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2007 J. Phys. A: Math. Theor. 40 11561

(http://iopscience.iop.org/1751-8121/40/38/008)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **40** (2007) 11561–11567 doi:10.1088/1751-8113/40/38/008

On the unitarity of higher derivative and nonlocal theories

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Received 24 April 2007, in final form 2 August 2007
Published 4 September 2007
Online at stacks.iop.org/JPhysA/40/11561

Abstract
We consider two simple models of higher derivative and nonlocal quantum systems. It is shown that, contrary to some claims found in literature, they can be made unitary.

PACS numbers: 03.65.−w, 04.60.Ds

Considerable attention has been paid recently to the problem of quantizing the theories which contain higher derivatives or are even nonlocal in time. This is mainly due to the fact that such theories arise naturally when one attempts to model the dynamics on noncommutative spacetime with the help of star product construction [1–3]. It has been shown that the field theories with spacetime noncommutativity lead to nonunitarity and acausality, at least when quantized with the help of naive Feynman rules [4–6]. There are several proposals of alternative quantization schemes which seem to cure the trouble with nonunitarity [7–10]. However, they give rise to other problems [11, 12] so the question of the existence of consistent quantum theory remains open. In view of that one is tempted to study simple models to gain more understanding of the problems we are faced with. However, even in the simplest cases there is some misunderstanding concerning the consistency of the relevant models. In order to clarify some issues we study two simple systems which are sometimes claimed to lead to nonunitary evolution.

Let us first consider the Lagrangian [13]

$$L = \tfrac{1}{2}(\ddot{q}^2 - \Omega^4 q^2). \qquad (1)$$

The corresponding classical equation of motion reads

$$q^{(IV)} - \Omega^4 q = 0. \qquad (2)$$

The general solution to equation (2) is a linear combination of $\exp(\pm \mathrm{i}\Omega t)$ and $\exp(\pm\Omega t)$. It is sometimes claimed [13] that due to the existence of exponentially rising solutions $\exp(\pm\Omega t)$ the quantum Hamiltonian of such type of systems is not Hermitean and the evolution operator $\exp\left(\frac{-\mathrm{i}tH}{\hbar}\right)$ is not unitary.

Let us consider this problem in some detail. In order to quantize the model we have to put it first into a Hamiltonian form. This can be done with the use of Ostrogradsky formalism [14–16]. One defines the canonical variables

$$
\begin{aligned}
&q_1 \equiv q, \qquad q_2 \equiv \dot{q} \\
&\Pi_1 \equiv \frac{\delta L}{\delta \dot{q}} = \frac{\partial L}{\partial \dot{q}} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \ddot{q}}\right) = -\dddot{q} \\
&\Pi_2 \equiv \frac{\delta L}{\delta \ddot{q}} = \frac{\partial L}{\partial \ddot{q}} = \ddot{q}
\end{aligned}
\tag{3}
$$

and the Hamiltonian

$$
H \equiv \Pi_1 \dot{q}_1 + \Pi_2 \dot{q}_2 - L = \Pi_1 q_2 + \frac{1}{2}\Pi_2^2 + \frac{\Omega^4}{2} q_1^2. \tag{4}
$$

It is straightforward to check that the canonical equations of motion imply the initial equation for q.

Our system, being linear, can be immediately quantized. The question we intend to solve is whether the resulting quantum system is unitary. The argument against unitarity based on the existence of exponentially growing solutions to classical equations of motion might go as follows. Let

$$
\hat{X} \equiv \hat{\Pi}_1 - \Omega\hat{\Pi}_2 - \Omega^3 \hat{q}_1 - \Omega^2 \hat{q}_2 \tag{5}
$$

then

$$
[\hat{X}, \hat{H}] = \mathrm{i}\hbar\Omega\hat{X} \tag{6}
$$

(which is equivalent to the existence of exponentially growing solutions to Heisenberg equations of motion). Assume now that $\hat{H}$ is self-adjoint and let $|E\rangle$ be the eigenvectors of $\hat{H}$ (possibly the generalized ones, corresponding to continuous spectrum). Then equation (6) implies

$$
(E - E' - \mathrm{i}\hbar\Omega)\langle E'|\hat{X}|E\rangle = 0. \tag{7}
$$

Equation (7) is fulfilled only provided

$$
\langle E'|\hat{X}|E\rangle = 0 \tag{8}
$$

for all E, E' which in turn means that the canonical variables are linearly dependent contradicting the canonical commutation rules.

