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1992 J. Phys. A: Math. Gen. 25 L1111

(http://iopscience.iop.org/0305-4470/25/18/004)

J. Phys. A: Math. Gen. 25 (1992) L1111–L1118. Printed in the UK

LETTER TO THE EDITOR

On a classical constrained system and its quantum mechanical counterpart

H Huber and H Büttner

Physikalisches Institut, Universität Bayreuth, W-8580 Bayreuth, Federal Republic of Germany

Received 30 March 1992, in final form 13 July 1992

Abstract. In this letter we discuss a non-integrable system of three coupled anharmonic oscillators with certain constraints, so that it is transformed into an integrable one. After having quantized the system with constraints and the classically equivalent unconstrained integrable system using the BFV algorithm and the EBK quantization method, respectively, the equivalence of the two quantization procedures is shown by explicitly performing the reduction to the physical subspace on the quantum level.

The interest in constrained systems is due to the fact that they can be related to systems with a local gauge invariance since both are described by singular Lagrangians. The freedom to choose a gauge is intimately related to the existence of unphysical degrees of freedom making the quantization of such systems extremely difficult. This results from the fact that by fixing the gauge in order to get rid of the unphysical modes one may destroy the relativistic covariance of the theory (see e.g. [1]).

In order to introduce the topic and to fix the notation we give a brief sketch of the most important contributions to the quantization of systems with constraints. According to Dirac we call a constraint T_α first class, if its Poisson brackets (denoted in the following as $\{\,,\}$) with all the other constraints vanish at least weakly, that is

$$\{T_\alpha, T_\beta\} = C^\gamma_{\alpha\beta} T_\gamma \qquad \text{for all } \beta \text{ and } \gamma \tag{1}$$

where the $C^\gamma_{\alpha\beta}$ are called the structure coefficients, which may depend on the phase space variables. Constraints for which (1) does not hold are called second class.

The efforts to quantize systems with constraints, started with the work of Dirac in 1950 [2,3]. In Dirac's canonical quantization method the Poisson brackets of classical mechanics are replaced by quantum commutators (denoted in the following as $[\,,]$). Subsequently the quantum analogues $\hat{T}_\alpha$ of the classical first-class constraints T_α are imposed as quantum operators on the physical states:

$$\{A, B\} \to \mathrm{i}[\hat{A}, \hat{B}] \qquad \hat{T}_\alpha \mid \mathrm{phys}\rangle = 0\,. \tag{2}$$

One of the difficulties arising in this quantization procedure is that the first-class character of the constraints is not necessarily preserved on the quantum level, i.e.

$$\{T_\alpha, T_\beta\} = C^\gamma_{\alpha\beta} T_\gamma \not\Rightarrow [\hat{T}_\alpha, \hat{T}_\beta] = \hat{C}^\gamma_{\alpha\beta} \hat{T}_\gamma \tag{3}$$

0305-4470/92/181111+08$04.50

due to the fact that the structure coefficients $C^{\gamma}_{\alpha\beta}$ become operator-valued. Obviously the problem turns out to be even more severe, if second class constraints are considered. One way to circumvent this lies in using Dirac brackets instead of Poisson brackets, since by definition the Dirac brackets of all constraints with one another vanish strongly. But among other reasons operator-ordering problems prevent the general applicability of the method (cf [4]).

Another approach proposed by Faddeev [5] consists in extracting first the true, gauge-invariant degrees of freedom of the theory with the help of additional gauge constraints Ω_α, called subsidary conditions. In a second step one performs a path-integral quantization, where δ-functions of both the original and the gauge constraints occuring in the measure determine the restriction to the physical paths. This formalism was generalized by Senjanovič [6] to systems including second-class constraints. The main disadvantage of this quantization procedure is the appearance of the constraints in the measure of the path integral destroying the relativistic covariance of the theory.

