Gauging non-Hermitian Hamiltonians

H F Jones

Physics Department, Imperial College, London SW7 2AZ, UK
E-mail: h.f.jones@imperial.ac.uk

Received 2 November 2008, in final form 12 February 2009
Published 6 March 2009
Online at stacks.iop.org/JPhysA/42/135303

Abstract
We address the problem of coupling non-Hermitian systems, treated as fundamental rather than effective theories, to the electromagnetic field. In such theories the observables are not the $x$ and $p$ appearing in the Hamiltonian, but quantities $X$ and $P$ constructed by means of the metric operator. Following the analogous procedure of gauging a global symmetry in Hermitian quantum mechanics we find that the corresponding gauge transformation in $X$ implies minimal substitution in the form $P \rightarrow P - eA(X)$. We discuss how the relevant matrix elements governing electromagnetic transitions may be calculated in the special case of the Swanson Hamiltonian, where the equivalent Hermitian Hamiltonian $h$ is local, and in the more generic example of the imaginary cubic interaction, where $H$ is local but $h$ is not.

PACS numbers: 03.65.Ca, 11.30.Er, 02.30.Mv

1. Introduction
Recent interest in Hamiltonians that are non-Hermitian but nonetheless have a real spectrum dates from the pioneering paper of Bender and Boettcher [1], which gave strong numerical and analytical evidence that the spectrum of the class of Hamiltonians

$$H = p^2 + m^2 x^2 - (ix)^N$$

(1)
was completely real and positive for $N \geq 2$, and attributed this reality to the (unbroken) $PT$ symmetry of the Hamiltonian. Subsequently a large number of $PT$-symmetric models were explored (see, e.g. [2]), and it was found that the phenomenon was rather general. The drawback that the natural metric on the Hilbert space, with overlap $\int \psi_i(-x)\psi_j(x) \, dx$, was not positive definite was overcome by the realization [3] that one could construct an alternative, positive-definite metric involving the so-called $C$ operator. The formalism was further developed by Mostafazadeh [4], building on earlier work by Scholtz et al [5]. In
particular he showed [6] that such a Hamiltonian $H$ was related by a similarity transformation to an equivalent Hermitian Hamiltonian $h$. The key relation is the quasi-Hermiticity of $H$:

$$H^\dagger = \eta H \eta^{-1},$$

(2)

where $\eta$ is Hermitian and positive definite. $\eta$ is related to the $C$ operator by $\eta = CP$, and it is frequently extremely useful [7] to write it in the exponential form $\eta = e^{-Q}$. Occasionally $\eta$ can be constructed exactly (see, for example, [8–12]), but more typically it can only be constructed in perturbation theory, for example for the $ix^3$ model [13].

From equation (2) we can immediately deduce that

$$h \equiv \rho H \rho^{-1}$$

(3)

is Hermitian, where $\rho = e^{-1/2Q}$. Other operators $A$ will also be observables, having real eigenvalues, if they are also quasi-Hermitian, i.e.

$$A^\dagger = \eta A \eta^{-1},$$

(4)

and they again are related by the similarity transformation to Hermitian counterparts $a$:

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

(5)

The similarity transformation also transforms the states of the Hermitian system, $|\psi\rangle$, to those of the quasi-Hermitian system, $|\psi\rangle$:

$$|\psi\rangle = \rho^{-1} |\phi\rangle.$$

(6)

This implies that the matrix element of an operator is

$$\langle O \rangle_{ij} = \langle \psi_i | \eta O | \psi_j \rangle.$$  

(7)

In particular, the matrix elements of an observable can be written as

$$\langle \psi_i | \eta A | \psi_j \rangle = \langle \psi_i | \rho^{-1} \eta (\rho^{-1} a \rho)\rho^{-1} | \psi_j \rangle = \langle \psi_i | a | \psi_j \rangle.$$  

(8)

A very important observation is that

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

(9)

Thus, an alternative way of finding $h$ is to calculate the observables $X$ and $P$ and then rewrite $H(x, p)$ in terms of them.

The above concerns quasi-Hermitian systems considered in isolation. However, important conceptual issues arise when one attempts to consider such systems in interaction with an otherwise Hermitian environment. For example, [14] examined a non-Hermitian analogue of the Stern–Gerlach experiment in which the role of the intermediate inhomogeneous magnetic field flipping the spin is taken over by an apparatus described by a non-Hermitian Hamiltonian. This type of set-up has been further discussed and elaborated in a series of papers by various authors [15–20].

