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On pseudo-Hermitian Hamiltonians and their Hermitian counterparts

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Abstract

In the context of two particularly interesting non-Hermitian models in quantum mechanics we explore the relationship between the original Hamiltonian H and its Hermitian counterpart h, obtained from H by a similarity transformation, as pointed out by Mostafazadeh. In the first model, due to Swanson, h turns out to be just a scaled harmonic oscillator, which explains the form of its spectrum. However, the transformation is not unique, which also means that the observables of the original theory are not uniquely determined by H alone. The second model we consider is the original PT-invariant Hamiltonian, with potential $V = \mathrm{i}gx^3$. In this case the corresponding h, which we are only able to construct in perturbation theory, corresponds to a complicated velocity-dependent potential. We again explore the relationship between the canonical variables x and p and the observables X and P.

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1. Introduction

There has recently been a great deal of interest in the properties of non-Hermitian Hamiltonians, particularly those which possess PT symmetry, of which the prototype is the Hamiltonian

$$H = \tfrac{1}{2}(p^2 + x^2) + \mathrm{i}gx^3, \tag{1}$$

first studied in detail by Bender and Boettcher [1], following an earlier suggestion by Bessis.

This Hamiltonian was shown numerically to have a real, positive spectrum, as indeed were its generalizations to

$$H = \tfrac{1}{2}(p^2 + x^2) + gx^2(\mathrm{i}x)^N. \tag{2}$$

A rigorous proof of the reality of the spectrum was subsequently given by Dorey *et al* [2].

In the intervening time many examples of non-Hermitian Hamiltonians were found, often complex generalizations of well-known soluble potentials such as the Morse potential, which all possessed real spectra for some range of the parameters. However, the focus then moved on to more difficult problems posed by such Hamiltonians, namely whether they possessed a consistent interpretational framework. The problem arises because in such theories the natural metric in the space of quantum mechanical states does not necessarily possess the attribute of positive definiteness which is the basis of the probabilistic interpretation of quantum mechanics.

In the context of *PT*-invariant theories a solution was proposed by Bender *et al* [3], who introduced a new operator C and a new scalar product, the *CPT* scalar product, which was indeed positive definite. This solves the problem in principle, but the difficulty is that the new product is dynamically determined; that is, one needs to know the eigenvalues and eigenvectors of the Hamiltonian in order to construct C. This can be done for soluble models, but for the prototype Hamiltonian of equation (1) only a perturbative expansion for C is available.

In a parallel development, Mostafazadeh [4] introduced the notion of pseudo-Hermiticity. A Hamiltonian is said to be pseudo-Hermitian with respect to a positive-definite, Hermitian operator η if it satisfies

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

In the case of *PT*-symmetric Hamiltonians the role of η is played by PC. In [5] it was found convenient to write C in the form $C = e^{Q}P$, where Q was a Hermitian operator satisfying $PQ = -QP$. Hence in this case $\eta = e^{-Q}$, which is indeed a positive-definite Hermitian operator.

The positive-definite metric takes the form

$$\langle\langle \varphi, \psi \rangle\rangle = \langle \varphi, \eta\psi \rangle, \tag{4}$$

where $\langle\,\rangle$ denotes the usual scalar product.

Further, the observables of the theory were identified as pseudo-Hermitian operators A with respect to η. In the case of *PT*-symmetric theories where the Hamiltonian is an even function of p, which includes the class of equation (2), this coincides with the definition [6] that A must satisfy $\tilde{A} = (CPT)A(CPT)$.

Mostafazadeh went on to show that under a similarity transformation implemented by $\rho = \sqrt{\eta}$ such a Hamiltonian is equivalent to a Hermitian Hamiltonian h, according to

$$H = \rho^{-1} h \rho. \tag{5}$$

Again, a similar relation holds for observables in general: if a is an observable in the Hermitian theory described by h, the corresponding observable in the pseudo-Hermitian theory is

$$A = \rho^{-1} a \rho. \tag{6}$$

In this paper we wish to explore these relationships in detail in two models. One, initially presented by Swanson [7], is a soluble model which can be transformed by a similarity transformation (in fact a whole class of such transformations) to a simple harmonic oscillator. Here we discuss the different possible similarity transformations, and in the simplest case, where $\eta = \eta(x)$, identify the observables. The second model, which can only be treated in perturbation theory, is the original $\mathrm{i}gx^3$ Hamiltonian of equation (1). In this case we construct h to order g^4 and the observables to order g^2. The resulting h is a complicated, momentum-dependent object, in contrast to the simple form of H. This means that although the two theories are formally equivalent, the non-Hermitian H is the only practical starting point.