In order to overcome the problems in quantizing systems with constraints Batalin, Fradkin and Vilkovisky (BFV) developed an operator quantization method, which neither depends on operator ordering nor fails in yielding a non-unitary or relativistic non-covariant S-matrix [7–10]. An excellent review of the BFV approach is given by Henneaux [11]. The main property of the method is that on the one hand the phase space is enlarged to permit relativistic covariance by treating the Lagrange parameters as dynamical variables, and on the other hand the number of physical degrees of freedom is reduced through the introduction of ghost variables obeying the opposite quantum statistic as the original variables and thus, loosley speaking, counting as negative degrees of freedom [4, 11].

BFV quantization provides a powerful tool to quantize a system with constraints preserving its constrained nature on the quantum level. In order to test this method and to get a somewhat deeper understanding we demonstrate in a first step for a simple model how the restriction of the Hilbert space in the BFV algorithm works and how it is related to the classical case. The essential property of our system will be that classically the imposion of a constraint causes it to turn from a non-integrable system to an integrable one thus becoming exactly solvable. We can therefore quantize the system directly and compare the two ways of quantization. The system considered consists of three coupled one-dimensional quartic oscillators with a constraint $\overline{T}$ and the Lagrangian

$$\overline{L} = \tfrac{1}{2}(\dot{q}_1{}^2 + \dot{q}_2{}^2 + \dot{q}_3{}^2) - \overline{V}(q) - \mu\overline{T}(q) \tag{4}$$

with

$$\overline{V}(q) = q_1^4 + c_2 q_2^4 + c_3 q_3^4 + c_4 q_1^2 q_2^2 + (24 - c_4) q_1^2 q_3^2 + [64 - (c_2 + c_3)] q_2^2 q_3^2$$

and

$$\overline{T}(q) = q_2 - q_3 \,.$$

In order to arrive at a Hamiltonian formulation of the problem, we forget about the constraint and interpret the Lagrange parameter μ as a dynamical variable with canonical conjugated momentum p_μ. A Legendre transformation in the eight-dimensional phase space formally yields

$$\overline{H} = \tfrac{1}{2}(p_1^2 + p_2^2 + p_3^2) + \dot{\mu} p_\mu + \overline{V}(q) + \mu\overline{T}(q)$$

and

$$T_{\rm p} \equiv p_\mu = \frac{\partial \overline{L}}{\partial \dot{\mu}} \stackrel{!}{=} 0$$

where $T_{\rm p}$ is now a primary constraint arising through the absence of a kinetic term belonging to the dynamical variable μ in (4). Since the Poisson bracket of $T_{\rm p}$ with $\overline{H}$ does not vanish, the demand on $T_{\rm p}$ to be zero for all times leads to a secondary constraint. The so-called Dirac–Bergmann algorithm [3, 4, 12] describes how this secondary constraint (and eventually tertiary constraints, etc) are to be handled in order to arrive at a new Hamiltonian H_0 together with a complete set of constraints, that is each having vanishing Poisson brackets with H_0. In our case these are a first-class constraint ($T' = T_{\rm p}$) and two second-class constraints ($T''_\alpha, \alpha = 1, 2$):

$$H_0 = \tfrac{1}{2}(p_1^2 + p_2^2 + p_3^2) + \dot{\mu} p_\mu + V_0(q) \tag{5}$$

with

$$\begin{aligned} V_0(q) = {} & q_1^4 + (2c_3 - c_2)q_2^4 + c_3 q_3^4 + (24 - c_4)q_1^2(q_2^2 + q_3^2) + [64 - (c_2 + c_3)]q_2^2 q_3^2 \\ & - 2[(12 - c_4)q_1^2 + (c_3 - c_2)q_2^2]q_2 q_3 \end{aligned}$$

$$T' = p_\mu \qquad T''_1 = q_2 - q_3 \qquad T''_2 = p_2 - p_3$$

$$\{T', H_0\} = 0 = \{T', T''_\alpha\} \qquad \{T''_\alpha, H_0\} = 0$$

but

$$\{T''_\alpha, T''_\beta\} = 2\delta_{\alpha\beta} \qquad \alpha, \beta = 1, 2 .$$

