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2005 J. Phys. A: Math. Gen. 38 6557

(http://iopscience.iop.org/0305-4470/38/29/010)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **38** (2005) 6557–6569 doi:10.1088/0305-4470/38/29/010

$\mathcal{PT}$-symmetric cubic anharmonic oscillator as a physical model

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Received 18 November 2004, in final form 1 June 2005
Published 6 July 2005
Online at stacks.iop.org/JPhysA/38/6557

Abstract

We perform a perturbative calculation of the physical observables, in particular, pseudo-Hermitian position and momentum operators, the equivalent Hermitian Hamiltonian operator and the classical Hamiltonian for the $\mathcal{PT}$-symmetric cubic anharmonic oscillator, $H = \frac{1}{2m}p^2 + \frac{1}{2}\mu^2x^2 + \mathrm{i}\epsilon x^3$. Ignoring terms of order ϵ^4 and higher, we show that this system describes an ordinary quartic anharmonic oscillator with a position-dependent mass, and real and positive coupling constants. This observation elucidates the classical origin of the reality and positivity of the energy spectrum. We also discuss the quantum–classical correspondence for this $\mathcal{PT}$-symmetric system, compute the associated conserved probability density and comment on the issue of factor ordering in the pseudo-Hermitian canonical quantization of the underlying classical system.

PACS number: 03.65.−w

1. Introduction

$\mathcal{PT}$-symmetric quantum mechanics was originated by the observation, initially made by Bessis and Zinn-Justin, that the Hamiltonian for a cubic anharmonic oscillator,

$$H = \frac{p^2}{2m} + \frac{\mu^2}{2}x^2 + \mathrm{i}\epsilon x^3, \tag{1}$$

with $\mu, \epsilon \in \mathbb{R}$, has a real, positive and discrete spectrum. During the last six years, there have appeared a number of publications [1–8] exploring the properties of the Hamiltonian (1). Yet the nature of the physical system described by this Hamiltonian has not been clarified. The present paper aims at addressing this basic issue. We will achieve this aim by computing the physical observables, the localization probability density and the underlying classical Hamiltonian for this system. This is the first example of a $\mathcal{PT}$-symmetric quantum system with configuration space $\mathbb{R}$ that allows such a computation.

0305-4470/05/296557+13$30.00

As the main technical tools used in our analysis have been developed in the study of the spectral properties of $\mathcal{PT}$-symmetric Hamiltonians, we will include here a brief account of the relevant developments.

The first convincing numerical evidence supporting the reality and positivity of the spectrum of (1) was provided by Bender and Boettcher [1] who made the important observation that this Hamiltonian was $\mathcal{PT}$-symmetric. Among dozens of publications on the subject that followed [1] was the paper by Dorey, Dunning and Tateo [9] that provided the first mathematically rigorous proof of the spectral properties conjectured by Bessis and Zinn-Justin (see also [10]). From a physicist's point of view, a more important development was the idea, put forward by Bender and his collaborators [1, 11], that such $\mathcal{PT}$-symmetric Hamiltonians might be used as the Hamiltonian operator for an extended/generalized quantum theory.

The main obstacle for realizing this idea was that a non-Hermitian Hamiltonian such as (1) generated a nonunitary time evolution. This was not compatible with the conventional probabilistic interpretation of quantum mechanics. The resolution of this problem came as a by-product of the attempts to characterize the non-Hermitian operators having a real spectrum [12–16].

Reference [13] lists the necessary and sufficient conditions that ensure the reality of the spectrum of a diagonalizable operator[1]. Among these is the condition that H must be Hermitian with respect to a positive-definite inner product $\langle\cdot,\cdot\rangle_+$. This inner product is generally different from the defining inner product $\langle\cdot,\cdot\rangle$ of the (reference) Hilbert space $\mathcal{H}$ in which the operator H acts. It can be conveniently expressed in terms of a positive-definite (metric) operator $\eta_+ : \mathcal{H} \to \mathcal{H}$ according to [12]

$$\langle\cdot,\cdot\rangle_+ = \langle\cdot,\eta_+\cdot\rangle. \tag{2}$$

The condition that H be Hermitian with respect to $\langle\cdot,\cdot\rangle_+$, i.e., $\langle\cdot, H\cdot\rangle_+ = \langle H\cdot,\cdot\rangle_+$, is equivalent to η_+-pseudo-Hermiticity of H [12]. This means that η_+ belongs to the set $\mathcal{U}_H$ of all Hermitian invertible operators $\eta : \mathcal{H} \to \mathcal{H}$ satisfying[2] [12]

$$H^\dagger = \eta H \eta^{-1}. \tag{3}$$

An interesting property of the set $\mathcal{U}_H$ of all metric operators η is that to each pair (η_1, η_2) of elements of $\mathcal{U}_H$ there corresponds a symmetry generator $\eta_2^{-1}\eta_1$ of H [12]. Furthermore, $\mathcal{PT}$-symmetric Hamiltonians H that act in $\mathcal{H} = L^2(\mathbb{R})$, e.g., (1), are $\mathcal{P}$-pseudo-Hermitian, i.e., $\mathcal{P} \in \mathcal{U}_H$. This in turn implies that if H has a real spectrum, then $\mathcal{P}^{-1}\eta_+ = \mathcal{P}\eta_+$ commutes with H. The construction of the physical Hilbert space $\mathcal{H}_{\rm phys}$ that is based on the $\mathcal{CPT}$-inner product [18] makes implicit use of this observation. As shown in [16] for theories defined on $\mathbb{R}$ and more recently generalized in [19] to theories defined on a complex contour, the $\mathcal{C}$ operator introduced in [18] is related to the metric operator η_+ according to

$$\mathcal{C} = \mathcal{P}\eta_+ = \eta_+^{-1}\mathcal{P}, \tag{4}$$

and the $\mathcal{CPT}$-inner product is precisely $\langle\cdot,\cdot\rangle_+$.

The recent approximate calculations of $\mathcal{C}$ for the anharmonic oscillator (1) and its analogues [8, 20] have also revealed the practical significance of the factorization (4) of $\mathcal{C}$. These calculations are based on equation (4) and the observation that (being a positive-definite operator) η_+ admits an exponential representation

$$\eta_+ = {\rm e}^{-Q}, \tag{5}$$

where Q is a Hermitian operator.

