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LETTER TO THE EDITOR

Time-sliced path integrals with stationary states**Chris M Field and Frank W Nijhoff**

Department of Applied Mathematics, University of Leeds, Leeds LS2 9JT, UK

E-mail: cfield@maths.leeds.ac.uk and nijhoff@maths.leeds.ac.uk

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Online at stacks.iop.org/JPhysA/39/L309**Abstract**

The path integral approach to the quantization of one degree-of-freedom Newtonian particles is considered within the discrete time-slicing approach, as in Feynman's original development. In the time-slicing approximation the quantum mechanical evolution will generally not have any stationary states. We look for conditions on the potential energy term such that the quantum mechanical evolution may possess stationary states without having to perform a continuum limit. When the stationary states are postulated to be solutions of a second-order ordinary differential equation (ODE) eigenvalue problem, it is found that the potential is required to be a solution of a particular first-order ODE. Similarly, when the stationary states are postulated to be solutions of a second-order ordinary difference equation (ODE) eigenvalue problem the potential is required to be a solution of a particular first-order ODE. The classical limits (which are at times very nontrivial) are integrable maps.

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1. Introduction

The path integral approach to quantum mechanics was developed by Feynman in the middle of the last century [4], building on an insight of Dirac's [2] (see also [3]). As described by Feynman [5], the path integral approach 'is another, a third way, of describing quantum mechanics, which looks quite different to that of Schrödinger and Heisenberg, but is equivalent to them'. There have now been thousands of papers on the application of path integral techniques to problems in quantum mechanics. This was recently surveyed in the monograph [8], where results on models that have been explicitly solved were classified and arranged in tabular form. In their practical application, however, path integrals are still usually performed via Feynman's original time-slicing approach (see, for instance, [11]).

This letter considers the time-sliced path integral of a non-relativistic particle with one degree of freedom, as described by a Lagrangian of the form

$$\mathcal{L}_0(\dot{q}, q) = \frac{1}{2}\dot{q}^2 - V(q), \quad (1.1)$$

and looks for potentials, $V(q)$, such that the quantum evolution may have stationary states whilst still within the discrete time-sliced approximation.

The results have relevance to various areas of research, including the study of lattice effects in Monte Carlo simulations, asymptotically long-time investigations of quantum systems, and the investigation of discrete-time quantum systems in their own right.

In section 2, the potential term is derived under the assumption that the preserved quantum mechanical stationary states of the discrete-time evolution are eigenfunctions of a linear second-order ODE.

In section 3, the potential term is derived under the assumption that the preserved quantum mechanical stationary states of the discrete-time evolution are eigenfunctions of a linear second-order $O\Delta E$.

2. Differential equation ansatz

Feynman's approach gives the one-step time evolution of a wavefunction $\psi(q_n, t_n)$ within the time-slicing approximation as

$$\psi(q_{n+1}, t_{n+1}) = N \int_C \exp\left[\frac{i}{\hbar} \varepsilon \mathcal{L}(q_{n+1}, q_n)\right] \psi(q_n, t_n) dq_n, \quad (2.1)$$

where C is some interval of \mathbb{R} , and n is a discrete time parameter. To obtain the wavefunction at later times the integrals are concatenated (i.e., iterated). In Feynman's original paper [4], the path integral is built up, and worked with throughout the paper, by employing a finite time interval $\varepsilon = t_{n+1} - t_n$, which is sent to zero at the end of the calculations. In this limit (where a finite time interval requires an infinite number of integrals) we obtain the path integral, see [4, 6]. This 'time-slicing' approach is still the method that is usually employed in the evaluation of path integrals. As we are studying phenomena within the time-slicing approximation we set $\varepsilon = 1$ without loss of generality. The discrete-time Lagrangian is (see [4])

$$\mathcal{L}(q_{n+1}, q_n) = \frac{1}{2}(q_{n+1} - q_n)^2 - V(q_n). \quad (2.2)$$

(The discrete-time Lagrangian (2.2) follows from the original Lagrangian (1.1) by the replacement $\dot{q} = (q_{n+1} - q_n)/\varepsilon$, see [4].) For $C = \mathbb{R}$, unitarity shows that $|N|^2 = (2\pi\hbar)^{-1}$ (in [4] N is found by considering the zeroth-order term of an expansion in the time-step parameter). At this stage we refrain from stipulating the range of integration and the normalization constant N .