2. The Swanson Hamiltonian

An interesting Hamiltonian, which is PT-symmetric, but not symmetric, is that considered by Swanson [7]:

$$H = \omega a^\dagger a + \alpha a^2 + \beta \alpha^{\dagger 2}, \tag{7}$$

where a and $a^\dagger$ are harmonic oscillator annihilation and creation operators for unit frequency and ω, α and β are real constants. This Hamiltonian has a real, positive spectrum in a certain range of the parameters.

In fact for $\omega > \alpha + \beta$, the spectrum of equation (7) is that of the simple harmonic oscillator with frequency $\Omega = \sqrt{\omega^2 - 4\alpha\beta}$. Swanson showed this by constructing a transformation operator $U(= \eta)$ of Bogoliubov type which reduced the original problem to that of the simple harmonic oscillator. This gave the following form[1] for U:

$$U = \exp\left\{\frac{1}{2}\left(\frac{g_3}{g_1} - \frac{g_2}{g_4}\right)a^{\dagger 2}\right\}\exp\left(\frac{1}{2}\,wd^2\right)\exp(cd\ln z), \tag{8}$$

where $w = (g_3g_4 - g_1g_2)/g_4^2$, $z = g_4/g_1$, and c and d are Bogoliubov transforms of a and $a^\dagger$:

$$c = g_1a^\dagger - g_3a, \qquad d = g_4a - g_2a^\dagger.$$

The g_i are subject to the three conditions

$$g_1g_4 - g_2g_3 = 1, \qquad g_2g_4\omega + g_2^2\alpha + g_4^2\beta = 0, \qquad g_1g_3\omega + g_1^2\alpha + g_3^2\beta = 0,$$

which means that there is a one-parameter family of solutions, depending on g_1, say. Geyer *et al* [8] noted this non-uniqueness of U, in contrast to the uniquely defined operator C, or Q, of [3, 5], and proposed that the ambiguity could be removed by the requirement that not only the Hamiltonian but a given observable (or in general an 'irreducible set of observables') should be pseudo-Hermitian with respect to η.

In fact what this amounts to in this case is that η is a function of that particular observable. A very simple form of η can be found [8] by requiring it to be a function of the number operator $N = a^\dagger a$. In fact, with $S(= \rho = \eta^{\frac{1}{2}})$ given by

$$S = \exp\left[\tfrac{1}{4}N\ln(\alpha/\beta)\right], \tag{9}$$

it is easy to see, using the commutation relations $[N, A] = 2B, [N, B] = 2A$, where $A := a^{\dagger 2} + a^2$, $B := a^{\dagger 2} - a^2$, that

$$h = SHS^{-1} = \tfrac{1}{2}p^2(\omega - 2\sqrt{\alpha\beta}) + \tfrac{1}{2}x^2(\omega + 2\sqrt{\alpha\beta}), \tag{10}$$

a scaled harmonic oscillator with frequency Ω.

The condition $[S, N] = 0$ gives the additional constraint $g_1g_3 = g_2g_4$ on the parameters g_i: however, it is still not easy to see the equivalence between the three-exponential form of Swanson, equation (8) and the single-exponential form of equation (9).

While this transformation is adequate to obtain the spectrum of H, it is not suitable for calculations in wave mechanics, where explicit eigenfunctions are needed. An alternative transformation, which immediately gives the form of the wavefunctions, is obtained by choosing η to be a function of x. Indeed, it is easily seen that the required form of ρ is

$$\rho = \exp\left[\tfrac{1}{2}\lambda x^2\right], \tag{11}$$

where

$$\lambda = \frac{\beta - \alpha}{\omega - \alpha - \beta}.$$

[1] Taking the g_i as real.

By virtue of the commutation relations $[x^2, A] = 2B, [x^2, B] = 2A + 4C, [x^2, C] = -B$, where $C := N + \frac{1}{2}$, the similarity transformation $\rho H \rho^{-1}$ now gives

$$h = \rho H \rho^{-1} = \frac{1}{2} p^2(\omega - \alpha - \beta) + \frac{1}{2} x^2 \frac{\omega^2 - 4\alpha\beta}{\omega - \alpha - \beta}, \tag{12}$$

a different scaled harmonic oscillator with the same frequency Ω.