In our simple example the reduction of the phase space can be done explicitly by carrying out the canonical transformation $(q_i, \mu, p_i, p_\mu) \rightarrow (Q_i, Q_\mu, P_i, P_\mu)$, $i = 1, \ldots, 3$, generated by

$$S = q_1 P_1 + \mu P_\mu + \frac{1}{\sqrt{2}}(P_2 + P_3)q_2 + \frac{1}{\sqrt{2}}(P_2 - P_3)q_3$$

which yields

$$\begin{aligned} H_0 = {} & \tfrac{1}{2}(P_1^2 + P_2^2 + P_3^2) + \dot{Q}_\mu P_\mu + Q_1^4 + 16Q_2^4 + [16 - (c_2 - c_3)]Q_3^4 + 12Q_1^2 Q_2^2 \\ & + 2(18 - c_4)Q_1^2 Q_3^2 + (5c_3 - c_2 - 32)Q_2^2 Q_3^2 + 2(c_3 - c_2)Q_2 Q_3^3 \end{aligned} \tag{6}$$

$$T' = P_\mu \qquad T''_1 = Q_3 \qquad T''_2 = P_3 .$$

On the physical subspace the constraints are valid for all times and therefore the system is described by

$$H^\star = \tfrac{1}{2}(P_1^2 + P_2^2) + Q_1^4 + 12Q_1^2 Q_2^2 + 16Q_2^4 \tag{7}$$

which is integrable [13] due to the existence of a second integral of the motion

$$F = -Q_2 P_1^2 + Q_1 P_1 P_2 + Q_1^2 Q_2 (8Q_2^2 + 4Q_1^2) . \tag{8}$$

So far the classical system is considered and our calculation shows that the system H_0 in eight-dimensional phase space together with the constraints T', T_1'' and T_2'' is equivalent to the unconstrained system $H^\star$ in four-dimensional phase space, reflecting the fact that each first-class constraint reduces the dimension of the phase space by two and each second-class constraint reduces it by one.

Before we determine the quantum version of the constrained system H_0 we want to calculate the quantum mechanical energy eigenvalues of the unconstrained system $H^\star$. This can be done using the Einstein–Brillouin–Keller (EBK) quantization rule [15–17]

$$I_k = \hbar\left(n_k + \frac{\alpha_k}{4}\right) \qquad k = 1, \ldots, N \tag{9}$$

for an N-dimensional integrable, but not necessarily separable system. The n_k are integers and the α_k are the Maslov indices belonging to the kth irreducible closed path by means of which the kth action variable I_k is defined:

$$I_k = \frac{1}{2\pi}\oint_{\gamma_k} p(q, F)\,\mathrm{d}q \qquad k = 1, \ldots, N\,. \tag{10}$$

Here F is an N-dimensional vector containing the N constants of motion and γ_k stands for the kth irreducible closed path on the N-torus [18]. For the two-dimensional system $H^\star$ the Maslov indices α_1 and α_2 are equal to 2 [19] and the discrete energy values are given by

$$E_{n_1 n_2} = H^\star(I_1, I_2) = H^\star\left[\hbar(n_1 + \tfrac{1}{2}), \hbar(n_2 + \tfrac{1}{2})\right]. \tag{11}$$

Figure 1 shows the energy eigenvalues of the system $H^\star$ up to $E = 100$. There are no lower eigenvalues for higher quantum numbers n_1, n_2 since it can be shown that $\partial E(n_k, n_l)/\partial n_k > 0$ for $k \neq l,\ k, l = 1, 2$.