The only weak point in the above reasoning is the assumption on the existence (even in distributional sense) of the matrix elements $\langle E'|\hat{X}|E\rangle$. In fact, we shall show below that the theory is unitary while $\langle E'|\hat{X}|E\rangle$ are not well defined.

To this end we make a simple canonical (hence unitary) transformation

$$
\begin{aligned}
&\hat{q}_1 = \frac{1}{\sqrt{2}\Omega}(\hat{X}_1 + \hat{X}_2), \qquad \hat{q}_2 = \frac{1}{\sqrt{2}\Omega}(\hat{P}_1 - \hat{P}_2) \\
&\Pi_1 = \frac{\Omega}{\sqrt{2}}(\hat{P}_1 + \hat{P}_2), \qquad \hat{\Pi}_2 = \frac{\Omega}{\sqrt{2}}(-\hat{X}_1 + \hat{X}_2).
\end{aligned}
\tag{9}
$$

Then the Hamiltonian takes the following form:

$$
\hat{H} = \left(\frac{1}{2}\hat{P}_1^2 + \frac{\Omega}{2}\hat{X}_1^2\right) - \left(\frac{1}{2}\hat{P}_2^2 - \frac{\Omega}{2}\hat{X}_2^2\right). \tag{10}
$$

Here $\hat{H}$ is the difference of the harmonic oscillator and the inverted harmonic oscillator. Both terms depend on different variables so if they are self-adjoint and generate unitary dynamics so is $\hat{H}$. Only the second piece calls for some explanation. It is unbounded from below but only quadratically. Therefore, it defines a self-adjoint operator with purely continuous spectrum covering the whole real axis [17].

In order to find the coordinate representation for eigenvectors of $\hat{H}$ we have only to find the corresponding wavefunctions for the inverted harmonic oscillator. This is quite straightforward [18] and results in the following final formula for eigenfunctions of $\hat{H}$:

$$\langle X_1, X_2|n, \varepsilon; \pm\rangle = \left(\frac{1}{\sqrt{\sqrt{\pi}2^n n!}}\sqrt[4]{\frac{\Omega}{\hbar}}H_n\left(\sqrt{\frac{\Omega}{\hbar}}X_1\right)\mathrm{e}^{-\frac{\Omega X_1^2}{2\hbar}}\right)$$
$$\times\left(\sqrt[4]{\frac{2\Omega}{\hbar}}\frac{\mathrm{e}^{\frac{\varepsilon\pi}{4\hbar\Omega}}}{\sqrt{4\pi\, ch\left(\frac{\pi\varepsilon}{\hbar\Omega}\right)}}D_{-\frac{\mathrm{i}\varepsilon}{\hbar\Omega}-\frac{1}{2}}\left(\pm\sqrt{\frac{2\Omega}{\hbar}}\left(\frac{1+\mathrm{i}}{\sqrt{2}}\right)X_2\right)\right). \tag{11}$$

Here H_n are Hermite polynomials, while D_ν being the parabolic cylinder functions. The energies of the above states are given by

$$E \equiv E(n, \varepsilon) = \hbar\Omega\left(n + \frac{1}{2}\right) - \varepsilon. \tag{12}$$

Consider now the matrix elements $\langle E'|\hat{X}|E\rangle$. By virtue of equations (5) and (9) we find

$$\hat{X} = \sqrt{2}\Omega(\hat{P}_2 - \Omega\hat{X}_2). \tag{13}$$

Now, using (11), (13) and the asymptotic form of parabolic cylinder functions [18] we find that the matrix elements $\langle n', \varepsilon', \lambda'|\hat{X}|n, \varepsilon, \lambda\rangle$, $\lambda, \lambda' = \pm 1$, are expressed, apart from regular contributions, in terms of badly divergent integrals of the form

$$\int^{\infty}\mathrm{d}x\exp\left(\frac{\mathrm{i}(\varepsilon' - \varepsilon)}{\hbar\Omega}\ln x\right) \sim \int^{\infty}\mathrm{d}y\exp\left(y\left(1 + \mathrm{i}\frac{(\varepsilon - \varepsilon')}{\hbar\Omega}\right)\right). \tag{14}$$

Therefore, the matrix elements under consideration are not well defined even in the distributional sense.