Again, scattering gives rise to problems, since unitarity, as conventionally defined, is generically not satisfied for a $PT$-symmetric Hamiltonian. Unitarity can be restored, by use of the $\eta$ metric, but then the concept of ‘in’ and ‘out’ states has to be drastically [21, 22], or in some cases [23] less drastically, revised.

This paper is concerned with another such issue, namely how one couples a charged particle described by a quasi-Hermitian Hamiltonian to the electromagnetic field, following as closely as possible the well-known gauging procedure for a Hermitian Hamiltonian. This
problem has been previously dealt with by Fariah and Fring [24] in a treatment which in many ways is more sophisticated than this paper, dealing with pulses rather than plane waves and going beyond first-order perturbation theory. However, the subtleties arising from the difference between \( x \) and \( X \) (see equation (22)) were not encountered there because the calculations were done entirely within the framework of the dipole approximation, where the electromagnetic potential \( A \) is just a function of time.

2. Brief review of the standard procedure

In standard quantum mechanics the probability density is just \( |\psi(x)|^2 \), which is unchanged under a change of phase of the wavefunction: \( \psi \rightarrow e^{i\alpha}\psi \) provided that \( \alpha \) is a real constant. If we try to extend this to \( \alpha = \alpha(x) \), a real function of \( x \), an extra term appears in the Schrödinger equation, because now \( \hat{p}e^{i\alpha}\psi = e^{i\alpha}(\hat{p} + e\nabla)\psi \). We cancel this additional \( \nabla \alpha \) term by \( \text{minimal substitution} \):

\[
p \rightarrow p - eA. \tag{10}
\]

Then under the combined transformations

\[
\begin{align*}
\psi & \rightarrow \psi' = e^{i\alpha}\psi \\
A & \rightarrow A' = A - \nabla \alpha,
\end{align*} \tag{11}
\]

we obtain \( (\hat{p} - eA)\psi \rightarrow e^{i\alpha}(\hat{p} - eA)\psi \), as required. Moreover, the electric and magnetic fields are unchanged by the gauge transformation (22).

So for a normal Hamiltonian of the form

\[
H = \frac{p^2}{2m} + V(x), \tag{12}
\]

the coupling to the vector potential is \(-e(A \cdot p + p \cdot A)/(2m)\). In first-order perturbation theory a standard procedure then gives the transition rate between the states \( |i\rangle \) and \( |j\rangle \) induced by a plane wave

\[
A(x, t) = \int d\omega \tilde{A}(\omega)e^{i(k \cdot x - \omega t)} + c.c. \tag{13}
\]

as

\[
wij \propto \frac{e^2}{m^2} |\langle i | p_A | j \rangle|^2 \tag{14}
\]

in the dipole approximation \( e^{ik \cdot x} \approx 1 \) over the range of the interaction. Here the constant of proportionality is \((2\pi/\hbar^2)\tilde{A}(\omega_i^2)\), where \( \omega_i = (E_i - E_j)/\hbar \) and \( p_A \) is the projection of \( p \) in the direction of \( A \).

The matrix element \( \langle i | p_A | j \rangle \) can be recast in terms of \( \langle i | x_A | j \rangle \), where \( x_A \) is similarly defined, by

\[
(E_i - E_j)\langle i | x | j \rangle = \langle i | [H, x] | j \rangle = -\frac{i\hbar}{m} \langle i | p | j \rangle, \tag{15}
\]

so that

\[
\langle i | p_A | j \rangle = im\omega_i \langle i | x_A | j \rangle. \tag{16}
\]
3. Quasi-Hermitian quantum mechanics

The total probability is now \( \langle \psi | \eta | \psi \rangle \), where \( \eta \) is the metric operator. This is no longer invariant under \( |\psi\rangle \rightarrow e^{i\varphi(x)}|\psi\rangle \), except in the special case where \( \eta = \eta(x) \) so that \( [\eta, x] = 0 \).

