^3y) + \tilde{v}_{4+4}(x^4 + y^4) \right\}. \quad (15)
$$

We have determined numerically the parameters of the quantum action for transition time $T = 0.5$, corresponding to temperature $\tau = 2$, and find

\begin{align*}
\tilde{m}_{2+2} & = 0.9998(2) \\
\tilde{m}_{11} & = 0.0000(3) \\
\tilde{v}_0 & = 1.1875(32) \\
\tilde{v}_{11} & = 0.0105(31) \\
\tilde{v}_{2+2} & = 0.5098(63) \\
\tilde{v}_{22} & = 0.0523(15) \\
\tilde{v}_{1+3} & = 0.0016(12) \\
\tilde{v}_{4+4} & = 0.0017(30). \quad (16)
\end{align*}

The data are consistent with vanishing parameters $\tilde{m}_{11}$, $\tilde{v}_{1+3}$ and $\tilde{v}_{4+4}$. The quantum action slightly modifies the parameters $\tilde{v}_{2+2}$ and the parameter $\tilde{v}_{22}$. We computed the Poincaré sections for the quantum action at temperature $\tau = 2$, corresponding to energies $E = 10, 20, 50$. They are shown in Figs.[2b,3b,4b]. One observes that the quantum system also displays chaos, and the Poincaré sections are slightly different from those of the classical action. One should note that the classical action at $T = 0$ is equivalent to a quantum action at temperature $\tau = \infty$.

## 5 Discussion

We have discussed the use of the quantum action, which can be considered as a renormalized classical action at finite temperature. We found that the quantum action solves the problem of proper definitions of quantum instantons and quantum chaos. As an example, we have considered harmonic oscillators with a weak anharmonic coupling ($V_{\text{coup}} \sim x^2y^2$) and computed
the quantum action at temperature $\tau = 2$. We compared Poincaré sections at temperature $\tau = \infty$ and $\tau = 2$ and found that both display chaos.

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Figure caption

Fig.[1] Quantum action parameters corresponding to classical double well potential

\[ V(x) = \frac{1}{2}(x^2 - 1)^2. \] 

Quantum action parameters \( \tilde{m} \) (full diamond, full dot), \( \tilde{v}_0 \) (open diamond, open dot), \( \tilde{v}_2 \) (full triangles), \( \tilde{v}_4 \) (open triangles) versus transition time \( T \) (inverse temperature).

Fig.[2a] Classical Poincaré sections corresponding to the classical potential

\[ V(x, y) = \frac{1}{2}(x^2 + y^2) + 0.05x^2y^2. \] 

Energy \( E = 10 \).

Fig.[2b] Poincaré sections from the quantum action corresponding to the classical potential

\[ V(x, y) = \frac{1}{2}(x^2 + y^2) + 0.05x^2y^2. \] 

Energy \( E = 10 \).

Fig.[3a] Like Fig.[2a], but energy \( E = 20 \).

Fig.[3b] Like Fig.[2b], but energy \( E = 20 \).

Fig.[4a] Like Fig.[2a], but energy \( E = 50 \).

Fig.[4b] Like Fig.[2b], but energy \( E = 50 \).
POINCARÉ SECTION

QUANTUM
POINCARÉ SECTION

CLASSICAL

E = 20
POINCARÉ SECTION

QUANTUM
POINCARÉ SECTION

CLASSICAL

-10  -5   0   5   10

-10  -5   0   5   10

\( E = 50 \)
POINCARÉ SECTION