[1] In view of the requirements of the standard quantum measurement theory, physical observables, in general, and the Hamiltonian, in particular, must be diagonalizable operators [17].

[2] Here and throughout this paper, the adjoint of an operator $A : \mathcal{H}_1 \to \mathcal{H}_2$ between two Hilbert spaces $\mathcal{H}_1$ (with inner product $\langle\cdot,\cdot\rangle_1$) and $\mathcal{H}_2$ (with inner product $\langle\cdot,\cdot\rangle_2$) is defined to be the unique operator $A^\dagger : \mathcal{H}_2 \to \mathcal{H}_1$ satisfying $\langle\cdot, A\cdot\rangle_2 = \langle A^\dagger\cdot,\cdot\rangle_1$.

The metric operator η_+ (which is generally unique up to symmetries of H [15, 16, 21]), not only determines the structure of the physical Hilbert space but also fixes the observables of the theory as well [22, 23, 17]. By definition (definition 1), *physical observables are the Hermitian operators acting in the physical Hilbert space* $\mathcal{H}_{\rm phys}$ [22, 23, 17], i.e., $A : \mathcal{H} \to \mathcal{H}$ is an observable if[3]

$$\langle \cdot, A\cdot\rangle_+ = \langle A\cdot, \cdot\rangle_+. \tag{6}$$

Alternatively, *physical observables A are* η_+*-pseudo-Hermitian operators acting in* $\mathcal{H}$, i.e., $A^\dagger = \eta_+ A \eta_+^{-1}$.

In order to see the central role played by the metric operator η_+ in the construction of the observables, we recall that as an operator mapping $\mathcal{H}_+$ onto $\mathcal{H}$ the unique positive square root $\rho = \sqrt{\eta}_+$ of η_+ is a unitary operator [26, 17], i.e.,

$$\langle \rho\cdot, \rho\cdot\rangle = \langle \cdot, \cdot\rangle_+. \tag{7}$$

Hence, the Hermitian operators O acting in $\mathcal{H}_{\rm phys}$ (i.e., the physical observables) may be obtained from the Hermitian operators o acting in $\mathcal{H}$ according to

$$O = \rho^{-1} o \rho. \tag{8}$$

This is also consistent with the condition [13] that H is related to a Hermitian operator $h : \mathcal{H} \to \mathcal{H}$ by a similarity transformation

$$h = \rho H \rho^{-1}. \tag{9}$$

The mapping $\rho : \mathcal{H}_{\rm phys} \to \mathcal{H}$ establishes the unitary equivalence of the $\mathcal{PT}$-symmetric quantum system $\mathcal{S}_{PT}$ having $\mathcal{H}_{\rm phys}$, H and O as the physical Hilbert space, the Hamiltonian and the physical observables, and the quantum system $\mathcal{S}$ having $\mathcal{H}$, h and o as the physical Hilbert space, the Hamiltonian and the physical observables, respectively [22, 17]. $\mathcal{S}_{PT}$ and $\mathcal{S}$ describe the same physical system because the physical quantities such as the expectation values and transition amplitudes are independent of the choice of $\mathcal{S}_{PT}$ and $\mathcal{S}$.

The advantage of the $\mathcal{PT}$-symmetric description provided by $\mathcal{S}_{PT}$ over the Hermitian description provided by $\mathcal{S}$ is that unlike H, the Hermitian Hamiltonian h is generally nonlocal. This advantage is, however, balanced by the disadvantage that the physical (pseudo-Hermitian) position X and momentum operators P of $\mathcal{S}_{PT}$ are also generally nonlocal. These operators are defined by [19]

$$X := \rho^{-1} x \rho, \qquad P := \rho^{-1} p \rho, \tag{10}$$

where x and p are the conventional position and momentum operators. The main advantage of the Hermitian description is that it provides means for identifying the underlying classical system [17]. The classical Hamiltonian is obtained by expressing h in terms of x and p and replacing the latter with the classical (real-valued) position x_c and momentum p_c observables. In general, this yields an expression that may involve powers of $\hbar$. The classical Hamiltonian H_c is then obtained by evaluating this expression in the limit $\hbar \to 0$, i.e., assuming that this limit exists,

$$H_c(x_c, p_c) := \lim_{\hbar\to 0} h(x_c, p_c). \tag{11}$$

The initial Hamiltonian H may be recovered by performing the so-called η_+-pseudo-Hermitian canonical quantization of H_c and adopting an appropriate factor-ordering prescription [17].

[3] As argued in [22], identifying observables with $\mathcal{CPT}$-invariant operators as initially done in [18] leads to a dynamical inconsistency. The latter is avoided if one modifies this definition as proposed in [24]. This modified definition is equivalent to definition 1 for symmetric Hamiltonians H (satisfying $\langle x|H|x'\rangle = \langle x'|H|x\rangle$) and cannot be applied for nonsymmetric Hamiltonians [25].

Disregarding the complications due to the factor-ordering problem and assuming that H_c is an analytic function of x_c and p_c, we have

$$H_c(X, P) = h(X, P) = h(\rho^{-1}x\rho, \rho^{-1}p\rho) = \rho^{-1}h(x, p)\rho = H. \tag{12}$$

Having introduced the η_+-pseudo-Hermitian position operator X, we can also address the issue of determining the conserved probability density ρ for the localization of the system in the configuration space. This requires the identification of the physical localized states of the system. Being (the generalized [27]) eigenvectors of X, the localized state vectors are given by

$$|\xi^{(x)}\rangle = \rho^{-1}|x\rangle, \tag{13}$$

where $|x\rangle$ are the conventional position eigenvectors. The conserved probability density associated with a given state vector $\psi \in \mathcal{H}_{\rm phys}$ has the form [17]

$$\varrho(x) = N^{-1}|\Psi(x)|^2, \tag{14}$$

where $\Psi(x)$ is the physical position wavefunction for the state vector ψ, i.e.,

$$\Psi(x) := \langle \xi^{(x)}, \psi\rangle_+ = \langle x|\rho\psi\rangle, \tag{15}$$

where $\langle\cdot|\cdot\rangle$ is the usual L^2-inner product on $\mathcal{H} = L^2(\mathbb{R})$ and $N := \langle\psi, \psi\rangle_+ = \int_{-\infty}^{\infty} |\Psi(x)|^2\, {\rm d}x$.[4]

An important feature of the exponential representation (5) of the metric operator η_+ is that it reduces the calculation of ρ and ρ^{-1} to that of Q, for

$$\rho^{\pm 1} = {\rm e}^{\mp Q/2}. \tag{16}$$

We will use this observation together with the approach pursued in [8] to perform a perturbative calculation of X, P, h, H_c and ϱ for the $\mathcal{PT}$-symmetric Hamiltonian (1).

