Energy-dependent Hamiltonians and their pseudo-Hermitian interpretation

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Abstract

The concept of energy-dependent forces in quantum mechanics is re-analysed. We suggest a simplification of their study via the representation of each self-adjoint and energy-dependent Hamiltonian $H = H(E)$ with real spectrum by an auxiliary non-Hermitian operator $K$ which remains energy-independent. Practical merits of such an approach to the Schrödinger equations with energy-dependent potentials are illustrated using their quasi-exactly solvable example.

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1 Introduction

An introduction of phenomenological potentials which vary with the energy of the system proved useful in atomic, molecular as well as nuclear and particle physics. Quite often, a certain energy-dependence of the parameters results from their physical meaning – the best known illustrations are provided by the Klein-Gordon equation (where the potential happens to be a quadratic function of the energy [1]) and by the Bethe-Salpeter equations (where the relativistic kinematics is partially incorporated in the description of the two-body systems [2]). Another elementary sample of such a motivation of the work with an energy-dependent Hamiltonian $H = H(E)$ may be found outlined here in Appendix A.

In another group of phenomenological models, the energy-dependence in the “realistic” Hamiltonians $H = H(E)$ remains artificial and serves as a mere ad hoc simulation of certain complicated and not too well understood effects within a sufficiently transparent model. In the similar pragmatic simulations, the fit of the experimental data is often unexpectedly successful [3]. Although the consequent theoretical foundation of the explicit construction of the energy-dependent components of the interactions may be missing, the procedure of the (variational or numerical) fitting itself usually offers a useful guidance towards an optimal choice of the form of $H = H(E)$ [4]. In such a situation, one can only regret that the merits of the simplified physics are sometimes counterbalanced by perceivable growth of mathematical difficulties. In this sense, the energy-dependent forces attract attention as a purely mathematical challenge [5].

From an abstract point of view, one of the most common theoretical sources of the energy-dependent potentials may be sought in a tentative projection of wavefunctions $|\Psi\rangle$ on a certain “model” subspace of Hilbert space. After such a projection the unitarity of the time evolution is broken of course. The microscopic and energy-independent Hamiltonians $H$ are being replaced by their so called effective reduced forms $H_{\text{eff}} = H_{\text{eff}}(E)$ [6]. Some of the key technical details of such a re-definition of the system may be found summarized in Appendix B. Within its overall framework, the development of a sufficiently flexible treatment of specific models seems to be an urgent task. For this reason, we decided to re-analyze here the general Schrödinger energy-dependent bound-state problem

$$H(E_\alpha)|\phi_\alpha\rangle = E_\alpha|\phi_\alpha\rangle \quad (1)$$

keeping in mind, first of all, the new possibilities which were opened by the recent growth of interest in the systems where the time evolution need not necessarily be purely unitary [7].

In section 2 we shall start our considerations by summarizing a few known facts about the models with the general $H = H(E)$. We shall show there how the major part of the difficulties introduced by the energy-dependence of the Hamiltonian may be formally eliminated by the introduction of a suitable bi-orthogonal basis. In the new language, the enhanced flexibility of the basis
becomes reflected by the possibility of a modification of the scalar product in Hilbert space. In this manner, one may even try to control the physical contents of the theory [8].

In section 3 we shall pay attention to the demonstration of the applicability of the formalism of section 2 to a specific class of the energy dependent Hamiltonians. We decided to pay attention to the next-to-solvable potentials which form the so called quasi-exactly solvable (QES, [9]) family. A sketchy review of their basic properties is presented as a separate Appendix C. The main consequence of our present energy-dependent re-interpretation of the popular QES Hamiltonians may be seen in the establishment of their new role of a source of non-orthogonal bases in Hilbert space.

In the short summary of our effort in section 4 we shall emphasize that our Appendices A and B stressed the immediate physical and pragmatic appeal of the energy-dependence in \( H = H(E) \). Our subsequent choice of the QES illustrations of Appendix C may then play the role of their sophisticated and more flexible mathematical complement, showing that although our present interpretation of the effective and other energy-dependent Hamiltonians seems to be a fairly universal recipe, its various implementations may differ in the degree of the insight they are able to offer. In this sense, any continuation of their study would be welcome.

