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Gauging non-Hermitian Hamiltonians

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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 $\boldsymbol{x}$ and $\boldsymbol{p}$ appearing in the Hamiltonian, but quantities $\boldsymbol{X}$ and $\boldsymbol{P}$ 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 $\boldsymbol{X}$ implies minimal substitution in the form $\boldsymbol{P} \to \boldsymbol{P} - e\boldsymbol{A}(\boldsymbol{X})$. 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.

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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

$$H = p^2 + m^2x^2 - (\mathrm{i}x)^N \tag{1}$$

was completely real and positive for $N \geqslant 2$, 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 $\int \psi_i(-x)\psi_j(x)\,\mathrm{d}x$, 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:

$$H^\dagger = \eta H \eta^{-1}, \tag{2}$$

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

From equation (2) we can immediately deduce that

$$h \equiv \rho H \rho^{-1} \tag{3}$$

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

$$A^\dagger = \eta A \eta^{-1}, \tag{4}$$

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

$$A = \rho^{-1} a \rho. \tag{5}$$

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

$$|\psi\rangle = \rho^{-1}|\varphi\rangle. \tag{6}$$

This implies that the matrix element of an operator is

$$\langle \mathcal{O} \rangle_{ij} = \langle \psi_i | \eta \mathcal{O} | \psi_j \rangle. \tag{7}$$

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

$$\begin{aligned} \langle \psi_i | \eta A | \psi_j \rangle &= \langle \varphi_i | \rho^{-1} \eta (\rho^{-1} a \rho) \rho^{-1} | \varphi_j \rangle \\ &= \langle \varphi_i | a | \varphi_j \rangle. \end{aligned} \tag{8}$$

A very important observation is that

$$\begin{aligned} H(\boldsymbol{x}, \boldsymbol{p}) &= H(\rho \boldsymbol{X} \rho^{-1}, \rho \boldsymbol{P} \rho^{-1}) \\ &= \rho H(\boldsymbol{X}, \boldsymbol{P}) \rho^{-1} \\ &= h(\boldsymbol{X}, \boldsymbol{P}). \end{aligned} \tag{9}$$

Thus, an alternative way of finding h is to calculate the observables $\boldsymbol{X}$ and $\boldsymbol{P}$ and then rewrite $H(\boldsymbol{x}, \boldsymbol{p})$ 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 η 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 $\boldsymbol{x}$ and $\boldsymbol{X}$ (see equation (22)) were not encountered there because the calculations were done entirely within the framework of the dipole approximation, where the electromagnetic potential $\boldsymbol{A}$ is just a function of time.

2. Brief review of the standard procedure

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

$$\boldsymbol{p} \to \boldsymbol{p} - e\boldsymbol{A}. \tag{10}$$

Then under the combined transformations

$$\begin{cases} \psi \to \psi' = \mathrm{e}^{\mathrm{i}e\alpha}\psi \\ \boldsymbol{A} \to \boldsymbol{A}' = \boldsymbol{A} - \nabla\alpha, \end{cases} \tag{11}$$

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

So for a normal Hamiltonian of the form

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

the coupling to the vector potential is $-e(\boldsymbol{A}\cdot\boldsymbol{p} + \boldsymbol{p}\cdot\boldsymbol{A})/(2m)$. 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

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

as

$$w_{ij} \propto \frac{e^2}{m^2}|\langle i|p_A|j\rangle|^2 \tag{14}$$

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

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

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

so that

$$\langle i|p_A|j\rangle = \mathrm{i}m\omega_{ij}\langle i|x_A|j\rangle. \tag{16}$$

3. Quasi-Hermitian quantum mechanics

The total[1] probability is now $\langle\psi|\eta|\psi\rangle$, where η is the metric operator. This is no longer invariant under $|\psi\rangle \to \mathrm{e}^{\mathrm{i}e\alpha(\boldsymbol{x})}|\psi\rangle$, except in the special case where $\eta = \eta(\boldsymbol{x})$ so that $[\eta, \boldsymbol{x}] = 0$.