Because we are interested in the issue of finding the classical limit of the $\mathcal{PT}$-symmetric theory based on the Hamiltonian (1), we wish to retain the factors of $\hbar$. However, for the simplicity of the calculations and ease of the comparison with the known results, we will introduce and employ the following dimensionless quantities:

$$\mathrm{x} := \ell^{-1}x, \qquad \mathrm{p} := \ell\hbar^{-1}p, \tag{17}$$

$$\mathcal{M} := \ell^2\hbar^{-1}\sqrt{m}\mu, \qquad \varepsilon := \ell^5\hbar^{-2}m\epsilon, \tag{18}$$

$$\mathrm{H}_0 := \frac{1}{2}\mathrm{p}^2 + \frac{\mathcal{M}^2}{2}\mathrm{x}^2, \qquad \mathrm{H}_1 := \mathrm{i}\mathrm{x}^3, \tag{19}$$

$$\mathrm{H} := \ell^2\hbar^{-2}mH = \frac{1}{2}\mathrm{p}^2 + \frac{\mathcal{M}^2}{2}\mathrm{x}^2 + \mathrm{i}\varepsilon\mathrm{x}^3 = \mathrm{H}_0 + \varepsilon\mathrm{H}_1, \tag{20}$$

where ℓ is an arbitrary length scale which may be taken as μ^2/ϵ. Clearly, we have $[\mathrm{x}, \mathrm{p}] = \mathrm{i}$.

2. Calculation of Q

In [8] the authors outline a perturbative calculation of Q for the Hamiltonian (20) taking ε as the perturbation parameter. They use the identities $[\mathcal{C}, \mathcal{PT}] = 0$ and $\mathcal{C}^2 = 1$ to infer that as a

[4] The physical position wavefunctions evolve in time according to the Schrödinger equation with h being the Hamiltonian operator. In general, one can express h in the form $p^2/(2m) + W$, where W is a nonlocal potential (an infinite series in p with x-dependent coefficients). This in turn implies that the probability current density that together with ϱ satisfies the continuity equation has a nonlocal dependence on $\Psi(x)$; it is not given by the standard formula, unless H is Hermitian. This is especially significant in the study of tunnelling and scattering for pseudo-Hermitian Hamiltonians (having scattering states).

function of x and p, Q must be even in x and odd in p. Furthermore, imposing $[C, \mathrm{H}] = 0$ and making use of the fact that H_1 is an imaginary cubic potential, they find the operator equation

$$2\varepsilon\, \mathrm{e}^{Q}\mathrm{H}_1 = [\mathrm{e}^{Q}, \mathrm{H}], \tag{21}$$

and that Q may be expanded in an odd power series in ε,

$$Q = Q_1\varepsilon + Q_3\varepsilon^3 + Q_5\varepsilon^5 + \cdots, \tag{22}$$

where $Q_{2i+1} = Q_{2i+1}(x, p)$ with $i = 0, 1, 2, \ldots$ are ε-independent. Next, they expand e^{Q} in power series in ε, substitute the result in (21) and demand that this equation be satisfied at each order of ε. This yields a series of operator equations that they iteratively solve for Q_{2i+1}.

The operator equations whose solution yields Q_{2i+1} may be more conveniently obtained from the η_+-pseudo-Hermiticity of H,

$$\mathrm{H}^{\dagger} = \eta_+\mathrm{H}\eta_+^{-1}. \tag{23}$$

Substituting $\eta_+ = \mathrm{e}^{-Q}$ in this equation and noting that $\mathrm{H}^{\dagger} = \mathrm{H}_0 - \epsilon\mathrm{H}_1$, we have

$$\mathrm{H}_0 - \mathrm{e}^{-Q}\mathrm{H}_0\,\mathrm{e}^{Q} = \epsilon(\mathrm{H}_1 + \mathrm{e}^{-Q}\mathrm{H}_1\,\mathrm{e}^{Q}). \tag{24}$$

Next, we employ the Baker–Campbell–Hausdorff identity,

$$\mathrm{e}^{-A}B\,\mathrm{e}^{A} = B + [B, A] + \frac{1}{2!}[[B, A], A] + \frac{1}{3!}[[[B, A], A], A] + \cdots, \tag{25}$$

(where A and B are linear operators) to express (24) as

$$\begin{aligned} &-[\mathrm{H}_0, Q] - \frac{1}{2!}[[\mathrm{H}_0, Q], Q] - \frac{1}{3!}[[[\mathrm{H}_0, Q], Q], Q] - \cdots \\ &\qquad = \varepsilon\left(2\mathrm{H}_1 + [H_1, Q] + \frac{1}{2!}[[\mathrm{H}_1, Q], Q] + \frac{1}{3!}[[[\mathrm{H}_1, Q], Q], Q] + \cdots\right). \end{aligned} \tag{26}$$

Now, in view of (22), we can easily identify the terms in (26) that are of the same order in powers of ε. Enforcing (26) at each order, we find the desired operator equations for Q_{2i+1}. Matching the terms of order $\varepsilon, \varepsilon^2, \ldots, \varepsilon^5$, we find in this way the following independent operator equations which agree with those obtained in [8][5]:

$$[\mathrm{H}_0, Q_1] = -2\mathrm{H}_1, \tag{27}$$

$$[\mathrm{H}_0, Q_3] = -\frac{1}{6}[[\mathrm{H}_1, Q_1], Q_1], \tag{28}$$

$$[\mathrm{H}_0, Q_5] = -\frac{1}{6}([[\mathrm{H}_1, Q_1], Q_3] + [[\mathrm{H}_1, Q_3], Q_1]) + \frac{1}{360}[[[[\mathrm{H}_1, Q_1], Q_1], Q_1], Q_1]. \tag{29}$$

The higher order terms in ε similarly yield operator equations for Q_{2i+1} with $i \geqslant 3$. As noted in [8], one can iteratively solve these equations to obtain Q_{2i+1}.