Let us add some general remarks concerning our model. It provides a particular example of the so-called Pais–Uhlenbeck quartic oscillator [19]. For the general Pais–Uhlenbeck oscillator the differential operator entering the Euler–Lagrange equation is a fourth-order linear one containing only even powers of time derivative. It can be factorized into the product of two second-order operators; the corresponding frequencies squared may be either real or complex conjugated (in particular, they may coincide). The general solution to the dynamical equation is a sum of two terms each describing a second-order system. Therefore, the Ostrogradski Hamiltonian is a linear combination of two commuting pieces. In particular, for real positive frequencies squared the Hamiltonian is a difference of two harmonic oscillators [19, 20] (the difference is due to the fact that Ostrogradski Hamiltonian is always unbounded from below). For other values of frequencies the commuting pieces represent inverted oscillators, two-dimensional angular momentum and dilatation operators or kinetic energy of free particle on the plane [19] (see also equation (26) below). One should also note that due to the existence of two globally defined independent integrals of motion there exists a large variety of canonically/unitary inequivalent Hamiltonian formulations [21]. Whatever Hamiltonian formalism one starts with, the resulting quantum theory is unitary. This is due to the fact that the Hamiltonian is always a linear combination of two commuting pieces, each of them generating unitary evolution (the latter can be shown by referring to relevant mathematics [17]). Considering any such piece from the point of view of Heisenberg matrix mechanics one notes that its eigenvalues are complex (i.e. the evolution is not unitary) if, on the classical level, the relevant dynamics contains exponentially growing terms. This conclusion is, however, wrong because the relevant matrix elements simply do not exist. On the other hand, the matrix elements are well defined and Heisenberg method leads to real energies if the classical solutions are oscillatory functions multiplied by at most polynomial functions of time.

As a second model we consider the nonlocal harmonic oscillator [22, 23]

$$L = \frac{1}{2}\dot{q}(t)^2 - \frac{\omega^2}{2} q\left(t - \frac{T}{2}\right) q\left(t + \frac{T}{2}\right). \tag{15}$$

The Euler–Lagrange equation

$$\int \mathrm{d}t' \frac{\delta L(t')}{\delta q(t)} = 0 \tag{16}$$

reads

$$\ddot{q}(t) + \frac{\omega^2}{2}\,(q(t-T) + q(t+T)) = 0. \tag{17}$$

This theory can be quantized using the method of Pais and Uhlenbeck [19]. To this end we rewrite the Lagrangian in an equivalent form

$$L = -\frac{1}{2} q(t)\ddot{q}(t) - \frac{\omega^2}{4}((q(t)q(t-T) + q(t)q(t+T)) \tag{18}$$

or

$$L = -\frac{1}{2} q(t) \left(\left(\frac{\mathrm{d}}{\mathrm{d}t} \right)^2 + \omega^2 ch\left(T \frac{\mathrm{d}}{\mathrm{d}t} \right) \right) q(t). \tag{19}$$

According to the prescription given in [19] we consider the entire function

$$\Phi(u) \equiv z^2 + \omega^2 ch(Tz), \qquad u = z^2. \tag{20}$$

It is not difficult to verify that (i) $\Phi(u)$ has no multiple zeros except a discrete set of values of ωT; in the latter case the double zeros are real and negative, (ii) there is a finite nonempty set of real negative zeros, $z^2 = -\Omega_i^2, i = 1, \ldots, m, m \geqslant 1$, (iii) there is an infinite number of complex pairwise conjugated zeros, $z^2 = -\omega_k^2, z^2 = -\overline{\omega}_k^2, k = 1, 2, \ldots$ and $\sum_{k=1}^{\infty} \omega_k^{-2}$ is absolutely convergent.

By virtue of the above properties one can write

$$\frac{\omega^4}{\Phi(z^2)} = \sum_{i=1}^{m} \frac{\eta_i \Omega_i^2}{1 + \frac{z^2}{\Omega_i^2}} + \sum_{k=1}^{\infty} \left(\frac{\eta_k \omega_k^2}{1 + \frac{z^2}{\omega_k^2}} + \frac{\overline{\eta}_k \overline{\omega}_k^2}{1 + \frac{z^2}{\overline{\omega}_k^2}} \right). \tag{21}$$

