Closed Path Integrals and Renormalisation in Quantum Mechanics

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We suggest a closed form expression for the path integral of quantum transition amplitudes. We introduce a quantum action with renormalized parameters. We present numerical results for the $V \sim x^4$ potential. The renormalized action is relevant for quantum chaos and quantum instantons.

1. Introduction

The path integral has become a standard method to quantize classical theories. The class of systems for which the path integral can be computed analytically is ridiculously small. Examples are quadratic Lagrangians, e.g., for free motion and the harmonic oscillator [1]. Let us consider the Q.M. transition amplitude from $x_{in}, t_{in}$ to $x_{fi}, t_{fi}$ given by

$$G(x_{fi}, t_{fi}; x_{in}, t_{in}) = \int [dx] \exp \left[ \frac{i}{\hbar} S[x] \right]_{x_{in}, t_{in}}^{x_{fi}, t_{fi}}, \tag{1}$$

where $S = \int dt \frac{m\dot{x}^2}{2} - V(x)$ denotes the classical action. In some cases this path integral can be expressed as a sum over classical paths only

$$G(x_{fi}, t_{fi}; x_{in}, t_{in}) = \sum_{\{x_{cl}\}} Z \exp \left[ \frac{i}{\hbar} S[x_{cl}] \right]_{x_{in}, t_{in}}^{x_{fi}, t_{fi}}, \tag{2}$$

where $S[x_{cl}]$ is the classical action evaluated along the classical trajectory from $x_{in}, t_{in}$ to $x_{fi}, t_{fi}$. There may be infinitely many classical paths for a given pair of boundary points $(x_{in}, t_{in}), (x_{fi}, t_{fi})$. Different paths then correspond to different values of the action. The factor $Z$ represents some (time-dependent) normalisation factor, enforced by the unitarity of the amplitude. Eq.(2) holds, e.g., for quadratic Lagrangians, where the sum runs over a single path where the action is minimal. In the case of the harmonic oscillator $V(x) = \frac{m\omega^2}{2} x^2$, one has

$$S[x_{cl}]|_{x_{in}, t_{in}}^{x_{fi}, t_{fi}} = \frac{m\omega}{2 \sin(\omega T)} \left[ x_{fi}^2 + x_{in}^2 \right] \cos(\omega T) - 2x_{in} x_{fi},$$

$$Z = \sqrt{\frac{m\omega}{2\pi i \hbar \sin(\omega T)}}, \quad T = t_{fi} - t_{in}.$$ 

Another example where the sum over classical paths is exact is the path integral of the quantum mechanical top, which mathematically corresponds to free motion on the group manifold of $SU(2) \otimes \mathbb{R}^2$. Eq.(3) is a well known but remarkable result. It is possible that there are other systems, where the path integral is given by a sum over classical paths. However, the result is not true in general. A simple counter example is given by Nelson [1].

In the following we will explore if the validity of Eq.(3) can be extended to a wider class of quantum systems, if we allow the classical action to be replaced by a renormalized action. The motivation comes from perturbative renormalisation in Q.F.T. Recall that a theory is called renormalizable, if a fixed finite number of counter terms of the action allows to make the Q.F.T. finite to any given order. The renormalized action is different from the bare action, due to quantum loop corrections, which exist for interacting theories. The action and also Green’s functions have the same structure in its bare and renormalized form. Quantum mechanics can be viewed as Q.F.T. in $0 + 1$ dimension. Here we suggest for Q.M. the existence of a renormalized/quantum action, which describes the transition amplitude (Green’s function), having the same structure but parameters different from the classical action.

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

$$G(x_{fi}, t_{fi}; x_{in}, t_{in}) = \tilde{Z} \exp \left[ \frac{i}{\hbar} \tilde{S}[\tilde{x}_{cl}] \right]_{x_{in}, t_{in}}^{x_{fi}, t_{fi}}, \tag{3}$$

Here $\tilde{x}_{cl}$ denotes the classical path corresponding to the action $\tilde{S}$, 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.(3) 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 renormalized action

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depend on the time $T$. The renormalized 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 $x_{fi}, x_{in}$.

Why is such result of physical interest? (i) Having constructed the action $\tilde{S}$ gives a closed form solution for the path integral. (ii) The action $\tilde{S}$ defines a renormalized action in Q.M. (iii) Gutzwiller’s trace formula has been used widely to study quantum chaos in a semi-classical regime (e.g., highly excited states in atoms). Eq.(3) establishes a simple relation between the transition amplitude and some action $\tilde{S}$ which mathematically has the form of the classical action. Eq.(3) allows to define quantum chaos in an unambiguous way. (iv) Eq.(3) allows to study quantum descendants of classical instanton solutions. We have no proof of this conjecture. However, we will give numerical evidence in support of the conjecture. We will elaborate on the topic (ii), while (iii,iv) will be discussed in another letter.