A variation of the approach of [8] is to substitute the ansatz[6]

$$Q_{2i+1} = \sum_{j,k=0}^{i+1} c_{ijk}\{x^{2j}, p^{2k+1}\} \tag{30}$$

in the operator equations for Q_{2i+1} and to solve for the coefficients c_{ijk}. In this way, we have found the following solutions for (27) and (28), respectively:

$$Q_1 = -\frac{1}{\mathcal{M}^4}\left[\frac{4}{3}\mathrm{p}^3 + \mathcal{M}^2\{\mathrm{x}^2, \mathrm{p}\}\right] = -\frac{1}{\mathcal{M}^4}\left(\frac{4}{3}\mathrm{p}^3 + 2\mathcal{M}^2\mathrm{xpx}\right), \tag{31}$$

[5] These equation are obtained at the orders ε, ε^3 and ε^5, respectively.

[6] Here $\{\cdot, \cdot\}$ stands for the anticommutator, $\{A, B\} = AB + BA$.

$$Q_3 = \frac{4}{\mathcal{M}^{10}}\left[\frac{32}{15}\mathrm{p}^5 + \frac{5}{3}\mathcal{M}^2\{\mathrm{x}^2, \mathrm{p}^3\} + \mathcal{M}^4\{\mathrm{x}^4, \mathrm{p}\} + 2\mathcal{M}^2\mathrm{p}\right]$$
$$= \frac{128}{15\mathcal{M}^{10}}\mathrm{p}^5 + \frac{40}{3\mathcal{M}^8}\mathrm{xp}^3\mathrm{x} + \frac{8}{\mathcal{M}^6}\mathrm{x}^2\mathrm{px}^2 - \frac{32}{\mathcal{M}^8}\mathrm{p}. \tag{32}$$

These confirm the results of [8] except for the coefficient of the last term in (32). We have checked the validity of (32) by inserting this relation in (28) and affecting both sides of the resulting equation on the function $f_1(\mathrm{x}) = \mathrm{x}$. Using the fact that in the x-representation $\mathrm{p} = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{dx}}$, we could easily perform the necessary calculations (without having to use any commutation relations) and check the validity (32).

In fact, we can obtain the coefficients c_{ijk} using this method. In order to do this, we can substitute (30) in the operator equations for Q_{2i+1} (rather than trying to use the complicated commutation relations for powers of x and p), affect both sides of these equations on $f_n(\mathrm{x}) = \mathrm{x}^n$ and demand that they are equal for all $n = 0, 1, 2, 3, \ldots$.

3. The equivalent Hermitian Hamiltonian

Having obtained Q, we can easily calculate the Hermitian Hamiltonian

$$\mathrm{h} = \rho\mathrm{H}\rho^{-1} \tag{33}$$

associated with the dimensionless Hamiltonian H. Using (16), (25) and (33), we have

$$\mathrm{h} = \mathrm{H} + \frac{1}{2}[\mathrm{H}, Q] + \frac{1}{2!2^2}[[\mathrm{H}, Q], Q] + \frac{1}{3!2^3}[[[\mathrm{H}, Q], Q], Q] + \cdots. \tag{34}$$

Now, in view of (20) and (22), it is very easy to identify the perturbative expansion of h, i.e., find ε-independent operators $\mathrm{h}^{(j)}$ such that

$$\mathrm{h} = \sum_{i=0}^{\infty}\mathrm{h}^{(j)}\varepsilon^j. \tag{35}$$

This yields

$$\mathrm{h}^{(0)} = \mathrm{H}_0, \qquad \mathrm{h}^{(1)} = \mathrm{H}_1 + \frac{1}{2}[\mathrm{H}_0, Q_1], \tag{36}$$

$$\mathrm{h}^{(2)} = \frac{1}{2}[\mathrm{H}_1, Q_1] + \frac{1}{8}[[\mathrm{H}_0, Q_1], Q_1], \tag{37}$$

$$\mathrm{h}^{(3)} = \frac{1}{2}[\mathrm{H}_0, Q_3] + \frac{1}{8}[[\mathrm{H}_1, Q_1], Q_1] + \frac{1}{48}[[[\mathrm{H}_0, Q_1], Q_1], Q_1], \tag{38}$$

$$\mathrm{h}^{(4)} = \frac{1}{4}[\mathrm{H}_1, Q_3] - \frac{1}{192}[[[\mathrm{H}_1, Q_1], Q_1], Q_1], \tag{39}$$

$$\mathrm{h}^{(5)} = \frac{1}{2}[\mathrm{H}_0, Q_5] + \frac{1}{12}([[\mathrm{H}_1, Q_1], Q_3] + [[\mathrm{H}_1, Q_3], Q_1]) + \frac{1}{120}[[[\mathrm{H}_0, Q_3], Q_1], Q_1]. \tag{40}$$

In view of the fact that Q_1, Q_3 and Q_5 are Hermitian while H_1 is anti-Hermitian, it is not difficult to see that the terms contributing to $\mathrm{h}^{(j)}$ with even j are Hermitian while those contributing to $\mathrm{h}^{(j)}$ with odd j are anti-Hermitian. The fact that h is a Hermitian operator then suggests that the $\mathrm{h}^{(j)}$ with odd j must vanish. There is another argument supporting this expectation, namely, that because H_1 is a cubic potential, the perturbation series for the ground state energy of H and consequently (the isospectral operator) h must only include even powers of the perturbation parameter ε [5].