A simple gauge transformation allows us to consider, instead of (2.2), the (gauge equivalent):

$$\mathcal{L}(q_{n+1}, q_n) = -q_n q_{n+1} + q_n^2 - V(q_n) =: -q_n q_{n+1} - W(q_n). \quad (2.3)$$

In this section, we look for forms of the potential, $V(q)$ (or, equivalently, $W(q)$), such that after evolution by equation (2.1) the new wavefunction is a solution to the same eigenvalue problem of a second-order ODE, with the same eigenvalue (and so will be for any number of evolutions). We write the eigenvalue problem as

$$M_q \psi(q) = E \psi(q), \quad (2.4)$$

where M_q is an arbitrary linear second-order ODE (which for convenience is written as a partial differential operator)

$$M_q = p_0(q) \frac{\partial^2}{\partial q^2} + p_1(q) \frac{\partial}{\partial q} + p_2(q). \quad (2.5)$$

The new wavefunction, evolved by (2.1), although required to be a solution of the same eigenvalue problem, is not necessarily the same function. However, the requirement of unitarity will remove the possibility that the evolved wavefunction becomes the identically zero solution.

Over-tildes will now be used to denote time updates, i.e., $q = q_{n-1}$, $q := q_n$, $\tilde{q} := q_{n+1}$, etc. It is required that

$$M_{\tilde{q}} \tilde{\psi}(\tilde{q}) = E \tilde{\psi}(\tilde{q}). \quad (2.6)$$

However, by definition

$$\begin{aligned} E \tilde{\psi}(\tilde{q}) &= N \int_C \exp \left[\frac{i}{\hbar} \mathcal{L}(\tilde{q}, q) \right] E \psi(q) dq = N \int_C \exp \left[\frac{i}{\hbar} \mathcal{L}(\tilde{q}, q) \right] \{M_q \psi(q)\} dq \\ &= N \int_C \left\{ \overline{M_q} \exp \left[\frac{i}{\hbar} \mathcal{L}(\tilde{q}, q) \right] \right\} \psi(q) dq + S, \end{aligned} \quad (2.7)$$

where S is the surface term

$$S = \left[p_0(q) \exp \left[\frac{i}{\hbar} \mathcal{L}(\tilde{q}, q) \right] \left(\frac{i}{\hbar} \tilde{q} \psi(q) + \frac{\partial \psi(q)}{\partial q} \right) \right]_C, \quad (2.8)$$

and $\overline{M_q}$ is the adjoint of M_q . For (2.7) to hold it is required that the integral in equation (2.1) exists, and, furthermore, the integral converges uniformly with respect to \tilde{q} in an appropriate region and the integrand of the integral relation is an analytic function of \tilde{q} in this region when q is on the line of integration. It will be assumed that these analytic requirements hold. The surface term vanishing, i.e., $S = 0$, seems to be generally in accord with physical requirements (for instance, if $C = \mathbb{R}$, then $S = 0$ is achieved by requiring that $\psi(q)$ and $\frac{\partial \psi(q)}{\partial q}$ tend to zero as $|q| \rightarrow \infty$). If the surface term vanishes then it is required that

$$\overline{M_q} \left(\exp \left[\frac{i}{\hbar} \mathcal{L}(\tilde{q}, q) \right] \right) = M_{\tilde{q}} \left(\exp \left[\frac{i}{\hbar} \mathcal{L}(\tilde{q}, q) \right] \right). \quad (2.9)$$

This PDE is a functional equation for both M_q and $\mathcal{L}(\tilde{q}, q)$. It can be solved as follows.