## 2 Mathematical consequences of the energy-dependence of \( H(E) \)

In the spirit of the recent review [10], many (though not all of the) mathematical puzzles related to eq. (1) may be clarified when one contemplates an auxiliary family of the Hermitian Hamiltonians \( H(z) \) which depend on a real parameter \( z \). Let this value be temporarily disentangled from the energy eigenvalues. Then, all the Hamiltonians \( H = H(z) \) may be assigned their respective spectral representations,

\[
H(z) = \sum |n(z)\rangle E_n(z) \langle n(z)|.
\]

Only within such a broader framework, we impose the constraint \( E_n(z) = z \) at the very end of all the necessary constructions and for all the indices \( n \). The latter constraint may happen to be satisfied at an empty or non-empty set of roots \( z = z_1(n), z_2(n), \ldots, z_{m(n)}(n) \). With their knowledge at our disposal (see an elementary example in Appendix A), one may pick up a suitable subset \( A \) of the “allowed” multiindices \( \alpha = (n, i) \in A \) and abbreviate \( z_i(n) = E_\alpha \) and \( |n(z_i)\rangle = |\phi_\alpha\rangle \). By such a construction we arrive at a formal solution of our energy-dependent problem (1) under very general assumptions and/or for the various particular choices of the parameter-dependence in \( H = H(z) \).
2.1 Non-orthogonal wave functions

There exist several difficulties which arise in connection with the generalized Schrödinger equation (1). First of all, the standard orthogonality relations between the separate bound states are lost. Even though the norm of each state may be fixed via a suitable re-scaling of $||\phi_\alpha|| = \langle \phi_\alpha | \phi_\alpha \rangle$, it is necessary to know and evaluate also all the off-diagonal non-vanishing overlaps

$$\langle \phi_\alpha | \phi_\beta \rangle = R_{\alpha,\beta}, \quad \alpha, \beta \in A.$$  \hspace{1cm} (2)

Under certain (nontrivial) assumptions this matrix has an inverse which enters the decomposition of the identity projector

$$\tilde{I} = \sum_{\alpha,\beta \in A} |\phi_\alpha\rangle \left( R^{-1} \right)_{\alpha,\beta} \langle \phi_\beta |.$$  \hspace{1cm} (3)

The practical value of such a completeness of our basis (or, at least, its completeness in the whole “relevant” Hilbert space) is significantly lowered by the non-diagonality of the matrix $R$. The sufficiently precise evaluation of this matrix and of its inverse $R^{-1}$ may happen to become prohibitively time-consuming. The practical applicability of the completeness relations (3) with a non-diagonal $R$ is further lowered in all the applications of the energy-dependent potentials which would rely upon a purely numerical solution of eq. (1). Within the framework of our present considerations, at least a partial return to semi- and non-numerical techniques will be advocated, therefore.

2.2 Biorthogonal basis in the Hilbert space

An inspection of the action of our family of the operators $H(E)$ on the separate elements of our basis set of kets $|\phi_\alpha\rangle \equiv |n(z_i)\rangle$ with $\alpha = (n, i) \in A$ reveals that the new operator $K$ defined by its generalized spectral representation

$$K = \sum_{\alpha,\beta \in A} |\phi_\alpha\rangle E_\alpha \left( R^{-1} \right)_{\alpha,\beta} \langle \phi_\beta |$$  \hspace{1cm} (4)

may be interpreted as equivalent to our Hamiltonian family whenever their action within our “allowed” space is concerned,

$$K |\phi_\alpha\rangle = E_\alpha |\phi_\alpha\rangle.$$  \hspace{1cm} (5)