Using (27)–(29), we can easily show that indeed $\mathrm{h}^{(1)}$, $\mathrm{h}^{(3)}$ and $\mathrm{h}^{(5)}$ vanish identically. This may be viewed as a consistency check of our calculations. The perturbative expansion of h valid up to and including terms of order ε^5 is, therefore, given by

$$\mathrm{h} = \mathrm{H}_0 + \mathrm{h}^{(2)}\varepsilon^2 + \mathrm{h}^{(4)}\varepsilon^4 + \mathcal{O}(\varepsilon^6), \tag{41}$$

$$\mathrm{h}^{(2)} = \frac{1}{4}[\mathrm{H}_1, Q_1], \tag{42}$$

$$\mathrm{h}^{(4)} = \frac{1}{4}[\mathrm{H}_1, Q_3] - \frac{1}{192}[[[\mathrm{H}_1, Q_1], Q_1], Q_1], \tag{43}$$

where we have made use of (27). Next, we use (31) and (32) to obtain the explicit form of $\mathrm{h}^{(2)}$ and $\mathrm{h}^{(4)}$. After a lengthy calculation, we find

$$[H_1, Q_1] = \frac{6}{\mathcal{M}^4}\left(\{\mathrm{x}^2, \mathrm{p}^2\} + \mathcal{M}^2\mathrm{x}^4 + \frac{2}{3}\right), \tag{44}$$

$$[H_1, Q_3] = -\frac{4}{\mathcal{M}^{10}}(16\{\mathrm{x}^2, \mathrm{p}^4\} + 15\mathcal{M}^2\{\mathrm{x}^4, \mathrm{p}^2\} + 64\mathrm{p}^2 + 6\mathcal{M}^4\mathrm{x}^6 + 76\mathcal{M}^2\mathrm{x}^2), \tag{45}$$

$$\begin{aligned}[[[H_1, Q_1], Q_1], Q_1] = -\frac{48}{\mathcal{M}^{12}}&(8\mathrm{p}^6 - 8\mathcal{M}^2\{\mathrm{x}^2, \mathrm{p}^4\} + 9\mathcal{M}^4\{\mathrm{x}^4, \mathrm{p}^2\} \\ &- 68\mathcal{M}^2\mathrm{p}^2 + 10\mathcal{M}^6\mathrm{x}^6 + 28\mathcal{M}^4\mathrm{x}^2).\end{aligned} \tag{46}$$

Therefore, in view of (42) and (43),

$$\mathrm{h}^{(2)} = \frac{3}{2\mathcal{M}^4}\left(\{\mathrm{x}^2, \mathrm{p}^2\} + \mathcal{M}^2\mathrm{x}^4 + \frac{2}{3}\right), \tag{47}$$

$$\mathrm{h}^{(4)} = \frac{2}{\mathcal{M}^{12}}\left(\mathrm{p}^6 - 9\mathcal{M}^2\{\mathrm{x}^2, \mathrm{p}^4\} - \frac{51}{8}\mathcal{M}^4\{\mathrm{x}^4, \mathrm{p}^2\} - \frac{81}{2}\mathcal{M}^2\mathrm{p}^2 - \frac{7}{4}\mathcal{M}^6\mathrm{x}^6 - \frac{69}{2}\mathcal{M}^4\mathrm{x}^2\right). \tag{48}$$

A simple application of (41) is in the calculation of the energy eigenvalues E_n of the Hamiltonian H. If we denote by $|n\rangle$ the normalized eigenvectors of the harmonic oscillator Hamiltonian H_0, then we can easily calculate E_n up to and including terms of order ε^3. This is done using the first-order Rayleigh–Schrödinger perturbation theory which yields

$$\mathrm{E}_n = \mathcal{M}\left(n + \tfrac{1}{2}\right) + \langle n|\mathrm{h}^{(2)}|n\rangle + \mathcal{O}(\varepsilon^4). \tag{49}$$

Substituting (47) in this relation and doing the necessary algebra, we find

$$\mathrm{E}_n = \mathcal{M}\left(n + \frac{1}{2}\right) + \frac{1}{8\mathcal{M}^4}(30n^2 + 30n + 11)\varepsilon^2 + \mathcal{O}(\varepsilon^4). \tag{50}$$

This is in complete agreement with the earlier calculations reported in [4, 7].

Next, we use (17)–(19) to obtain the expression for the unscaled Hermitian operator h that is associated with the original Hamiltonian H. This results in

$$\begin{aligned}h = \frac{p^2}{2m} + \frac{1}{2}\mu^2x^2 + \frac{3}{2\mu^4}&\left(\frac{1}{m}\{x^2, p^2\} + \mu^2x^4 + \frac{2\hbar^2}{3m}\right)\epsilon^2 + \frac{2}{\mu^{12}}\left(\frac{p^6}{m^3} - \frac{9\mu^2}{m^2}\{x^2, p^4\}\right. \\ &\left. - \frac{51\mu^4}{8m}\{x^4, p^2\} - \frac{7\mu^6}{4}x^6 - \frac{81\hbar^2\mu^2}{2m^2}p^2 - \frac{69\hbar^2\mu^4}{2m}x^2\right)\epsilon^4 + \mathcal{O}(\epsilon^6)\end{aligned} \tag{51}$$

$$= \frac{p^2}{2m} + \frac{1}{2}\mu^2 x^2 + \frac{1}{m\mu^4}\left(\{x^2, p^2\} + px^2p + \frac{3m\mu^2}{2}x^4\right)\epsilon^2 + \frac{2}{\mu^{12}}\left(\frac{p^6}{m^3} - \frac{63\mu^2}{16m^2}\{x^2, p^4\}\right.$$
$$\left. - \frac{81\mu^2}{8m^2}p^2x^2p^2 - \frac{33\mu^4}{16m}\{x^4, p^2\} - \frac{69\mu^4}{8m}x^2p^2x^2 - \frac{7\mu^6}{4}x^6\right)\epsilon^4 + \mathcal{O}(\epsilon^6), \tag{52}$$

where we have used the identities

$$px^2p - \tfrac{1}{2}\{x^2, p^2\} = \hbar^2, \qquad x^2p^2x^2 - \tfrac{1}{2}\{x^4, p^2\} = 4\hbar^2x^2,$$
$$p^2x^2p^2 - \tfrac{1}{2}\{x^2, p^4\} = 4\hbar^2p^2.$$

Note that if one does not truncate the perturbation expansion of h, one finds that it is an infinite series in powers of p. This confirms the assertion that the Hermitian Hamiltonian for a non-Hermitian Hamiltonian with a real spectrum is, in general, a nonlocal (pseudo-differential) operator [26, 17]. A remarkable property of the cubic anharmonic oscillator (1) is that the corresponding Hermitian Hamiltonian h turns out to be a local (differential) operator once one truncates its perturbation expansion. This is not generally the case.