With this result in mind we now turn to the original problem, i.e. the quantization of the constraint system (5). As mentioned at the beginning, BFV quantization of constrained systems requires the introduction of some extra degrees of freedom including ghosts. In particular [8] for each of the constraints there is one (bosonic) Lagrange multiplier λ with conjugate momentum π, one (fermionic) cononical conjugated ghost pair $(\mathcal{C}, \bar{\mathcal{P}})$ and one (fermionic) anti-ghost pair $(\mathcal{P}, \bar{\mathcal{C}})$. Furthermore, since the construction of the gauge algebra of a constraint system strongly depends on the first-class character of the constraints [8], for each of the second-class constraints being at hand one canonical conjugated pair of (bosonic) auxiliary variables $(\xi\,,\,\eta)$ is needed in order to convert the second-class constraints into effectively first-class ones [10]. Thus our enlarged phase space (Σ, Π) becomes 15-dimensional $(i = 1, 2, 3,\ \alpha = 1, 2)$:

$$\Sigma = (q_i, \mu, \lambda', \lambda''_\alpha, \xi''_\alpha, \mathcal{C}', \mathcal{P}', \mathcal{C}''_\alpha, \mathcal{P}''_\alpha)$$
$$\Pi = (p_i, p_\mu, \pi', \pi''_\alpha, \eta''_\alpha, \bar{\mathcal{P}}', \bar{\mathcal{C}}', \bar{\mathcal{P}}''_\alpha, \bar{\mathcal{C}}''_\alpha)\,.$$

From now on all commutators are to be understood as supercommutators in the sense of

$$[A, B] = AB - (-1)^{\epsilon_A \epsilon_B} BA \tag{12}$$

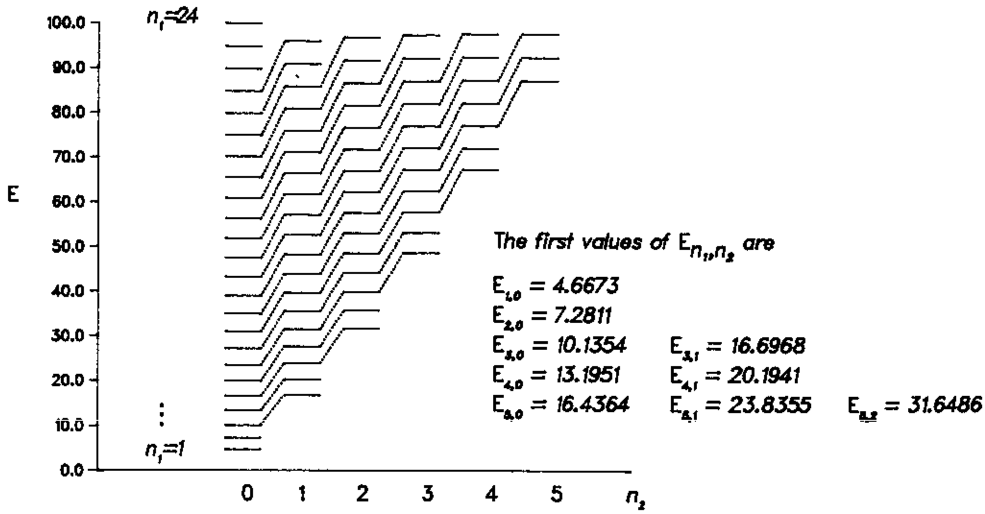

Figure 1. The numerically exact eigenvalues of the system $H^\star$ up to $E = 100$ ($\hbar = 1$). The quantum numbers n_k, $k = 1, 2$, correspond to the kth irreducible closed path on the 2-torus (see text). Eigenvalues belonging to the same n_1 are connected by dotted lines and ordered by increasing n_1 from the bottom to the top. The first values of E_{n_1,n_2} are:

$E_{1,0} = 4.6673$ $E_{2,0} = 7.2811$ $E_{3,0} = 10.1354$ $E_{4,0} = 13.1951$ $E_{5,0} = 16.4364$
$E_{3,1} = 16.6968$ $E_{4,1} = 20.1941$ $E_{5,1} = 23.8355$
$E_{5,2} = 31.6486$