2. Construction of renormalized action

We know the quantum action for the harmonic oscillator.

What does perturbation theory predict for the quantum action in the presence of a small anharmonic perturbation $S[x] = \int_0^T \frac{\dot{x}^2}{2m} + \frac{\omega_0^2 x^2}{2} + \lambda V(x)$, $\lambda << 1$? Using the saddle point method one obtains up to order $O(\lambda^2)$

$$\tilde{S} = S + S_1 + S_2,$$

$$S_1[x] = \frac{\lambda}{2m} \int_0^T dt \ G(t,t) \ V''(x(t)),$$

$$S_2[x] = \frac{\lambda^2}{4m^2} \int_0^T dt dt' \ G(t,t')G(t',t) V''(x(t))V''(x(t')),$$

$$G(t,t') = \frac{1}{\omega sh(\omega T)} \begin{bmatrix} sh(\omega t) & sh(\omega t' - T) : t \leq t' \\ sh(\omega t') & sh(\omega t - T) : t' \leq t \end{bmatrix},$$

where $G(t,t')$ denotes the Euclidean Green’s function. This shows that the quantum action contains terms beyond that occurring in the classical action.

In the following we want to determine numerically the renormalized action, Eq.(3), for the case of a quartic potential. In this work, we search for renormalized parameters, neglecting potential terms higher than fourth order in a first step. This search requires to calculate the transition amplitude, Eq.(3). We have chosen to compute the path integral via Monte Carlo with importance sampling. This requires to go over to imaginary time (Euclidean path integral) $t \to -it$. Then Eq.(3) becomes

$$G_E(x_{fi}, t_{fi}; x_{in}, t_{in}) = \int [dx] \exp[-\frac{1}{\hbar} S_E[x]] \bigg|_{x_{fi}, t_{fi}}^{x_{in}, t_{in}},$$

where the Euclidean classical action is given by $S_E = \int dt \frac{\dot{x}^2}{2} + V(x)$. Correspondingly, Eq.(3) becomes

$$G_E(x_{fi}, t_{fi}; x_{in}, t_{in}) = \tilde{Z}_E \exp \bigg[ -\frac{1}{\hbar} \tilde{S}_E[\tilde{x}_{cl}] \bigg|_{x_{in}, t_{in}}^{x_{fi}, t_{fi}} \bigg],$$

where the Euclidean quantum action is given by $\tilde{S}_E = \int dt \frac{\dot{x}^2}{2} + \tilde{V}(x)$. The transition to imaginary time causes a sign change of the mass term, besides that the action parameters keep its absolute and relative values. In the sequel of the paper we will work in imaginary time. We drop the subscript $E$ in what follows.

We consider a particle of mass $m$ moving in the presence of a local potential $V(x)$, given in polynomial form $V(x) = \sum_{n=0}^N v_n x^n$, with the parameters $m, v_0, \ldots, v_N$. We write the potential of the quantum action $\tilde{V}(x) = \sum_{n=0}^N \tilde{v}_n x^n$, being parametrized by $\tilde{m}, \tilde{v}_0, \ldots, \tilde{v}_N$. We choose a value for the time $T$ and a set of boundary points $\{x_1, \ldots, x_J\}$. For all pairs of $x_{in}, x_{fi}$ from that set we compute the Euclidean transition amplitude $G_{ij} \equiv G(x_i, x_j, T)$. We denote the Euclidean action $\tilde{S}$ along its classical path $\tilde{x}_{cl}$ by $\tilde{\Sigma}_{ij} = \tilde{S}[\tilde{x}_{cl}]_{t_{ij}, 0}^{t_{ij}, 0}$. Because $\tilde{Z}$ does not depend on $x_{in}, x_{fi}$, we subsume it into $\tilde{\Sigma}_{ij}^{ab} = \tilde{\Sigma}_{ij} - \ln \tilde{Z}$. Then Eq.(3) takes the form

$$G_{ij} = \exp[-\tilde{\Sigma}_{ij}^{ab}], \quad i, j = 1, \ldots, J.$$ (5)

While the quantum action has $N+2$ parameters, Eq.(5) represents $J^2/2 + O(J)$ independent equations to determine the quantum action. We have chosen a larger number of equations than parameters (over-determined) requiring that the error in Eq.(5) becomes globally minimal. I.e., we make a $\chi^2$-fit,

$$\chi^2 = \sum_{i,j=1,\ldots,J} (G_{ij} - \exp[-\tilde{\Sigma}_{ij}^{ab}])^2 / \sigma_{ij}^2,$$

which is a function of the parameters of the quantum action. A solution for the quantum action is considered as consistent, if we find the same action parameters for different sets of boundary points.