By construction, the new operator $K$ is energy-independent (i.e., no nonlinearity is encountered) and non-Hermitian (this is the price we decided to pay). The latter property of $K \neq K^\dagger$ is unexpected but its origin is clear after we abbreviate

$$\langle \langle \phi_\alpha | = \sum_{\beta \in A} \left( R^{-1} \right)_{\alpha,\beta} \langle \phi_\beta |$$  \hspace{1cm} (6)

and re-interpret the above eq. (4) as a diagonal-type spectral representation of our auxiliary non-Hermitian quasi-Hamiltonian,

$$K = \sum_{\alpha \in A} |\phi_\alpha\rangle E_\alpha \langle \langle \phi_\alpha |.$$  \hspace{1cm} (7)
The simplicity and transparency of such a notation is based on the consequent use of the double-bra symbol for the left eigen-vectors. This convention introduces a basis which happens to be, by construction, bi-orthogonal,

\[ \langle \langle \phi_\alpha | \phi_\beta \rangle \rangle = \delta_{\alpha, \beta}, \quad \alpha, \beta \in A. \]  (8)

Similarly, the abbreviated eq. (3),

\[ \hat{I} = \sum_{\alpha \in A} |\phi_\alpha\rangle \langle \langle \phi_\beta| \]  (9)

represents the maximally compact form of completeness relations.

### 2.3 Pseudo-Hermiticity

In a way paralleling the recent interest in certain specific non-Hermitian (for example, $\mathcal{PT}$-symmetric) systems with real spectra [11], we may expect that there exists an invertible and Hermitian “auxiliary metric” operator $\eta = \eta^\dagger$ such that our new operators $K \neq K^\dagger$ will satisfy the following quasi- or pseudo-Hermiticity relations

\[ K^\dagger \eta = \eta K \]  (10)

[7]. After the insertion of an ansatz

\[ \eta = \sum_{\alpha, \beta \in A} |\phi_\alpha\rangle \langle \langle \phi_\beta| U_{\alpha, \beta} \langle \langle \phi_\beta|, \]  (11)

relation (10) degenerates to the mere algebraic equation

\[ E_\alpha U_{\alpha, \beta} = U_{\alpha, \beta} E_\beta, \quad \alpha, \beta \in A. \]  (12)

It implies that under the non-degeneracy assumption $E_\beta \neq E_\alpha$ for $\alpha \neq \beta$, all the off-diagonal elements of $U$ must vanish while the diagonal elements $U_{\alpha, \alpha} = d_\alpha = d_\alpha^* \neq 0$ remain variable. This defines the large set of the metrics

\[ \eta = \sum_{\alpha \in A} |\phi_\alpha\rangle d_\alpha \langle \langle \phi_\alpha| \]  (13)

which are self-adjoint and invertible,

\[ \eta^{-1} = \sum_{\alpha \in A} |\phi_\alpha\rangle d_\alpha^{-1} \langle \langle \phi_\alpha|. \]  (14)

In this language each energy-dependent Hamiltonian $H(E)$ may be better understood via its $\eta$–pseudo-Hermitian representation $K$ using an arbitrary auxiliary metric $\eta$ defined by eq. (13). Its role becomes clear after we introduce the Hermitian conjugate of eq. (5), $\langle \phi_\alpha| K^\dagger = \langle \phi_\alpha| E_\alpha^*$. At the real energies $E_\alpha^* = E_\alpha$ it enables us to re-write this equation in the spirit of eq. (10),

\[ \langle \langle \phi_\alpha| \eta \rangle \rangle K = \langle \langle \phi_\alpha| \eta \rangle \rangle E_\alpha. \]
The non-degeneracy assumption immediately implies that
\[ \langle \phi_{\alpha} | = \text{const} \langle \phi_{\alpha} | \eta. \tag{15} \]

We see that the knowledge of the (non-singular) operator \( \eta \) is, up to a re-normalization (15), equivalent to the knowledge of the matrix \( R \) [cf. eq. (6)]. The main meaning of the use of \( \eta \) follows from the fact that in the hypothetical Hilbert space where the metric would be given by the operator \( \eta \), the operator \( K \) would become, in the light of eq. (10), “Hermitian”.