where ϵ_A denotes the Grassmann parity of the operator A and takes the value 0 or 1, if A is a bosonic or fermionic operator respectively. A detailed discussion of the application of the BFV algorithm to our model will be given in a forthcoming publication. Here we merely want to stress the fact that in our case all generalized structure functions of rank higher than one can be chosen to vanish. The generalized structure functions appear in the BFV algorithm as coefficients in the expansion of the generators of the (generalized) constraint algebras into a $\bar{\mathcal{P}}\mathcal{C}$-normal-ordered series of powers of the ghost operators [8–10]. For systems with only first-class constraints it is stated in [11] that all structure functions of rank higher than one vanish, if the algebra of the constraints is a true algebra, i.e. when their structure coefficients (see (1)) are actually true constants. Up to now there is no such statement known to the authors in the presence of second-class constraints. But a similar rule also seems to be valid, if the generalized algebra of the second class constraints involves only true constants (for a further example see ref. [20]). The BFV algorithm ends up with the so-called unitarizing Hamiltonian H (that means that the corresponding S-matrix is unitary) together with a BFV–BRST charge Ω:

$$H = H_0(q_i, \mu, p_i, p_\mu) + \sum_{k=1}^{2} \Gamma''_{1k}(\xi_1 + \eta_2)^k + \sum_{k=1}^{4} \Gamma''_{2k}(\eta_1 - \xi_2)^k$$
$$+ \lambda' p_\mu + \chi'\pi' + \sum_{\alpha=1}^{2}(\lambda''_\alpha T_\alpha + \chi''_\alpha \pi''_\alpha) + \bar{\mathcal{P}}'\mathcal{P}' + \bar{\mathcal{C}}'\mathcal{C}' + \sum_{\alpha=1}^{2}(\bar{\mathcal{P}}''_\alpha \mathcal{P}''_\alpha + \bar{\mathcal{C}}''_\alpha \mathcal{C}''_\alpha) \qquad (13)$$

with

$$\chi' = \mu \qquad \chi_1'' = p_3 \qquad \chi_2'' = q_2 \qquad .$$

$$\Gamma''_{\alpha k} = \frac{1}{k!}\underbrace{[\ldots[\ldots[H_0, T''_\alpha], T''_\alpha], \ldots], T''_\alpha]}_{k \text{ times}} .$$

The T_α are the new effectively first-class constraints

$$T_1 = T_1'' + 2(\eta_1 - \xi_2) \qquad T_2 = T_2'' - 2(\xi_1 + \eta_2) . \tag{14}$$

It is pointed out in [7] that the theory does not depend on a suitable choice of the gauge functions χ. The selection of the physical states of the system is enabled through the existence of a nilpotent fermionic BFV–BRST charge Ω, which commutes with H:

$$\Omega = T'\mathcal{C}' + \pi'\mathcal{P}' + \sum_{\alpha=1}^{2}(T_\alpha \mathcal{C}''_\alpha + \pi''_\alpha \mathcal{P}''_\alpha) \qquad [\Omega, \Omega] = 0 \qquad [H, \Omega] = 0 \tag{15}$$

and by which physical states are annihilated:

$$\Omega \mid \text{phys}\rangle = 0 . \tag{16}$$

Since Ω is nilpotent, every state $|\psi\rangle = \Omega \mid \text{any state}\rangle$ should be a physical one. However, Ω is also Hermitian, so that these states have zero norm and, for Ω commuting with H, they can be factored out of the physical sector of the Hibert space [11]:

$$\Omega \mid \text{any state}\rangle \neq |\text{phys}\rangle . \tag{17}$$

The two conditions (16) and (17) completely define the set of physical states of the theory. In this sense the system (H, Ω) represents the quantum mechanical version of the classical constrained system (H_0, T', T_1'', T_2''). Since fermionic operators have no effect on bosonic states and vice versa, it is clear by inspection that according to (16) all terms in the last two lines of H in (13) have to vanish acting on a physical state. In order to see how the restriction of the Hilbert space due to the new effectively first-class constraints T_α (14) works, it is useful to perform a unitary transformation leading to new variables