3. Numerical results

We have computed the Euclidean propagator in two ways: (i) We use Monte Carlo with importance sampling. The trick is to write the propagator matrix element as a ratio of two path integrals. This corresponds to splitting the action $S = S_0 + S_1$, chosen such that the path integral for $S_0$ is analytically known, $\exp[-S_0/\hbar]$ is treated as weight and $\exp[-S_1/\hbar]$ is treated as observable. (ii) According to the Feynman-Kac formula, the propagator for large time is asymptotically given by the ground state contribution. We have solved the stationary Schrödinger equation, computing a number $M$ (of lowest lying) energies and wave functions, and expressed the propagator as a spectral sum over those states.

(a) To test our algorithms, we considered the harmonic oscillator $V(x) = v_2 x^2$, $v_2 = 1/2$ (with parameters $m = \omega = \hbar = 1$). The classical path, the transition amplitude and the renormalized action are analytically
known, giving $\tilde{S} = S$. The results are found within statistical errors to be consistent with $\tilde{S} = S$.

(b) Next we have considered the quartic interaction $V(x) = v_4 x^4$, $v_4 = 1$, with parameters $m = h = 1$. We have computed numerically the ground state energy, $E_{gr} = 0.667986$, and the variance of the ground state wave function, $\text{var}_{gr} = 0.287333$. From those we introduce dynamically a time scale and a length scale (corresponding to the Bohr radius), $T_{sc} = \hbar/E_{gr} = 1.497$, $L_{sc} = \sqrt{\text{var}_{gr}} = 0.5360$. We have computed the propagator for $0 < T < 2$ via Monte Carlo runs with $N_{therm} = 4000$, $N_{skip} = 2000$ and $N_{conf} = 1000$. For $T > 1$ we also computed the propagator by solving the stationary Schrödinger equation and calculating the wave function and energy of the lowest $M$ states of the spectrum. We used $M = 30$ for $1 < T < 2$ and $M = 7$ for $T > 2$. We used up to 20 000 mesh points to solve the classical equation of motion in the determination of $S[\tilde{x},\tilde{p}]$. For the time interval $T = 0.5$, the numerical results are shown in Tab.[1]. The following observations are made: (i) The linear and the cubic renormalized potential term are compatible within statistical error with the value zero, expected from parity conservation of the quantum system.

(ii) The renormalized action generates a quadratic potential term, absent in the classical action. With respect to variation of the interval, most coefficients vary very little and are compatible within statistical errors with each other. The quadratic term is more sensitive, showing fluctuations from its average value of up to two standard deviations. In general we find for $J = 6$ that the numerical values of $\chi^2$ lie in the order of the value $\chi^2 = 36$, which means that the fits are acceptable. We found that the intervals, where the algorithms work, lie in the range of $[-1.0, +1.0]$ to $[-3.6, +3.6]$. If the interval is too small, with boundary points $x_i < < 1$, then the potential terms $x^2$ and $x^4$ are difficult to distinguish. On the other hand, if the interval is too large, with boundary points $x_i >> 1$, then the observable $\exp[-x^4]$ (of the Monte Carlo algorithm) becomes very small. In the renormalized action the quartic term dominates strongly over the quadratic term, which makes the latter difficult to discriminate. Stability of the renormalized parameters under variation of the interval of boundary points has been observed also for other values of the time $T$. The dependence on $T$ is shown in Fig.[1]. The error bars are estimated systematically (statistical errors of Monte Carlo data are of the size of symbols). We distinguish three regimes: (i) $0 < T << T_{sc}$, (ii) $T \approx T_{sc}$, and (iii) $T >> T_{sc}$. For $T$ close to zero, the renormalized parameters are close to those of the classical action. An exception is $\tilde{v}_4$ at $T = 0.1$, which is about 10% off the classical value. We believe that this does not reflect physics but is a fault due to limited numerical precision (recall that the propagator becomes $\delta(x_{f i} - x_{i n})$ when $T \rightarrow 0$). At about $T \approx T_{sc}$, $\tilde{m}_n$, $\tilde{v}_2$ and $\tilde{v}_4$ change noticeably. For large $T >> T_{sc}$ the renormalized parameters converge asymptotically. When increasing $T$ beyond $T_{sc}$ one observes that the stability of results requires an exponential increase in the number of mesh points. This can be traced to the fact that the classical trajectory covers several orders of magnitude (and the order increases with $T$). This observation, similar to critical slowing down observed in simulating critical phenomena in lattice field theory, puts an upper limit on the time parameter used in this investigation ($T \leq 5$).