4. Physical observables

The calculation of the physical observables $O : \mathcal{H}_{\rm phys} \to \mathcal{H}_{\rm phys}$ mimics that of h. As we discussed in section 1, because the reference Hilbert space $\mathcal{H}$ for the system is $L^2(\mathbb{R})$, the observables O are obtained from the Hermitian operators $o : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ according to (8). Substituting (16) in this relation and using (25), we have

$$O = o - \frac{1}{2}[o, Q] + \frac{1}{2!2^2}[[o, Q], Q] - \frac{1}{3!2^3}[[[o, Q], Q], Q] \pm \cdots. \tag{53}$$

Moreover, due to the particular ε-dependence of Q as given by (22), we can easily determine the following perturbation expansion for O:

$$O = o - \tfrac{1}{2}[o, Q_1]\varepsilon + \tfrac{1}{8}[[o, Q_1], Q_1]\varepsilon^2 - \tfrac{1}{2}\big([o, Q_3] + \tfrac{1}{24}[[[o, Q_1], Q_1], Q_1]\big)\varepsilon^3 + \mathcal{O}(\varepsilon^4). \tag{54}$$

Next, we calculate the dimensionless η_+-pseudo-Hermitian position and momentum operators

$$\mathrm{X} := \rho^{-1}\mathrm{x}\rho = \ell^{-1}X, \qquad \mathrm{P} := \rho^{-1}\mathrm{p}\rho = \ell\hbar^{-1}P. \tag{55}$$

This is done by substituting x and p for o in (54). Doing the necessary calculations, we obtain

$$\mathrm{X} = \mathrm{x} + \frac{2\mathrm{i}}{\mathcal{M}^4}\left(\mathrm{p}^2 + \frac{1}{2}\mathcal{M}^2\mathrm{x}^2\right)\varepsilon + \frac{1}{\mathcal{M}^6}(\{\mathrm{x}, \mathrm{p}^2\} - \mathcal{M}^2\mathrm{x}^3)\varepsilon^2 + \mathcal{O}(\varepsilon^3), \tag{56}$$

$$\mathrm{P} = \mathrm{p} - \frac{\mathrm{i}}{\mathcal{M}^2}\{\mathrm{x}, \mathrm{p}\}\varepsilon + \frac{1}{\mathcal{M}^6}\left(2\mathrm{p}^3 - \frac{1}{2}\mathcal{M}^2\{\mathrm{x}^2, \mathrm{p}\}\right)\varepsilon^2 + \mathcal{O}(\varepsilon^3). \tag{57}$$

We can directly read the expression for the η_+-pseudo-Hermitian position operator X and momentum operator P from these equations provided that we let $\mathrm{X} \to X$, $\mathrm{P} \to P/\sqrt{m}$, $\mathrm{x} \to x$, $\mathrm{p} \to p/\sqrt{m}$, $\mathcal{M} \to \mu$, $\varepsilon \to \epsilon$. As expected, X and P do not involve $\hbar$.

Equations (56) and (57) show that, as operators acting in $L^2(\mathbb{R})$, X and P are not Hermitian. The fact that by construction they are η_+-pseudo-Hermitian implies that as operators acting in $\mathcal{H}_{\rm phys}$ they are Hermitian [12]. Furthermore, these operators furnish an irreducible unitary representation of the Heisenberg–Weyl algebra, $[X, P] = i\hbar$, on the physical Hilbert space $\mathcal{H}_{\rm phys}$. They form an irreducible set of basic operators for the quantum system, i.e., other

observables may be constructed as power series in X and P. For instance, we can express the Hamiltonian (1) according to

$$H = \frac{P^2}{2m} + \frac{1}{2}\mu^2 X^2 + \frac{1}{m\mu^4}\left(\{X^2, P^2\} + PX^2P + \frac{3m\mu^2}{2}X^4\right)\epsilon^2 + \frac{2}{\mu^{12}}\left(\frac{P^6}{m^3} - \frac{63\mu^2}{16m^2}\{X^2, P^4\} - \frac{81\mu^2}{8m^2}P^2X^2P^2 - \frac{33\mu^4}{16m}\{X^4, P^2\} - \frac{69\hbar^2\mu^4}{8m}X^2P^2X^2 - \frac{7\mu^6}{4}X^6\right)\epsilon^4 + \mathcal{O}(\epsilon^6), \tag{58}$$

where we have made use of (9), (10) and (52). This is the manifestly Hermitian representation of the original Hamiltonian (1).

Another interesting implication of equations (56) and (57) is that if $\epsilon \neq 0$, the physical position (X) and momentum (P) operators do not satisfy the transformation rules of the usual position (x) and momentum (p) operators under $\mathcal{P}$ and $\mathcal{T}$ separately,

$$\mathcal{P}X\mathcal{P} \neq -X, \qquad \mathcal{P}P\mathcal{P} \neq -P, \qquad \mathcal{T}X\mathcal{T} \neq T, \qquad \mathcal{T}P\mathcal{T} \neq -P.$$

However, they share the same transformation rule under $\mathcal{PT}$,

$$\mathcal{PT}X\mathcal{PT} = -X, \qquad \mathcal{PT}P\mathcal{PT} = P.$$

This is consistent with the fact that unlike $\mathcal{P}$ and $\mathcal{T}$, $\mathcal{PT}$ is an antilinear η_+-pseudo-unitary operator [21][7]. In particular, it implies that, as an operator acting in $\mathcal{H}_{\rm phys}$, $\mathcal{PT}$ is an antilinear unitary operator. This in turn implies, in view of Wigner's classification of symmetries in quantum mechanics [28], that unlike $\mathcal{P}$ and $\mathcal{T}$, $\mathcal{PT}$ defines a physical symmetry of the quantum system. The fact that $\mathcal{P}$ does not correspond to a physical symmetry was to be expected, for its definition is intertwined with that of x which is not a physical observable for the system unless $\epsilon = 0$.