3 Illustration: Partially solvable potentials

The Hautot’s QES model (30) of Appendix C is an example of the well-motivated choice of the quantum system where, by definition, a suitable selection of the energy-dependent Hamiltonian \( H(E) = H_F + F W \) [with \( W = 1/r \) and \( F = F^{(QES)}(E) \)] is dictated by the feasibility of the evaluation of the overlaps (2). This means that the selected bound states \( \psi_{n,\ell}^{(QES)}(r) \) remain represented by polynomials of a finite degree \( N \geq n \). While we may drop the information about the value of the nodal count \( n \) and of the angular momentum \( \ell \) as redundant, we still have to keep in mind our choice of the subscript \( j \) which numbers all the eligible QES charges \( e = F_{N,j} \) with \( j = 0,1,\ldots,N \). This allows us to compactify our notation, \( \psi_{n,\ell} \equiv \psi_{n,\ell,N,j} \to |N,j) \), with the main purpose of using a suitable subset of the overcomplete family of these QES bound states as a non-orthogonal basis in the physical Hilbert space.

3.1 QES basis and orthogonality-type relations

Let us re-write eq. (30) as the following set of equations in the Dirac’s bra-ket notation,
\[ H(0) |M,k\rangle + W |M,k\rangle F_{M,k} = |M,k\rangle E_M \tag{16} \]
\[ k = 1,2,\ldots,L(M), \quad M = 0,1,\ldots. \]

In our particular example we shall prefer the one-charge-per-energy choice of \( L(M) = 1 \). The left and right eigenstates do not differ (or at least need not differ – see the non-Hermitian generalization of eq. (30) in ref. [13]). Thus, we may complement eq. (16) by its conjugate counterpart
\[ \langle N,j | H(0) + F_{N,j} \langle N,j |W = E_N \langle N,j |, \tag{17} \]
\[ j = 1,2,\ldots,L(N), \quad N = 0,1,\ldots. \]

There is no a priori reason for an orthogonality between multi-indexed bra vectors \( \langle N,k | \equiv \langle A | \) and ket vectors \( |N',k'| \equiv |b) \). Their overlaps \( R_{A,b} = \langle A | b) \) form a non-diagonal matrix (2) in general. We only have to
assume that this matrix remains invertible. Only in such a case we may employ eq. (3) and introduce the identity projector

\[ I = \sum_{a \in J_{ket}, B \in J_{bra}} |a\rangle \left( R^{-1} \right)_{a,B} \langle B | . \]  

(18)

As long as equations (16) and (17) share all their eigen-energies and eigen-charges, we may write down the following two alternative projected equations

\[ \langle N, j | H(0) | M, k \rangle = \langle N, j | M, k \rangle E_M - \langle N, j | W | M, k \rangle F_{M,k} \]  

(19)

\[ \langle N, j | H(0) | M, k \rangle = E_N \langle N, j | M, k \rangle - F_{N,j} \langle N, j | W | M, k \rangle \]  

(20)

with \((N, j) \in J_{bra}\) and \((M, k) \in J_{ket}\). Their subtraction gives the constraint

\[ (F_{M,k} - F_{N,j}) \langle N, j | W | M, k \rangle = (E_M - E_N) R_{(N,j),(M,k)} . \]  

(21)

This relation may be understood as the energy-dependence-related generalization of the usual orthogonality of the eigenvectors. All the matrix elements of \(H_0\) dropped out. For the so called Sturmian multiplets (i.e., within each subspace where \(M = N\)), the left-hand-side expression must be a diagonal matrix with respect to its second indices \(j\) and \(k\). For our present purposes we shall abbreviate \(\langle N, j | W | N, j \rangle \equiv w_{N,j}\). All the other matrix elements of \(W\) may be treated as defined by eq. (21). Once we know all the overlap matrix \(R\), just the diagonal elements \(w_{N,j}\) remain unspecified and, whenever needed, their values must be generated by an independent calculation.