4. Interpretation

How can we understand the behavior of the renormalized parameters? Why does the renormalized action depend on $T$? Consider the $n$-point function of a scalar field,
\[ \Gamma = \langle \text{vac}|t.o.(\Phi(x_1) \cdots \Phi(x_n))|\text{vac} \rangle. \]

This is the vacuum expectation value of a time-ordered \( n \)-fold product of the field. It corresponds to the transition from the physical vacuum at \( t = -\infty \), to the physical vacuum at \( t = +\infty \) with intermediate creation (annihilation) of particles at \( t_1, \ldots, t_n \). In order to obtain finite expressions, one introduces a regularisation parameter, say \( \mu \). Then \( \Gamma = \Gamma(x_1, \mu) \), i.e. the result depends on \( \mu \). In Q.M., we consider the propagator from \( x_{in}, t_{in} \) to \( x_{fi}, t_{fi} \). \( T = t_{fi} - t_{in} \). The analogue in Q.F.T. is

\[ \langle \text{vac}, t = T|t.o.(\Phi(x_1) \cdots \Phi(x_n))|\text{vac}, t = 0 \rangle. \]

Then the \( n \)-point function \( \Gamma(x_1, \mu, T) \) depends also on the time \( T \). The computation of renormalized parameters from \( \Gamma(x_1, \mu, T) \) then gives mass, coupling constants etc. as function of \( T \). Thus it is no surprise that the renormalized parameters in Q.M. also depend on \( T \).

Fig.\[1\] Renormalized parameters (in dimensionless units) versus time \( T \). Transition amplitude obtained by Monte Carlo (dots and circles) and by stationary Schrödinger equation (other symbols).

How can we understand the behavior of the renormalized parameters changing qualitatively in the investigated time interval? (i) For sufficiently small \( T \), one has \( S < h \), i.e. we are in the quantum regime. However, according to Dirac \[8\] (see also Ref. \[6\]), \( \exp(iS/h) \) is a good approximation of the propagator \( G \), when the time interval \( T \) over which \( G \) is supposed to propagate goes to zero. This is consistent with our numerical observation \( \bar{S} \approx S \) in this regime. (ii) For sufficiently large time \( T \) one has \( S > h \), i.e. one is in the semi-classical (WKB) regime. In imaginary time, the Feynman-Kac formula describes the propagator asymptotically,

\[ G(x_{fi}, T; x_{in}, 0) \sim_{T \to \infty} \psi_{gr}(x_{fi}) \exp(-E_{gr}T/h)\psi_{gr}(x_{in}). \]

For the harmonic oscillator \( (E_{gr} = \hbar\omega/2) \) one can show

\[ \tilde{v}_0 \sim_{T \to \infty} E_{gr}. \]

For the quartic potential one observes also a smooth behavior of \( \tilde{v}_0 \). We have fitted \( \tilde{v}_0 \) by the function \( A + B/T \). We obtain \( \tilde{v}_0 \to 0.6868 \), compatible with Eq.(6). Then using the definition of the renormalized action, Eq.(4), splitting the renormalized action into a \( \tilde{v}_0 \) part and a rest, and using the Feynman-Kac formula implies

\[ \exp[-\frac{1}{\hbar} \int_0^T dt \tilde{v}_0] \exp[-\frac{1}{\hbar} \int_0^T dt \frac{\tilde{m}}{2} \dot{x}^2 + \tilde{V}(\tilde{x})] \rightarrow_{T \to \infty} \psi_{gr}(x_{fi}) \exp(-E_{gr}T/h)\psi_{gr}(x_{in}). \]

Consequently, the renormalized action, when excluding the \( \tilde{v}_0 \) term, has an asymptotic limit for large \( T \)

\[ -\frac{1}{\hbar} \int_0^T dt \frac{\tilde{m}}{2} \dot{x}^2 + \tilde{V}(\tilde{x}) \rightarrow_{T \to \infty} \ln[\psi_{gr}(x_{fi}) \psi_{gr}(x_{in})]. \]

This is a strong indication (no proof) that the renormalized parameters of \( \tilde{S} \) converge asymptotically in \( T \). This is what has been observed in the data. It corresponds in Q.F.T. to the infinite volume limit.

In conclusion, we have computed numerically for the quartic potential a quantum corrected action, and find parameters being quite different from the classical values. Hence, quantum fluctuations can change the classical behavior drastically. This has been observed (in preliminary results) also for the instantons solutions of the double well potential.

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[1] L.S. Schulman, *Techniques and Applications of Path Integration*, John Wiley&Sons, New York (1981).
[2] L.S. Schulman, Phys. Rev. A35(1987)4956.
[3] L.S. Schulman, Phys. Rev. 176(1968)1558.
[4] Private communication by E. Nelson. See \[1\].
[5] M.C. Gutzwiller, *Chaos in Classical and Quantum Mechanics*, Springer, Berlin (1990), and references therein.
[6] P.M.A. Dirac, Physikalishe Zeitschrift der Sowjetunion, 3, No. 1 (1933); reprinted in: J. Schwinger, *Quantum Electrodynamics*, Dover, New York (1958); see also P.M.A., *The Principles of Quantum Mechanics*, Oxford, London (1958).