5. The classical limit

The phase space of the underlying classical Hamiltonian for the cubic anharmonic oscillator (1) is clearly $\mathbb{R}^2$. Having calculated the Hermitian operator h, we can determine the classical Hamiltonian H_c for this system using (11). In view of (51), the evaluation of the limit in (11) is trivial. Up to and including terms of order ϵ^5, H_c is given by

$$H_c = \frac{p_c^2}{2m} + \frac{1}{2}\mu^2 x_c^2 + \frac{3}{2\mu^4}\left(\frac{2}{m}x_c^2p_c^2 + \mu^2 x_c^4\right)\epsilon^2 + \frac{2}{\mu^{12}}\left(\frac{p_c^6}{m^3} - \frac{18\mu^2}{m^2}x_c^2p_c^4 - \frac{51\mu^4}{4m}x_c^4p_c^2 - \frac{7\mu^6}{4}x_c^6\right)\epsilon^4 + \mathcal{O}(\epsilon^6). \tag{59}$$

We shall first explore the consequences of neglecting the terms of order ϵ^4 and higher. Then, we can express H_c in the form

$$H_c = \frac{p_c^2}{2M(x_c)} + \frac{\mu^2}{2}x_c^2 + \frac{3\epsilon^2}{2\mu^2}x_c^4 + \mathcal{O}(\epsilon^4), \tag{60}$$

$$M(x_c) := \frac{m}{1 + 3\mu^{-4}\epsilon^2x_c^2} = m\left(1 - 3\mu^{-4}\epsilon^2x_c^2\right) + \mathcal{O}(\epsilon^4). \tag{61}$$

[7] This can be easily checked using the approach of [16].

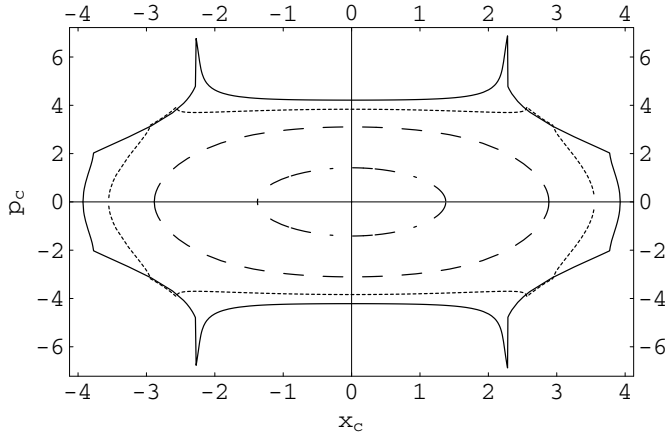

Figure 1. Graph of the orbits in phase space for the Hamiltonian (59) with $\mathcal{O}(\epsilon^6)$ neglected, $m = \mu = 1, \epsilon = 0.1$ and $E = 1$ (dashed–dotted curve), $E = 5$ (dashed curve), $E = 8$ (dotted curve) and $E = 10$ (full curve). The horizontal and vertical axes are those of x_c and p_c, respectively. Note that $E_\star = 50/3 \approx 16.7$. Hence, our perturbative calculation of the classical orbit for $E = 10$ is not as reliable as that for $E = 1$ and $E = 5$. In particular, the elliptic shape of the $E = 1$ orbit is consistent with equation (62).

Therefore, for sufficiently small ϵ, H_c describes the dynamics of a point particle with a position-dependent mass $M(x_c)$ that interacts with a quartic anharmonic potential. This statement provides a physical interpretation of the original $\mathcal{PT}$-symmetric cubic anharmonic oscillator (1). Obviously, this is a valid approximation as long as we can neglect the contribution from the terms of order ϵ^4 and higher, $\mathcal{O}(\epsilon^4) \approx 0$.

Under this assumption, H_c takes non-negative values; the classically allowed energies E are non-negative. This is the classical analogue of the fact that the $\mathcal{PT}$-symmetric quantum Hamiltonian (1) has a positive spectrum. Moreover, it is not difficult to show that the classical orbits in the phase space for the Hamiltonian (60) are ellipses determined by

$$\frac{p_c^2}{2m} + \left(\frac{\mu^2}{2} + \frac{3\epsilon^2 E}{\mu^4}\right) x_c^2 = E. \tag{62}$$

The coupling of the energy E and the perturbation parameter ϵ is an indication that the above approximation is valid for low energies, i.e.,

$$E \ll E_\star := \tfrac{1}{6}\mu^6\epsilon^{-2}. \tag{63}$$

The inclusion of the terms of order ϵ^4 distorts the above picture. However, as long as condition (63) holds, the classical (phase-space) orbits are closed curves. Figure 1 shows the graph of such orbits.

If we perform the η_+-pseudo-Hermitian quantization of the classical Hamiltonian (59), namely, let $x_c \to X$, $p_c \to P$ and $\{\cdot,\cdot\}_c \to -i\hbar^{-1}[\cdot,\cdot]$, where $\{\cdot,\cdot\}_c$ is the classical Poisson bracket, we recover the expression (58) for the original Hamiltonian (1), provided that we adopt the correct factor-ordering prescription. This observation underlines the importance of the issue of factor-ordering ambiguity in pseudo-Hermitian and, in particular, $\mathcal{PT}$-symmetric quantum mechanics.

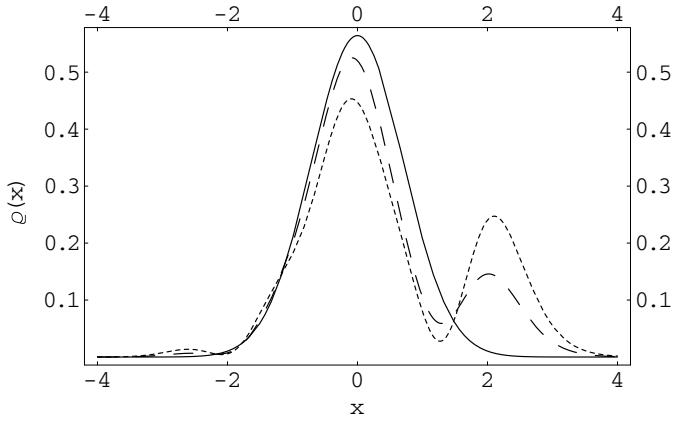

Figure 2. Graph of the invariant probability density ϱ for $\psi(x) = \mathrm{e}^{-x^2/2}$, $\hbar = m = \mu = 1$ and $\epsilon = 0$ (full curve), $\epsilon = 0.2$ (dashed curve) and $\epsilon = 0.25$ (dotted curve).