It is, however, invariant under

\[
|\psi\rangle \rightarrow e^{i\varphi(x)}|\psi\rangle, \tag{17}
\]

where \( X \) is the observable \( X = \rho^{-1} x \rho \). For then

\[
\langle \psi | \eta | \psi \rangle \rightarrow \langle \psi | e^{-i\varphi(X)} \eta e^{i\varphi(X)} | \psi \rangle = \langle \psi | \eta | \psi \rangle, \tag{18}
\]

since \( X^\dagger \eta = \eta X \). Note that, in terms of the eigenstates \( |\varphi\rangle \) of \( h \), equation (17) corresponds to

\[
|\varphi\rangle \rightarrow \rho e^{i\varphi(X)} \rho^{-1} |\varphi\rangle = e^{i\varphi(x)} |\varphi\rangle. \tag{19}
\]

Since we are using \( X \) in the exponent in equation (17), we will also need to write \( H \) in terms of \( X \) and the corresponding conjugate observable \( P \), according to equation (9), i.e.

\[
H(x, p) = h(X, P). \tag{20}
\]

The minimal substitution we require, in \( h(X, P) \), is then

\[
P \rightarrow P - eA(X), \tag{21}
\]

with the combined transformations

\[
\begin{aligned}
|\psi\rangle &\rightarrow |\psi'\rangle = e^{i\varphi(X)}|\psi\rangle \\
A(X) &\rightarrow A'(X) = A(X) - \nabla X \alpha(X).
\end{aligned} \tag{22}
\]

It is important to note that because \( X \) and \( x \) do not commute, the argument of \( A \) in equation (21) must be \( X \) rather than \( x \) in order to ensure that

\[
e^{-i\varphi(X)}(P - eA) e^{i\varphi(X)} = P - eA.
\]

Given the gauge transformation of equation (22), we are obliged to define \( B(X) = \nabla X \times A(X) \), and the Fourier transform of equation (13) will also have to be rewritten in terms of \( X \). How are we to interpret this, when \( X \) is a complicated non-local operator? The answer is that the external, classical electromagnetic potential is in reality \( A(\xi) \), where \( \xi \) is a real vector of position. Then \( B(\xi) = \nabla \xi \times A(\xi) \), and equation (13) becomes

\[
A(\xi, t) = \int d\omega \; A(\omega) \; e^{i(k \cdot \xi - \omega t)} + c.c. \tag{23}
\]

Then, in the interaction with the non-Hermitian system, \( \xi \) is replaced by the operator \( X \), of which it is the eigenvalue. This is in parallel with the normal practice whereby in equation (13) it is understood that \( x \) is a numerical vector, but in its interaction with a Hermitian system \( x \) is interpreted as the operator \( \hat{x} \).

If \( h \) is of standard form, \( p^2 / (2\mu) + U(x) \), the scattering rate is

\[
w_{ij} \propto \frac{e^2}{\mu^2} |\langle \psi_i | \eta P_A | \psi_j \rangle|^2 = \frac{e^2}{\mu^2} |\langle \psi_i | P_A | \psi_j \rangle|^2, \tag{24}
\]

and the second form of the matrix element can then be rewritten, as in the Hermitian case, as a matrix element of \( x_A \), namely

\[
\langle \psi_i | P_A | \psi_j \rangle = i\mu \alpha_{ij} \langle \psi_i | x_A | \psi_j \rangle. \tag{25}
\]

Note that the probability density \( \omega(x) = \langle \psi | x | \rho | x | \psi \rangle \) is also invariant under the transformation of equation (17).
3.1. The Swanson model

A much-studied example where \( h \), but not \( H \), is of standard form is the Swanson Hamiltonian [8], whose three-dimensional version reads

\[
H = \frac{p^2}{2m_1} + \frac{1}{2}i\omega \{x, p\} + \frac{1}{2}m_2\omega^2 x^2,
\]

with \( m_2 = (1 - \epsilon^2)m_1 \). There is actually a one-parameter family [25] of \( Q \)s, from which we consider just the two cases (i) \( Q = Q(x) \) and (ii) \( Q = Q(p) \). In either case the equivalent Hermitian Hamiltonian is just a harmonic oscillator of the form

\[
h(x, p) = \frac{p^2}{2\mu} + \frac{1}{2}\mu\omega^2 x^2.
\]

(i) \( Q = Q(x) = \epsilon m_1\omega x^2 \). This amounts to completing the square as

\[
H = \frac{(p + i\epsilon m_1\omega x)^2}{2m_1} + \frac{1}{2}m_1\omega^2 x^2,
\]

so that \( X = x \), while \( P = p + i\epsilon m_1\omega x \). Thus in this case

\[
h(x, p) = \frac{p^2}{2m_1} + \frac{1}{2}m_1\omega^2 x^2,
\]

so that \( \mu = m_1 \). The coupling to the vector potential is thus

\[
-\frac{e}{2m_1} (A \cdot P + P \cdot A) = -\frac{e}{2m_1} [(A \cdot p + p \cdot A) + i\epsilon m_1\omega (A \cdot x + x \cdot A)].
\]

The required matrix element,

\[
\langle \psi_i | \eta P_A | \psi_j \rangle = \langle \psi_i | p_A | \psi_j \rangle,
\]

is then found from expressing each component of \( p \) on the right-hand side in terms of creation and annihilation operators: \( p = i\sqrt{(m_1\omega/2)}(a^\dagger - a) \).