$$\begin{aligned} Q_2 &= (q_2 + q_3)/\sqrt{2} \qquad & P_2 &= (p_2 + p_3)/\sqrt{2} \\ Q_3 &= (q_2 - q_3)/\sqrt{2} \qquad & P_3 &= (p_2 - p_3]/\sqrt{2} \end{aligned} \tag{18}$$

by which all other operators are unaltered resulting in

$$\begin{aligned} H \mid \text{phys}\rangle = \{&\tfrac{1}{2}(p_1^2 + P_2^2) + q_1^4 + 12q_1^2Q_2^2 + 16Q_2^4 + \tfrac{1}{4}T_2^2 + \tfrac{1}{4}[16 - (c_2 + c_3)]T_1^4 \\ &+ (18 - c_4)q_1^2T_1^2 + \tfrac{1}{2}(5c_3 - c_2 - 32)Q_2^2T_1^2 + 1/\sqrt{2}(c_3 - c_2)Q_2T_1^3\} \mid \text{phys}\rangle . \end{aligned} \tag{19}$$

Note, that this is just the Hamiltonian H_0 in (6) when Q_3 is replaced by $T_2/\sqrt{2}$ and P_3 is replaced by $T_1/\sqrt{2}$. Thus the purpose of the Γ-terms appearing in the unitarizing Hamiltonian (13) becomes obvious: they define the Hamiltonian in the enlarged Hilbert space in a way such that the new effectively first-class constraints T_α

have the same physical effect on the enlarged Hilbert space as the original second-class constraints T''_α have on the original one. This should hold regardless of the complexity of the Γ-terms.

Applying (16) in (19) one finally gets

$$H \mid \text{phys}\rangle = [\tfrac{1}{2}(p_1^2 + P_2^2) + q_1^4 + 12q_1^2Q_2^2 + 16Q_2^4] \mid \text{phys}\rangle = H^\star \mid \text{phys}\rangle . \tag{20}$$

Since the classical limit of a quantum mechanical theory is well defined, this shows that the constrained system (H, Ω) (equation (13)) is the quantized version of the classical two-dimensional unconstrained system $H^\star$ (equation (20)). Thus the energy eigenvalues of (H, Ω) are given by the EBK quantization of $H^\star$ carried out above (11). An interesting question is related to the second classical constant of motion F (8): is it still a conserved quantity in the quantum mechanical system $H^\star$? For a general system (Hamiltonian K, constant of motion I, $\{K, I\} = 0$) the answer is highly non-trivial because due to the mixing of coordinates and momenta in I (and eventually in K) there may appear additional terms in the commutator $[K, I]$. But for Hamiltonian systems of the form $H = \frac{1}{2}\sum_i p_i^2 + V(q)$ it has been stated by Hietarinta [14] that constants of motion, which are of at most second-order in the momenta, quantum mechanically do commute with the Hamiltonian (to see what happens in other cases consult [14]). In this consideration the quantum operator corresponding to a classical quantity must be defined through any admissible operator ordering rule, e.g. the Weyl rule:

$$(p^k q^l)_W \equiv \frac{1}{\binom{k+l}{k}} \sum \text{all orderings of } p \text{ and } q .$$

Therefore one finds

$$[(F)_W, (H^\star)_W] = 0 \tag{21}$$

and

$$[(F)_W, (H_0)_W] = (\{F, H_0\})_W . \tag{22}$$

In general there is no definite way to relate a quantum operator to a given classical quantity. But once quantum and classical dynamics do correspond (as in (22)) the BFV algorithm seems to preserve this correspondence. The remarkable fact is that the influence of constraints on a quantum system is treated within the BFV algotrithm without any ambiguity in operator ordering and under full conservation of relativistic covariance making the theory applicable to a wide range of problems (see e.g. [20–23]). Apart from its applicability BFV quantization provides a useful tool to get some more insight into that what we have called the quantum mechanical constrained nature of a system. For future work it would be interesting to investigate how the non-integrable system (i.e. H_0 without constraints) is quantum mechanically related to that with constraints.

The authors would like to thank the referee for the suggestion to investigate the second constant of motion on the quantum level.

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