Following [19], we define new variables

$$\begin{aligned}
\tilde{Q}_i &\equiv \prod_{\substack{j=1 \\ j \neq i}}^{m} \left(1 + \frac{1}{\Omega_j^2}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\right) \prod_{k=1}^{\infty} \left(1 + \frac{1}{\omega_k^2}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\right)\left(1 + \frac{1}{\overline{\omega}_k^2}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\right) q \\
Q_k &\equiv \prod_{i=1}^{m} \left(1 + \frac{1}{\Omega_i^2}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\right) \prod_{\substack{l=1 \\ l \neq k}}^{\infty} \left(1 + \frac{1}{\omega_l^2}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\right) \prod_{l=1}^{\infty} \left(1 + \frac{1}{\overline{\omega}_l^2}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\right) q \\
\overline{Q}_k &\equiv \prod_{i=1}^{m} \left(1 + \frac{1}{\Omega_i^2}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\right) \prod_{l=1}^{\infty} \left(1 + \frac{1}{\omega_l^2}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\right) \prod_{\substack{l=1 \\ l \neq k}}^{\infty} \left(1 + \frac{1}{\overline{\omega}_l^2}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\right) q.
\end{aligned} \tag{22}$$

With the above definitions the Lagrangian takes the form

$$L = -\frac{1}{2}\sum_{i=1}^{m}\eta_i\tilde{Q}_i\left(\frac{d^2}{dt^2}+\Omega_i^2\right)\tilde{Q}_i - \frac{1}{2}\sum_{k=1}^{\infty}\left(\eta_k Q_k\left(\frac{d^2}{dt^2}+\omega_k^2\right)Q_k+\overline{\eta}_k\overline{Q}_k\left(\frac{d^2}{dt^2}+\overline{\omega}_k^2\right)\overline{Q}_k\right). \tag{23}$$

By rescaling $\tilde{Q}_i \to \frac{\tilde{Q}_i}{\sqrt{|\eta_i|}}$, $Q_k \to \frac{Q_k}{\sqrt{\eta_k}}$, $\overline{Q}_k \to \frac{\overline{Q}_k}{\sqrt{\overline{\eta}_k}}$, and passing to the Hamiltonian formalism we find

$$H = \frac{1}{2}\sum_{i=1}^{m}(\mathrm{sgn}\,\eta_i)\left(\tilde{P}_i^2+\Omega_i^2\tilde{Q}_i^2\right)+\frac{1}{2}\sum_{k=1}^{\infty}\left(\left(P_k^2+\omega_k^2Q_k^2\right)+\left(\overline{P}_k^2+\overline{\omega}_k^2\overline{Q}_k^2\right)\right). \tag{24}$$

This is, however, not the end of the story because the variables Q_k, P_k are complex. In order to find the relevant real variables we perform the following complex canonical transformation [19]:

$$\begin{aligned} P_k &= \frac{1}{2}\sqrt{\omega_k}((p_{1k}+\mathrm{i}q_{1k})+\mathrm{i}(p_{2k}-\mathrm{i}q_{2k})) \\ \overline{P}_k &= \frac{1}{2}\sqrt{\overline{\omega}_k}((p_{1k}-\mathrm{i}q_{1k})-\mathrm{i}(p_{2k}+\mathrm{i}q_{2k})) \\ Q_k &= \frac{\mathrm{i}}{2\sqrt{\omega_k}}((p_{1k}-\mathrm{i}q_{1k})+\mathrm{i}(p_{2k}+\mathrm{i}q_{2k})) \\ \overline{Q}_k &= \frac{-\mathrm{i}}{2\sqrt{\overline{\omega}_k}}((p_{1k}+\mathrm{i}q_{1k})-\mathrm{i}(p_{2k}-\mathrm{i}q_{2k})) \end{aligned} \tag{25}$$

which allows us to rewrite equation (24) as

$$H = \frac{1}{2}\sum_{i=1}^{m}(\mathrm{sgn}\,\eta_i)\left(\tilde{P}_i^2+\Omega_i^2\tilde{Q}_i^2\right)-\sum_{k=1}^{\infty}(\mathrm{Im}\,\omega_k(q_{1k}p_{1k}+q_{2k}p_{2k}) + \mathrm{Re}\,\omega_k(q_{1k}p_{2k}-q_{2k}p_{1k})). \tag{26}$$

So H is a sum (with an alternating sign) of a finite number of harmonic oscillators and an infinite number of terms which are linear combinations of dilatation and angular momentum in two dimensions. All terms depend on different variables and can be easily quantized; only dilatation calls for ordering rule—we adopt the simplest one: $q_1p_1+q_2p_2 \to \frac{1}{2}(\hat{q}_1\hat{p}_1+\hat{p}_1\hat{q}_1+\hat{q}_2\hat{p}_2+\hat{p}_2\hat{q}_2)$.