It is, however, invariant under

$$|\psi\rangle \to \mathrm{e}^{\mathrm{i}e\alpha(\boldsymbol{X})}|\psi\rangle, \tag{17}$$

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

$$\begin{aligned}\langle\psi|\eta|\psi\rangle &\to \langle\psi|\mathrm{e}^{-\mathrm{i}e\alpha(\boldsymbol{X})^\dagger}\eta\,\mathrm{e}^{\mathrm{i}e\alpha(\boldsymbol{X})}|\psi\rangle \\ &= \langle\psi|\eta|\psi\rangle,\end{aligned} \tag{18}$$

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

$$|\varphi\rangle \to \rho\mathrm{e}^{\mathrm{i}e\alpha(\boldsymbol{X})}\rho^{-1}|\varphi\rangle = \mathrm{e}^{\mathrm{i}e\alpha(\boldsymbol{x})}|\varphi\rangle. \tag{19}$$

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

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

The minimal substitution we require, in $h(\boldsymbol{X}, \boldsymbol{P})$, is then

$$\boldsymbol{P} \to \boldsymbol{P} - e\boldsymbol{A}(\boldsymbol{X}), \tag{21}$$

with the combined transformations

$$\begin{cases}|\psi\rangle \to |\psi'\rangle = \mathrm{e}^{\mathrm{i}e\alpha(\boldsymbol{X})}|\psi\rangle \\ \boldsymbol{A}(\boldsymbol{X}) \to \boldsymbol{A}'(\boldsymbol{X}) = \boldsymbol{A}(\boldsymbol{X}) - \nabla_{\boldsymbol{X}}\alpha(\boldsymbol{X}).\end{cases} \tag{22}$$

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

$$\mathrm{e}^{-\mathrm{i}e\alpha(\boldsymbol{X})}(\boldsymbol{P} - e\boldsymbol{A}')\,\mathrm{e}^{\mathrm{i}e\alpha(\boldsymbol{X})} = \boldsymbol{P} - e\boldsymbol{A}.$$

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

$$\boldsymbol{A}(\boldsymbol{\xi}, t) = \int \mathrm{d}\omega\, \tilde{\boldsymbol{A}}(\omega)\,\mathrm{e}^{\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{\xi} - \omega t)} + c.c. \tag{23}$$

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

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

$$\begin{aligned}w_{ij} &\propto \frac{e^2}{\mu^2}|\langle\psi_i|\eta P_A|\psi_j\rangle|^2 \\ &= \frac{e^2}{\mu^2}|\langle\varphi_i|p_A|\varphi_j\rangle|^2,\end{aligned} \tag{24}$$

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

$$\langle\varphi_i|p_A|\varphi_j\rangle = \mathrm{i}\mu\omega_{ij}\langle\varphi_i|x_A|\varphi_j\rangle. \tag{25}$$

[1] Note that the probability density $\varrho(\boldsymbol{x}) = \langle\psi|\rho|\boldsymbol{x}\rangle\langle\boldsymbol{x}|\rho|\psi\rangle$ 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

$$H = \frac{\boldsymbol{p}^2}{2m_1} + \frac{1}{2}\mathrm{i}\omega\varepsilon\{x_r,\, p_r\} + \frac{1}{2}m_2\omega^2\boldsymbol{x}^2, \tag{26}$$

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

$$h(\boldsymbol{x},\boldsymbol{p}) = \frac{\boldsymbol{p}^2}{2\mu} + \frac{1}{2}\mu\omega^2\boldsymbol{x}^2. \tag{27}$$

(i) $Q = Q(\boldsymbol{x}) = \varepsilon m_1\omega\boldsymbol{x}^2$. This amounts to completing the square as

$$H = \frac{(\boldsymbol{p}+\mathrm{i}\varepsilon m_1\omega\boldsymbol{x})^2}{2m_1} + \frac{1}{2}m_1\omega^2\boldsymbol{x}^2, \tag{28}$$

so that $\boldsymbol{X} = \boldsymbol{x}$, while $\boldsymbol{P} = \boldsymbol{p} + \mathrm{i}\varepsilon m_1\omega\boldsymbol{x}$. Thus in this case

$$h(\boldsymbol{x},\boldsymbol{p}) = \frac{\boldsymbol{p}^2}{2m_1} + \frac{1}{2}m_1\omega^2\boldsymbol{x}^2, \tag{29}$$