Substituting the form of the Lagrangian (2.3) into (2.9) and comparing coefficients of different powers of q reveals that $p_0(\tilde{q})$, $p_1(\tilde{q})$ and $p_2(\tilde{q})$ are quadratic polynomials. Hence, set

$$\begin{aligned} -\frac{1}{\hbar^2} p_0(\tilde{q}) &= A_0 \tilde{q}^2 + B_0 \tilde{q} + C_0, & -\frac{i}{\hbar} p_1(\tilde{q}) &= A_1 \tilde{q}^2 + B_1 \tilde{q} + C_1, \\ p_2(\tilde{q}) &= A_2 \tilde{q}^2 + B_2 \tilde{q} + C_2, \end{aligned}$$

and substitute this back into (2.9) to see how many of the coefficients are actually independent.

A comparison of the \tilde{q}^2 terms of (2.9) shows that

$$A_0 q^2 + A_1 q + A_2 = A_0 q^2 + B_0 q + C_0. \quad (2.10)$$

Comparing coefficients of different powers of q reveals $A_1 = B_0$ and $A_2 = C_0$.

A comparison of the \tilde{q} terms of (2.9) shows that

$$W'(q) = \frac{Dq^2 + Eq + F}{A_0 q^2 + B_0 q + C_0}, \quad (2.11)$$

where we have introduced

$$D := \frac{1}{2}(A_1 + B_0), \quad E := B_1 - i\hbar 2A_0, \quad F := \frac{1}{2}(B_2 + C_1) - i\hbar B_0. \quad (2.12)$$

A comparison of the \tilde{q}^0 terms of (2.9) is then made: the q^0 terms reveal that for (2.9) to hold, either $B_2 = C_1$ or $F = 0$. As $F = 0$ limits the form of the potential term, $B_2 = C_1$ is chosen. The q^1 terms reveal that for (2.9) to hold $D = A_1$. However, $A_1 = B_0$ and therefore $D = B_0$. The q^2 terms are trivial.

Taking the above findings together gives the form of M_q . For aesthetic reasons we make the replacements $\alpha := A_0$, $\beta := B_0$, $\gamma := C_0$, $\epsilon := E$, $\zeta := F$, and set $C_2 = i\hbar\epsilon/2$, so that M_q is formally Hermitian, to obtain

$$M_q = -\hbar^2(\alpha q^2 + \beta q + \gamma) \frac{\partial^2}{\partial q^2} + i\hbar(\beta q^2 + (\epsilon + 2i\hbar\alpha)q + i\hbar\beta + \zeta) \frac{\partial}{\partial q} + \gamma q^2 + (i\hbar\beta + \zeta)q + \frac{i\hbar\epsilon}{2}. \quad (2.13)$$

The potential term follows from the expression for $W(q)$, and we have

$$W'(q) = \frac{\beta q^2 + \epsilon q + \zeta}{\alpha q^2 + \beta q + \gamma}, \quad \text{where} \quad \alpha, \beta, \gamma, \epsilon, \zeta \in \mathbb{R}. \quad (2.14)$$

The quantum evolution given by equations (2.1), (2.3) and (2.14) (which is defined up to an unimportant constant of unit magnitude) sends the eigenfunctions of (2.4), where M_q is given by (2.13), to the eigenfunctions of the same eigenvalue problem (2.6) with the same eigenvalue, if the analytic requirements given between equations (2.7) and (2.9) hold. If the singularities of the rational function $W'(q)$, (2.14) (which are the singularities of the ODE given by (2.13)), occur on the real line, then there are also issues to be addressed in the integration of $W'(q)$ to obtain $W(q)$. (These are issues associated with the subset of \mathbb{R} on which the model is defined, which may have singularities of $W'(q)$ as boundaries. There are numerous possibilities here, which must be dealt with on a case by case basis.)