Let us consider one term of the second sum on the RHS of equation (26). It is of the form

$$\hat{h} = \frac{\mu}{2}(\hat{q}_1\hat{p}_1+\hat{p}_1\hat{q}_1+\hat{q}_2\hat{p}_2+\hat{p}_2\hat{q}_2)+\nu(\hat{q}_1\hat{p}_2-\hat{q}_2\hat{p}_1). \tag{27}$$

Dilatations commute with angular momentum so the spectrum of $\hat{h}$ reads

$$\varepsilon_{n,\lambda} = \mu\lambda+\nu n, \qquad n = 0, \pm 1, \ldots, -\infty < \lambda < \infty \tag{28}$$

and the corresponding wavefunctions (for example, in coordinate representation) can be easily found [19].

Now, let us consider the classical equations of motion implied by h. They read

$$\dot{q}_i = \mu q_i - \nu\varepsilon_{ik}q_k, \qquad \dot{p}_i = -\mu p_i + \nu\varepsilon_{ik}p_k. \tag{29}$$

The solutions are linear combinations of $\exp((\mu\pm\mathrm{i}\nu)t)$ (for $q's$) or $\exp((-\mu\pm\mathrm{i}\nu)t)$ (for $p's$). Therefore, we are dealing with exponentially growing solutions. Following the same line of reasoning as in the first example one could conclude that the energy must take complex values. Again this conclusion results from the assumption that the matrix elements of canonical variables in the energy representation are well defined, while it is straightforward to check that they are badly divergent (cf [19][equation (34)]).

Let us now make few remarks about path integral approach. Some care must be exercised when dealing with the Hamiltonians unbounded from below. Let us take as an example the inverted harmonic oscillator with the 'frequency' ω. As we have mentioned above the Hamiltonian is here a well-defined self-adjoint operator with purely continuous spectrum extending over the whole real line.

The propagator function

$$K(x, y; t) = \sum_{\lambda=\pm 1} \int_{-\infty}^{\infty} d\left(\frac{E}{\hbar\omega}\right) \mathrm{e}^{\frac{-\mathrm{i}Et}{\hbar}} \Psi_{E\lambda}(x)\overline{\Psi}_{E\lambda}(y) \tag{30}$$

cannot be continued to imaginary time whatever the sign of t is. On the level of path integration the Euclidean path integral is not well defined due to the fact that the integrand ceases to be of the form of the exponent of negative definite functional.

However, we can do the path integral directly (without referring to imaginary time approach) by applying Trotter formula and doing Fresnel integrals. The result, when extended to whole time axis, reads

$$K(x, y; t) = \frac{(1 - \mathrm{i}\,\mathrm{sgn}\, t)}{2\sqrt{\pi\hbar|t|}} \sqrt{\frac{\omega t}{sh\omega t}} \exp\left(\frac{\mathrm{i}\omega}{2\hbar sh\omega t}((x^2 + y^2)ch\omega t - 2xy)\right). \tag{31}$$

This result can be checked as follows. By virtue of equation (30) one gets

$$\int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\frac{\mathrm{i}\tilde{E}t}{\hbar}} K(0, 0; t) = \frac{2\pi}{\omega} \sum_{\lambda=\pm 1} |\Psi_{\tilde{E}\lambda}(0)|^2. \tag{32}$$

Using equation (31) and the explicit form of $\Psi_{\tilde{E}\lambda}$ (cf equation (11)) we find that (32) holds true.

Consider now $K(0, 0; t)$ for $t > 0$:

$$K(0, 0; t) = \frac{(1 - \mathrm{i})}{2} \sqrt{\frac{\omega}{\pi\hbar sh\omega t}}. \tag{33}$$

Let us forget for a moment that the imaginary time representation is ill defined. In order to extract the information about the spectrum of our Hamiltonian we continue (33) to imaginary time and consider the $t \to \infty$ behaviour. We find that $K(0, 0; t)$ becomes periodic in Euclidean regime which means that the energies are imaginary!

For our first example the propagator is simply the product of two propagators, one for harmonic oscillator and one for inverted harmonic oscillator. Therefore, we see that the improper application of the path integral method will result in wrong conclusions concerning the energy spectrum and unitarity.

The same applies to the nonlocal harmonic oscillator. We found that the Hamiltonian is a sum of commuting pieces, many of them having the spectrum unbounded from below. Again, it appears that an attempt to derive the energy eigenvalues from Euclidean version of path integral leads to complex energies, i.e. to the conclusion that the theory is not unitary.

Acknowledgment

PK thanks Barry Simon for kind and enlightening correspondence and bringing [17] to our attention. Supported by the grants 1 P03B 125 29 and 1 P03B 021 28 of the Polish Ministry of Science.

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