### 3.2 Perturbations and non-QES states

Whenever we leave the safe QES domain and contemplate the more general bound-state problem (30) at a generic charge \(F \neq F^{(QES)}\), we encounter a non-elementary (i.e., numerical or perturbative) diagonalization of Schrödinger equation

\[ \left[ H(0) + FW \right] |\Psi \rangle = E(F) |\Psi \rangle , \]

Assuming that \(F \neq F^{(QES)}\) and using eq. (18) we may insert

\[ |\Psi \rangle = \sum_{a \in J_{ket}, B \in J_{bra}} |a\rangle \left( R^{-1} \right)_{a,B} \langle B |\Psi \rangle = \sum_{a \in J_{ket}} |a\rangle h_a \]

and arrive at the infinite-dimensional linear algebraic equation

\[ \sum_{b \in J_{ket}, c \in J_{bra}} \langle A | H(F) | b \rangle R_{b,c} \langle C |\Psi \rangle = E \langle A |\Psi \rangle, \quad A \in J_{bra} \]

i.e., matrix equation

\[ \mathbf{Z}(E, F) \mathbf{h} = 0, \]  

(22)

where

\[ \mathbf{Z}_{A,b}(E, F) = \langle A | H(0) | b \rangle - E \langle A | b \rangle + F \langle A | W | b \rangle . \]
In the preparatory step we must evaluate all the input matrix elements. This step is usually the most time-consuming part of the algorithm. Fortunately, it can quite efficiently be optimized, in the present QES setting, by the use of all the available orthogonality-type identities. Thus, we recall eq. (20) and eliminate all the matrix elements of $H^{(0)}$. This means that in eq. (22) the costly input information becomes reduced to the mere evaluation of the matrix elements of the Coulombic $W(r) = 1/r$,

$$Z_{A\beta}(E, F) = (F - F_A) \langle A | W | b \rangle - (E - E_A) \langle A | b \rangle.$$ 

In the second step we keep $M \neq N$ (i.e., we stay out of the Sturmian subspaces or diagonal blocks in the matrix $Z$) and postulate the absence of a random degeneracy of charges. This means $F_{M,k} \neq F_{N,j}$ so that we are permitted to re-arrange the orthogonality-like relation (21) into definition representing a further vital reduction of the necessity of the excessive numerical integrations,

$$\langle N, j | W | M, k \rangle = \frac{E_M - E_N}{F_{M,k} - F_{N,j}} R_{(N,j),(M,k)}, \quad M \neq N.$$ 

The final, maximally reduced form of our linear Schrödinger non-QES algebraic problem then reads

$$w_{N,j} h_{N,j} + \sum_{K(\neq N),p} \frac{E_N - E_K}{F_{N,j} - F_{K,p}} R_{(N,j),(K,p)} h_{K,p} =$$

$$= \frac{E - E_N}{F - F_{N,j}} \sum_{M,k} R_{(N,j),(M,k)} h_{M,k} ,$$

$$j = 1, 2, \ldots, L(N), \quad N = 0, 1, \ldots .$$

Summarizing, any numerical or perturbative solution of this algebraic system requires just the knowledge of the overlaps $R$ and of the single array of the special diagonal Coulombic matrix elements $w_{N,j}$.

### 4 Summary

Whenever we try to parallel the orthogonality proof as it works in the standard energy-independent cases [1], we merely obtain a very formal relation [10]

$$\langle \phi_\beta | [H(E_\beta) - H(E_\alpha)] | \phi_\alpha \rangle = (E_\beta - E_\alpha) \langle \phi_\beta | \phi_\alpha \rangle .$$  

(23)

In spite of its comparative weakness (and in spite of its virtually negligible role in the purely theoretical considerations of section 2 above), we succeeded in demonstrating that its contents remain non-empty and that its practical implications may be very useful. First of all, this “weak orthogonality” relation has been shown to imply that whenever the energies coincide, $E_\beta = E_\alpha$, the self-overlaps $\langle \phi_\beta | \phi_\alpha \rangle$ remain undetermined. Less trivial is the observation that
for the non-degenerate spectra with $E_\beta \neq E_\alpha$, formula (23) admits the non-vanishing of the overlaps $R_{\beta,\alpha}$ and relates their values to the left-hand-side matrix elements. This is one of the key consequences of eq. (23), with practical merits which vary with the explicit form of $E$—dependence of the Hamiltonian operator $H(E)$. This point of view has been more explicitly supported by our illustrative energy-dependent re-interpretation of the current and popular QES examples.