This transformation corresponds to the method of reducing the original Schrödinger differential equation for ψ:

$$\left[\frac{1}{2}\omega\left(x^2 - \frac{\mathrm{d}^2}{\mathrm{d}x^2}\right) + \frac{1}{2}(\alpha + \beta)\left(x^2 + \frac{\mathrm{d}^2}{\mathrm{d}x^2}\right) + (\alpha - \beta)\left(x\frac{\mathrm{d}}{\mathrm{d}x} + \frac{1}{2}\right)\right]\psi = E\psi,$$

to that of a simple harmonic oscillator for φ by writing $\psi = W\varphi$ and choosing W so that there are no linear derivatives acting on φ. The resulting condition on W is $(\omega - \alpha - \beta)W' + (\beta - \alpha)xW = 0$, which gives $W = \rho^{-1}$. The resulting wavefunctions are

$$\psi_n = \mathcal{N}_n \, \mathrm{e}^{-\frac{1}{2}x^2(\lambda + \mu^2)} H_n(\mu x), \tag{13}$$

where

$$\mu = \frac{(\omega^2 - 4\alpha\beta)^{\frac{1}{4}}}{(\omega - \alpha - \beta)^{\frac{1}{2}}},$$

the H_n are the Hermite polynomials and $\mathcal{N}_n$ is the appropriate normalization factor. Clearly these are not orthonormal as they stand; rather they are orthonormal with respect to the weight factor $\eta = \rho^2 = \mathrm{e}^{\lambda x^2}$. That is,

$$\int \psi_m^*(x) \, \mathrm{e}^{\lambda x^2} \psi_n(x) \, \mathrm{d}x = \delta_{mn}, \tag{14}$$

in accordance with equation (4).

If one takes the point of view that the original Hamiltonian H is obtained by the inverse similarity transformation from the h of equation (12), then the independent observables of the non-Hermitian H theory are obtained by the same inverse transformation on those of h, which are x and p. Thus

$$X := \mathrm{e}^{-\frac{1}{2}\lambda x^2} x \, \mathrm{e}^{\frac{1}{2}\lambda x^2} = x, \qquad P := \mathrm{e}^{-\frac{1}{2}\lambda x^2} p \, \mathrm{e}^{\frac{1}{2}\lambda x^2} = p - \mathrm{i}\lambda x. \tag{15}$$

Equally H can be written in the form of equation (12), with p replaced by P. This approach, namely deriving a non-Hermitian Hamiltonian by the above transformation of p, was in fact originally taken by Ahmed [9] before the paper of Swanson.

However, a rather puzzling situation arises, in that what we define as the observables associated with H depends on the particular transformation ρ that is used to convert it to a simple harmonic oscillator. Thus, apart from the transformation used by Geyer *et al* and that just discussed, it would be equally possible to take ρ as a function of p alone. In that case we would have simple wavefunctions in momentum space, and the observables would be p and a transformed version of x. As already discussed above, there is in fact a one-parameter family of transformations, and hence of observables.

3. The igx^3 theory

For the Hamiltonian of equation (1) the Q operator has been constructed [3] up to $O(g^7)$ in the form $Q = \sum_r g^r Q_r$. To first order[2]

$$Q_1 = -\tfrac{4}{3}p^3 - 2xpx. \tag{16}$$

[2] In fact this result is accurate up to second order: Q contains only odd powers of g.

We are thus in a position to construct h, which to this order is given by

$$h = e^{-\frac{1}{2}gQ_1} H \, e^{\frac{1}{2}gQ_1}. \tag{17}$$

By virtue of the property $[Q_1, H_0] = 2H_1$, where $H_0 \equiv \frac{1}{2}(p^2 + x^2)$ and $H_1 \equiv \mathrm{i}x^3$, this becomes

$$\begin{aligned} h(x, p) &= H_0 - \tfrac{1}{4}g^2[Q_1, H_1] \\ &= H_0 + 3g^2\left(\tfrac{1}{2}x^4 + S_{2,2} - \tfrac{1}{6}\right) + O(g^4), \end{aligned} \tag{18}$$

where $S_{2,2} = (x^2p^2 + xp^2x + p^2x^2)/3$. As indicated, the next correction is of order g^4 by virtue of the structure of the commutation relations of the Q_r.