6. The conserved probability density

Expression (14) for invariant probability density for the localization of the quantum system under consideration involves the physical wavefunction (15). Given a state vector $\psi \in \mathcal{H}_{\rm phys}$, the perturbation expansion for the corresponding physical wavefunction is given by

$$\Psi(x) = \langle x|\,\mathrm{e}^{-Q/2}|\psi\rangle = \langle x|\sum_{k=0}^{\infty}\frac{(-1)^k Q^k}{2^k k!}|\psi\rangle$$
$$= \psi(x) - \tfrac{1}{2}\langle x|Q_1|\psi\rangle\varepsilon + \tfrac{1}{8}\langle x|Q_1^2|\psi\rangle\varepsilon^2 - \tfrac{1}{2}\left(\langle x|Q_3|\psi\rangle + \tfrac{1}{24}\langle x|Q_1^3|\psi\rangle\right)\varepsilon^3 + \mathcal{O}(\varepsilon^4), \tag{64}$$

where we have used (16) and (22). We can obtain the explicit form of the terms appearing on the right-hand side of (64) using (31), (32) and (17)–(19), and the identity $\langle x|p = -\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}\langle x|$. The result may be expressed as

$$\Psi(x) = (1 + \epsilon\hat{L}_1 + \epsilon^2\hat{L}_2 + \epsilon^3\hat{L}_3)\psi(x) + \mathcal{O}(\epsilon^4), \tag{65}$$

where

$$\hat{L}_1 := -\tfrac{1}{2}\hat{Q}_1, \qquad \hat{L}_2 := \tfrac{1}{8}\hat{Q}_1^2, \qquad \hat{L}_3 := -\tfrac{1}{2}\hat{Q}_3 - \tfrac{1}{48}\hat{Q}_1^3,$$

$$\hat{Q}_1 := \frac{2\mathrm{i}}{\mu^4}\left[-\frac{2\hbar^2}{3m}\frac{\mathrm{d}^3}{\mathrm{d}x^3} + \mu^2\left(x^2\frac{\mathrm{d}}{\mathrm{d}x} + x\right)\right],$$

$$\hat{Q}_3 := \frac{4\mathrm{i}}{\mu^{10}}\left[-\frac{32\hbar^4}{15m^2}\frac{\mathrm{d}^5}{\mathrm{d}x^5} + \frac{10\hbar^2\mu^2}{3m}\left(x^2\frac{\mathrm{d}^3}{\mathrm{d}x^3} + 3x\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right) - 2\mu^4\left(x^4\frac{\mathrm{d}}{\mathrm{d}x} + 2x^3\right) + \frac{8\hbar^2\mu^2}{m}\frac{\mathrm{d}}{\mathrm{d}x}\right].$$

Having obtained the general form of the physical wavefunction, we can calculate the invariant probability density ϱ according to (14). Figures 2 and 3 show the plots of ϱ for $\psi(x) = \mathrm{e}^{-x^2/2}$ and $x\,\mathrm{e}^{-x^2/2}$.

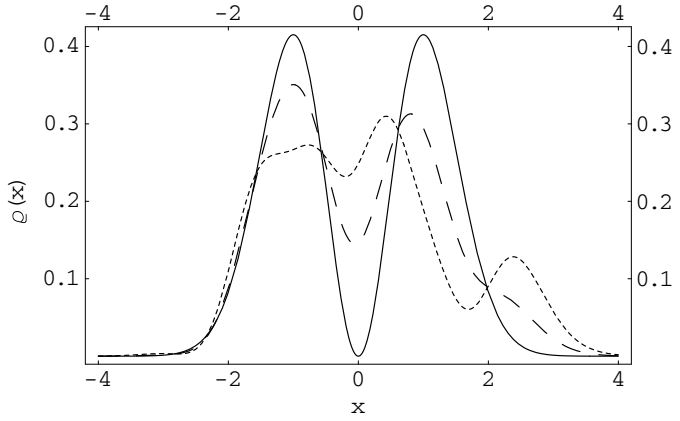

Figure 3. Graph of the invariant probability density ϱ for $\psi(x) = x\,\mathrm{e}^{-x^2/2}$, $\hbar = m = \mu = 1$ and $\epsilon = 0$ (full curve), $\epsilon = 0.1$ (dashed curve) and $\epsilon = 0.15$ (dotted curve).

7. Conclusion

We have performed a comprehensive study of the physical content of the $\mathcal{PT}$-symmetric quantum system based on the non-Hermitian cubic anharmonic oscillator (1). We showed how the general ideas developed within the framework of the pseudo-Hermitian quantum mechanics may be applied to this model. The result is an explicit characterization of the corresponding Hermitian Hamiltonian, physical observables, probability density and the underlying classical system. The only other $\mathcal{PT}$-symmetric system (with an infinite-dimensional state space) for which a similar treatment has been possible is the $\mathcal{PT}$-symmetric square well [17]. An important difference between the latter system and the anharmonic oscillator (1) is that the effects of non-Hermiticity of this oscillator do survive the classical limit; non-Hermiticity is not a by-product of the (pseudo-Hermitian) quantization.

Neglecting fourth and higher order terms in our perturbative treatment, we showed that the $\mathcal{PT}$-symmetric cubic anharmonic oscillator (1) describes a point particle having a position-dependent mass and interacting with a real quartic anharmonic potential. This provides a classical justification for the positivity of the spectrum of (1). The same argument applies to the cases where we should keep the terms of order up to (and including) five.

The pseudo-Hermitian quantization of the classical Hamiltonian defined by the appropriate metric operator together with a particular factor-ordering prescription yields the original local $\mathcal{PT}$-symmetric Hamiltonian while the usual canonical quantization of the same classical Hamiltonian with the appropriate factor-ordering prescription leads to the corresponding equivalent nonlocal Hermitian Hamiltonian.

The approach pursued in this paper may be applied to other $\mathcal{PT}$-symmetric and non-$\mathcal{PT}$-symmetric non-Hermitian Hamiltonians with a real spectrum. In general, however, the nonlocality of the corresponding equivalent Hermitian Hamiltonian may manifest itself at each order of the perturbation theory. This has already been the case for the $\mathcal{PT}$-symmetric square well studied in [17]. In view of the results of [8], the same is the case for the $\mathcal{PT}$-symmetric cubic potential, i.e., (1) with $\mu = 0$. An interesting subject of future study is to extend the approach pursued here to the field theoretical analogue of (1). Such a study should reveal the structure of the underlying classical field theory.

Note. After the online announcement of the preprint of this paper (quant-ph/0411137), Hugh Jones sent me his preprint: quant-ph/0411171, in part of which he also studies the $\mathcal{PT}$-symmetric cubic anharmonic oscillator.

Acknowledgments

I wish to thank Bijan Bagchi and Hugh Jones for their comments that helped me correct the minor errors in an earlier version of the paper.

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