With the parameters in generic position, the finite singularities of the ODE given by (2.13) are regular. According to the classification scheme of [15] they have s-rank= 1, while the singularity at infinity is irregular with s-rank= 2. Therefore the ODE given by (2.13) has s-rank multisymbol {1, 1, 2}; hence it is of confluent Heun class. As a consequence, the analytical work required to show that the quantum evolution sends an eigenfunction to the same eigenfunction will be quite involved in general. One subcase has already appeared in the literature; namely the case where $\alpha = \beta = \zeta = 0$ and $C = \mathbb{R}$. This is the discrete-time harmonic oscillator [1]. In exact analogy with the continuous-time quantum harmonic oscillator, the eigenfunctions are of the form $H_k(aq) e^{-b^2 q^2}$, $a, b \in \mathbb{R}$, where H_k denotes the k th Hermite polynomial. All analytical requirements are met in this case, and the path integral evolves eigenfunctions to the same eigenfunctions. That is, these are quantum mechanical stationary states of the system whilst still within the time-slicing approximation.

The classical limit of the quantum system given by equations (2.1), (2.3) and (2.14) is an integrable map of the plane known as the McMillan map [12] (see also [7]). The classical limit of the invariant is obtained using $-i\hbar \frac{\partial}{\partial q} = p$. In this connection it should be noted that integrable quantum mappings, in terms of Heisenberg operators, possessing exact quantum operator invariants have been proposed before, e.g., in [13, 14].

3. Difference equation ansatz

We now consider the quantum mechanical evolution associated with forms of the potential, $V(q)$ (or, equivalently, $W(q)$), such that the wavefunction is a solution to an eigenvalue problem of a second-order O Δ E, both before and after its time evolution within the time-slicing approximation. Furthermore, the original and evolved wavefunctions are associated with the same eigenvalue. We write the arbitrary linear second-order O Δ E eigenvalue problem as

$$N_q \psi(q) = E \psi(q), \quad N_q = p_1(q) \exp \left[a \frac{\partial}{\partial q} \right] + p_0(q) + p_{-1}(q) \exp \left[-a \frac{\partial}{\partial q} \right]. \quad (3.1)$$

Define, for convenience, $w(q) := e^{-\frac{i}{\hbar}W(q)}$. It is required that

$$N_{\tilde{q}}\tilde{\psi}(\tilde{q}) = E\tilde{\psi}(\tilde{q}). \tag{3.2}$$

And, by definition

$$E\tilde{\psi}(\tilde{q}) = N \int_C \exp\left[\frac{i}{\hbar}\mathcal{L}(\tilde{q}, q)\right] E\psi(q) dq. \tag{3.3}$$

It will be assumed that the integral in (3.3) exists, and, furthermore, that it converges uniformly with respect to \tilde{q} for $\tilde{q} \in \mathbb{R}$. It is also assumed that the integrand is an analytic function of \tilde{q} for all $q \in \mathbb{R}$. In this section the usual physical assumptions $C = \mathbb{R}$ and $\psi(q) \in L^2(\mathbb{R})$ are made, so that

$$\begin{aligned} E\tilde{\psi}(\tilde{q}) &= N \int_{-\infty}^{\infty} \exp\left[-\frac{i}{\hbar}q\tilde{q}\right] w(q)\{p_1(q)\psi(q+a) + p_0(q)\psi(q) + p_{-1}(q)\psi(q-a)\} dq \\ &= N \int_{-\infty}^{\infty} \exp\left[-\frac{i}{\hbar}q\tilde{q}\right] \left\{ w(q-a)p_1(q-a) \exp\left[\frac{i}{\hbar}a\tilde{q}\right] + w(q)p_0(q) \right. \\ &\quad \left. + w(q+a)p_{-1}(q+a) \exp\left[-\frac{i}{\hbar}a\tilde{q}\right] \right\} \psi(q) dq. \end{aligned} \tag{3.4}$$

Hence, for (3.2) to hold, it is required that

$$\begin{aligned} w(q-a)p_1(q-a) \exp\left[\frac{i}{\hbar}a\tilde{q}\right] + w(q)p_0(q) + w(q+a)p_{-1}(q+a) \exp\left[-\frac{i}{\hbar}a\tilde{q}\right] \\ = w(q) \exp\left[-\frac{i}{\hbar}aq\right] p_1(\tilde{q}) + w(q)p_0(\tilde{q}) + w(q) \exp\left[\frac{i}{\hbar}aq\right] p_{-1}(\tilde{q}). \end{aligned} \tag{3.5}$$

This is a functional equation that is solved in a similar manner to the development of the previous section to obtain $p_1(q)$, $p_0(q)$, $p_{-1}(q)$ and $w(q)$ (in this case using the independence of different powers of $e^{\frac{i}{\hbar}aq}$, rather than q).