(ii) \( Q = Q(p) = -\epsilon x^2/(m_2\omega) \).

This amounts to completing the square instead as

\[
H = \frac{p^2}{2m_2} + \frac{1}{2}m_2\omega^2 \left(x + \frac{i\epsilon p}{m_2\omega}\right)^2
\]

\[
= \frac{p^2}{2m_2} + \frac{1}{2}m_2\omega^2 X^2,
\]

so that \( P = p \), while \( X = x + i\epsilon p/(m_2\omega) \). Thus in this case

\[
h(x, p) = \frac{p^2}{2m_2} + \frac{1}{2}m_2\omega^2 x^2,
\]

with \( \mu = m_2 \). The coupling to the vector potential is thus

\[
-\frac{e}{2m_2} (A \cdot P + P \cdot A) = -\frac{e}{2m_2} (A \cdot p + p \cdot A).
\]

The matrix elements are still of the form of equation (31), but now the components of \( p \) on the right-hand side are expressed as \( p = i\sqrt{(m_2\omega/2)}(a^\dagger - a) \).

The important thing to note is that one will get different transition rates in the two cases. That is, the system is determined not only by the Hamiltonian \( H \), but also by the particular metric operator \( \eta \) used to restore unitarity.
3.2. Imaginary cubic interaction

The more common situation is that $H$ is of standard form, while $h$ is a complicated non-local object. For example, in the case of the (one-dimensional) prototype Hamiltonian

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

we have \[13\]

$$Q = -g \left( \frac{4}{3} p^3 + 2 xp \right) + O(g^3),$$

which gives rise \[26, 27\] to the observables

$$X = x + ig(x^2 + 2p^2) + g^2(-x^3 + 2pxp)$$
$$P = p - ig(xp + px) + g^2(2p^3 - xp^2) + O(g^3).$$

Referring to equation (9), we can write $H(x, p)$ as $h(X, P)$, where $h(x, p)$ has been calculated up to second order in $g$ as \[26, 27\]

$$h(x, p) = \frac{1}{2}(p^2 + x^2) + 3g^2 \left( \frac{1}{2} x^4 + S_{2,2}(x, p) - \frac{1}{6} \right) + O(g^4),$$

where $S_{2,2}(x, p) = (x^2 p^2 + xp^2 x + p^2 x^2)/3$.

From equation (38), we see that the minimal substitution $P \rightarrow P - eA(X)$ in $h(X, P)$ will give rise to additional couplings, of order $g^2$, arising from the mixed term $S_{2,2}(X, P)$.

To $O(g)$ the matrix elements will be just $\langle \psi_i | \eta P_A | \psi_j \rangle$. In order to calculate this we will need the corrected eigenfunctions, which have a first-order contribution, namely

$$\psi_i(x) = \psi_{i0}(x) + g \sum_{j \neq i} \langle \psi_{i0} | i x^3 | \psi_{j0} \rangle \psi_{j0}(x) + O(g^2).$$

In this case, it is much easier \[28\] to work with $H$ directly rather than with $h$.

4. Summary

For a standard Hermitian system the coupling to the electromagnetic potential, via the minimal substitution $p \rightarrow p - eA(x)$, is induced by implementing the position-dependent phase change $\psi \rightarrow e^{i\alpha(x)} \psi$ and demanding that the transformed Schrödinger equation be unchanged. For a quasi-Hermitian system we find instead that the phase must be taken as $\alpha(X)$, where $X$ is the observable associated with $x$. The coupling to the electromagnetic vector potential thus induced is via the minimal substitution $P \rightarrow P - eA(X)$ in $h(X, P)$ written in terms of $X$ and $P$, where $P$ is the observable associated with $p$.

The matrix elements governing electromagnetic transitions from one state of the system to another depend on both $H$ and the metric $\eta$. In the special case of the Swanson Hamiltonian, when the equivalent Hermitian Hamiltonian $h$ is local, this dependence is encoded in the mass of the particle, which cannot simply be read off from $H$. Generically $h$ is not local, and the coupling is considerably more complicated.

Acknowledgments

I am grateful to the referee for pointing out a serious mistake in the first version of this paper.
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