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

$$-\frac{e}{2m_1}(\boldsymbol{A}\cdot\boldsymbol{P} + \boldsymbol{P}\cdot\boldsymbol{A}) = -\frac{e}{2m_1}\left[(\boldsymbol{A}\cdot\boldsymbol{p} + \boldsymbol{p}\cdot\boldsymbol{A}) + \mathrm{i}\varepsilon m_1\omega(\boldsymbol{A}\cdot\boldsymbol{x} + \boldsymbol{x}\cdot\boldsymbol{A})\right]. \tag{30}$$

The required matrix element,

$$\langle\psi_i|\eta P_A|\psi_j\rangle = \langle\varphi_i|p_A|\varphi_j\rangle, \tag{31}$$

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

(ii) $Q = Q(\boldsymbol{p}) = -\varepsilon\boldsymbol{x}^2/(m_2\omega)$.
This amounts to completing the square instead as

$$\begin{aligned} H &= \frac{\boldsymbol{p}^2}{2m_2} + \frac{1}{2}m_2\omega^2\left(\boldsymbol{x} + \frac{\mathrm{i}\varepsilon\boldsymbol{p}}{m_2\omega}\right)^2 \\ &\equiv \frac{\boldsymbol{P}^2}{2m_2} + \frac{1}{2}m_2\omega^2\boldsymbol{X}^2, \end{aligned} \tag{32}$$

so that $\boldsymbol{P} = \boldsymbol{p}$, while $\boldsymbol{X} = \boldsymbol{x} + \mathrm{i}\varepsilon\boldsymbol{p}/(m_2\omega)$. Thus in this case

$$h(\boldsymbol{x},\boldsymbol{p}) = \frac{\boldsymbol{p}^2}{2m_2} + \frac{1}{2}m_2\omega^2\boldsymbol{x}^2, \tag{33}$$

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

$$-\frac{e}{2m_2}(\boldsymbol{A}\cdot\boldsymbol{P} + \boldsymbol{P}\cdot\boldsymbol{A}) = -\frac{e}{2m_2}(\boldsymbol{A}\cdot\boldsymbol{p} + \boldsymbol{p}\cdot\boldsymbol{A}). \tag{34}$$

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 $p = \mathrm{i}\sqrt{(m_2\omega/2)}(a^\dagger - a)$.

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 η 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

$$H = \tfrac{1}{2}(p^2 + x^2) + \mathrm{i}gx^3, \tag{35}$$

we have [13]

$$Q = -g\left(\tfrac{4}{3}p^3 + 2xpx\right) + O(g^3), \tag{36}$$

which gives rise [26, 27] to the observables

$$\left.\begin{aligned} X &= x + \mathrm{i}g(x^2 + 2p^2) + g^2(-x^3 + 2pxp) \\ P &= p - \mathrm{i}g(xp + px) + g^2(2p^3 - xpx) \end{aligned}\right\} + O(g^3). \tag{37}$$

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]

$$h(x, p) = \tfrac{1}{2}(p^2 + x^2) + 3g^2\left(\tfrac{1}{2}x^4 + S_{2,2}(x, p) - \tfrac{1}{6}\right) + O(g^4), \tag{38}$$

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

From equation (38), we see that the minimal substitution $P \to P - eA(X)$ 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

$$\psi_i(x) = \psi_i^0(x) + g\sum_{j\neq i}\left\langle\psi_j^0\middle|\mathrm{i}x^3\middle|\psi_i^0\right\rangle\psi_j^0(x) + O(g^2). \tag{39}$$

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

The matrix elements governing electromagnetic transitions from one state of the system to another depend on both H and the metric η. 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.

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