After some tedious but straightforward calculations the following first-order analytic OΔE for $W(q)$ is obtained:

$$W(q+a) - W(q) = i\hbar \ln \left(\frac{A_1 \exp\left[\frac{i}{\hbar}aq\right] + B_1 + C_1 \exp\left[-\frac{i}{\hbar}aq\right]}{A_{-1} \exp\left[\frac{i}{\hbar}aq + \frac{i}{\hbar}a^2\right] + A_0 + A_1 \exp\left[-\frac{i}{\hbar}aq - \frac{i}{\hbar}a^2\right]} \right). \tag{3.6}$$

The difference operator (3.1), of which the postulated quantum mechanical stationary states are eigenfunctions, is

$$\begin{aligned} N_q = \left\{ A_1 \exp\left[\frac{i}{\hbar}aq\right] + B_1 + C_1 \exp\left[-\frac{i}{\hbar}aq\right] \right\} \exp\left[a \frac{\partial}{\partial q} \right] + A_0 \exp\left[\frac{i}{\hbar}aq\right] + B_0 \\ + B_1 \exp\left[-\frac{i}{\hbar}aq\right] + \left\{ A_{-1} \exp\left[\frac{i}{\hbar}aq\right] + A_0 + A_1 \exp\left[-\frac{i}{\hbar}aq\right] \right\} \exp\left[-a \frac{\partial}{\partial q} \right]. \end{aligned} \tag{3.7}$$

The aim of this investigation is to find potentials of one degree-of-freedom Newtonian systems such that their quantum mechanical time evolution has stationary states even within the time-slicing approximation. Hence we wish to find explicitly real-valued expressions for $W(q)$ (and, consequently, $V(q)$). To this end, the following parameter replacements are made: $A_{-1} = \frac{1}{4} e^{-\frac{i}{\hbar}\frac{a^2}{2}} (\delta + \beta + 2i\alpha)$, $A_0 = \frac{1}{2} (\zeta + i\gamma)$, $A_1 = \frac{1}{4} e^{\frac{i}{\hbar}\frac{a^2}{2}} (\delta - \beta)$, $B_1 = \frac{1}{2} (\zeta - i\gamma)$, $C_1 = \frac{1}{4} e^{-\frac{i}{\hbar}\frac{a^2}{2}} (\delta + \beta - 2i\alpha)$; and substituting into (3.6) gives

$$W(q+a) - W(q) = 2\hbar \tan^{-1} \left(\frac{\beta \sin\left[\frac{a}{\hbar}\left(q + \frac{a}{2}\right)\right] + \alpha \cos\left[\frac{a}{\hbar}\left(q + \frac{a}{2}\right)\right] + \gamma}{\delta \cos\left[\frac{a}{\hbar}\left(q + \frac{a}{2}\right)\right] - \alpha \sin\left[\frac{a}{\hbar}\left(q + \frac{a}{2}\right)\right] + \zeta} \right). \tag{3.8}$$

The difference operator N_q is also easily rewritten in terms of the new parameters and trigonometric functions.

The first-order equation obtained by exponentiating (3.6) is easily solved, in a formal manner, by a product of four hyperbolic gamma functions [16, 17]. Ruijsenaars' hyperbolic gamma functions [16] are so-called minimal solutions that are essentially unique and have distinctive asymptotic properties ($w(q)$, of course, is only defined up to a factor with period a). Alternatively, in the difference case one may consider a scenario where the path integral is set up in terms of discrete summations, or Jackson q -integrals [10], and where the first-order O Δ E, (3.6) or (3.8), is solved by an iterative procedure. In a specific case there may be grounds for choosing a particular solution approach. This, however, falls outside of the remit of the current letter, which stops at giving the equation that the potential must obey (i.e., (3.6) or (3.8)).