This result is interesting in several respects. Firstly it is already quite complicated, compared with the simple form of H, and that complication only increases in higher orders. Secondly it has an x^4 component with a positive sign, as for a conventional quartic oscillator. Thirdly it is momentum dependent, containing a number of terms involving p.

The calculation can be continued, using

$$Q_3 = \frac{128}{15}p^5 + \frac{40}{3}S_{3,2} + 8S_{1,4} - 12p,$$

where the $S_{m,n}$ are fully symmetrized polynomials of degree m in x and n in p. The fourth-order contribution is

$$h_4 = g^4[-(7/2)x^6 - (51/2)S_{2,4} - 36S_{4,2} + 2p^6 + (15/2)x^2 + 27p^2],$$

which now has a negative coefficient for the x^6 term, but also contains a term in p^6. If we were able to sum up the perturbation series, the higher powers of $p = -\mathrm{i}\partial/\partial x$ would ultimately produce a non-local function. Clearly this is not a Hamiltonian that one would have contemplated in its own regard, were it not derived from equation (1). It is for this reason that we disagree with the contention of Mostafazadeh [10] that 'a consistent probabilistic *PT*-symmetric quantum theory is doomed to reduce to ordinary QM'.

Turning to the question of the independent observables of the system, these are obtainable from those of the Hermitian theory, namely x and p, by the transformations

$$X = e^{\frac{1}{2}Q} x \, e^{-\frac{1}{2}Q} \qquad P = e^{\frac{1}{2}Q} p \, e^{-\frac{1}{2}Q}. \tag{19}$$

To second order these are

$$\begin{aligned} X &= x + \mathrm{i}g(x^2 + 2p^2) + g^2(-x^3 + 2pxp), \\ P &= p - \mathrm{i}g(xp + px) + g^2(2p^3 - xpx). \end{aligned} \tag{20}$$

Again, these calculations can be carried out to higher order, but the results are not particularly illuminating.

It is, however, interesting to compare the ground-state expectation values

$$\langle\langle \psi_0, X\psi_0 \rangle\rangle = \left\langle \psi_0, e^{-\frac{1}{2}Q} x \, e^{-\frac{1}{2}Q} \psi_0 \right\rangle = 0$$

and

$$\langle\langle \psi_0, x\psi_0 \rangle\rangle = \langle \psi_0, e^{-Q} x\psi_0 \rangle = -\tfrac{3}{2}\mathrm{i}g + O(g^3).$$

The first must be real, and is in fact zero by symmetry, whereas the second is pure imaginary. This is unacceptable for an observable in quantum mechanics. In the generalization to quantum field theory, however, where $x(t) \to \varphi(\mathbf{x}, t)$, the field itself is not necessarily an observable, so a non-vanishing expectation value may be acceptable.

Note that Q itself is an observable, since it is Hermitian and commutes with itself. It also has the property that

$$Q(x, p) = e^{\frac{1}{2}Q} Q(x, p) \, e^{-\frac{1}{2}Q} = Q(X, P). \tag{21}$$

That is, Q, originally written as a function of x and p, is in fact the same function of the observables X and P.

Since X and P are the observables, it might be tempting to express H in terms of them, instead of the original x and p. Unfortunately this does not lead to any appreciable simplification, because in fact

$$H = \mathrm{e}^{\frac{1}{2}Q} h(x, p) \, \mathrm{e}^{-\frac{1}{2}Q} = h(X, P).$$

That is, the initial, non-Hermitian Hamiltonian H, when expressed in terms of the observables X and P, is of the same form as h: a complicated, momentum-dependent function.

4. Discussion

In the context of two particularly interesting models, we have discussed the relation between the original non-Hermitian Hamiltonian H and its Hermitian counterpart h, and have exhibited the observables of the theory. In the case of the Swanson Hamiltonian of equation (9), there is a one-parameter choice for the transformation operator η, and correspondingly the observables of the theory are not determined uniquely by the Hamiltonian but depend on that choice. For the $\mathrm{i}x^3$ model of equation (1) we explicitly constructed the corresponding Hermitian Hamiltonian in perturbation theory, noting its complicated, momentum-dependent character. We constructed the observables X and P in perturbation theory and discussed their relation to the canonical x, p.

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Note added in proof. After submission of this paper I became aware of a preprint by Mostafazadeh (quant-ph/0411137) which also deals with the topic of section 3. Where they overlap, the two papers are in complete agreement.

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