The classical limit of this system is found after first making the reverse Schrödinger replacement $-i\hbar \frac{\partial}{\partial q} = p$ (and $p = -q$ in this gauge). However, in a naive classical limit N_q trivializes. On making the replacement $a = a_S \hbar$, where a_S is independent of \hbar , the system now has a rich classical limit, namely the (integrable) Suris map [18]. The passage to the classical limit is nontrivial; the equation that the potential must obey is qualitatively changed by the process: the first-order difference equations that define $W(q)$ (either (3.6) or, equivalently, (3.8)) become first-order differential equations. From an alternative perspective to that of this letter, it can be remarked that we have an 'integrable quantization' of the Suris map, where, to retain integrability, the potential term has nontrivial quantum, $O(\hbar)$, corrections. (In other settings, it has long been realized that to retain integrability after quantization the potential term may need quantum deformations, see [9].)

It is satisfying to note that in both the cases the functional equations ((2.9) and (3.5)) give, in a straightforward manner, the specific form of the second-order differential or difference operator, as well as the equation for the potential term, such that the discrete-time quantum evolution may possess stationary states.

References

- [1] Berry M V, Balazs N L, Tabor M and Voros A 1979 Quantum maps *Ann. Phys., NY* **122** 26–63
- [2] Dirac P A M 1933 The Lagrangian in quantum mechanics *Physik. Z. Sowjetunion* **3** 64–72
- [3] Dirac P A M 1945 On the analogy between classical and quantum mechanics *Rev. Mod. Phys.* **17** 195–9
- [4] Feynman R P 1948 Space-time approach to non-relativistic quantum mechanics *Rev. Mod. Phys.* **20** 367–87
- [5] Feynman R P 1965 The development of the space-time view of quantum electrodynamics *Nobel Prize Award Address*
- [6] Feynman R P and Hibbs A 1965 *Quantum Mechanics and Path Integrals* (New York: McGraw-Hill)
- [7] Grammaticos B, Nijhoff F and Ramani A 1999 *The Painlevé Property: One Century Later* ed R Conte (New York: Springer) pp 413–516
- [8] Grosche C and Steiner F 1998 *Handbook of Feynman Path Integrals* (Berlin: Springer)
- [9] Hietarinta J 1984 Classical versus quantum integrability *J. Math. Phys.* **25** 1833–40
- [10] Jackson F H 1910 On q -definite integrals *Q. J. Pure Appl. Math.* **41** 163
- [11] Kleinert H 2004 *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets* 3rd edn (Singapore: World Scientific)
- [12] McMillan E M 1971 A problem in the stability of periodic systems *Topics in Modern Physics. A Tribute to E.U. Condon* ed W E Brittin and H Odabasi (Boulder: Colorado Associated University Press) pp 219–44
- [13] Nijhoff F W, Capel H W and Papageorgiou V G 1992 Integrable quantum mappings *Phys. Rev. A* **46** 2155–8
- [14] Quispel G R W and Nijhoff F W 1992 Integrable two-dimensional quantum mappings *Phys. Lett. A* **161** 419–22
- [15] Ronveaux A 1995 *Heun's Differential Equations* (New York: Oxford University Press)
- [16] Ruijsenaars S N M 1997 First order analytic difference equations and integrable quantum systems *J. Math. Phys.* **38** 1069–146
- [17] Ruijsenaars S N M 2001 Special functions defined by analytic difference equations *Proc. NATO Advanced Study Institute on Special Functions 2000 (Tempe, AZ, USA) (NATO Science Series II vol 30)* (Berlin: Springer) pp 281–333
- [18] Suris Yu B 1989 Integrable mappings of the standard type *Funct. Anal. Appl.* **23** 74–6