In the broader context involving the generic energy-dependence of virtually all the effective Hamiltonians we re-interpreted all the energy-dependent (i.e., in a way, non-linear) Schrödinger equations (1) as equivalent to the non-Hermitian but, by construction, fully linear algebraic eigenvalue problems (5). Such a step has been shown to facilitate our understanding of the theory as well as of the deeper mathematical nature of our original equation. The related possible scalar-product re-interpretations may make it more relevant in the context of physics, along the lines discussed much more thoroughly in the review of quasi-Hermiticity [8] as well as in its more recent continuations [7, 12].

In the future extensions of our present note one could select several interesting directions. Firstly, whenever the deviation $\lambda = F - F^{(QES)}$ of the charges remains sufficiently small, one feels tempted to construct the spectra $E = E(\lambda)$ perturbatively, in the form of a power series in $\lambda$. This could complement the existing QES-related perturbative studies based on different principles [14]. In a broader setting, our present recommendation of the use of unusual biorthogonal bases might also lead to a direct new progress in the area of perturbation theory itself.

As we already emphasized, the diagonalization of an operator which depends on its own eigenvalues is not, strictly speaking, a linear problem. In this sense the incompletely elementary QES class seems particularly suitable as an illustrative example at an introductory stage. In a way emphasized in ref. [10], all continuations of such a direction of development will be well motivated since even many apparently elementary energy-dependent interactions fail to admit a non-numerical treatment. Thus, a systematic classification of all the solvable cases would be of a paramount theoretical as well as practical importance.

Last but not least, we should not forget that also the recently popular replacements of the Hermitian $H = H(E)$ by their non-Hermitian descendants with real spectra [13] could offer another inspiration for a continuation of our present study.

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Appendix A: Energy dependence with an origin in physics

Under the influence of experimental data, even such a certainty as the energy-independence of the mass of a particle may require a critical re-evaluation. Such a critique finds its support in the decays of mesons \( K^+ \) where, traditionally, the vector-meson dominance offers a parameter-free explanation of the overall character of the data [15]. Still, the standard choice of the form factor \( F(t) \) of the \( \rho \) meson leads to a perceivable discrepancy between the parallel descriptions of the decays \( K^+ \to \pi^+\mu^+\mu^- \) and \( K^+ \to \pi^+e^+e^- \). The remedy of this discrepancy has been found [16] in the variability of the dilepton mass \( M = t_{\text{phys}} \) which is perceivably different in the above two processes. In accord with Isgur et al [17], one must work with the running mass \( m_{\rho}^2 \to \tilde{m}_{\rho}^2(t) \) in

\[
F(t) = \frac{m_{\rho}^2}{m_{\rho}^2 - t}. \tag{24}
\]

The variability of the running mass with the cross-channel energy \( t \) is necessary for a consistent interpretation of the analyticity of the propagators. Explicit calculations lead to the further modification of eq. (24) and an imaginary shift appears in

\[
F(t) = \frac{\tilde{m}_{\rho}^2(0)}{m_{\rho}^2(t) - t - i m_{\rho} \Gamma(t)}. \tag{25}
\]

The determination of the “realistic” running-mass function \( \tilde{m}_{\rho}^2(t) \) represents the main and challenging theoretical problem [18]. In the phenomenological considerations of ref. [16], a satisfactory agreement between the experiment and its description has been achieved via a selfconsistent determination of the energy dependence of the mass \( \tilde{m}_{\rho}^2(t) \) near the phenomenologically relevant dilepton invariant energies \( t \approx E_{\mu^+\mu^-} \) and \( t \approx E_{e^+e^-} \).

For a schematic clarification of some of the basic features of the above-mentioned energy dependence, the most elementary explicit toy model may be used and studied. Once we contemplate the Schrödinger equation in one dimension (in units \( \hbar = 2 \)) with the harmonic oscillator interaction,

\[
-\frac{1}{m(E)} \frac{d^2}{dr^2} \Psi(r) + r^2 \Psi(r) = E \Psi(r) \tag{26}
\]

the effects of the variability of the mass may be mimicked by an arbitrary simulation of its energy-dependence. For the most elementary illustrative ansatz

\[
m(E) = A^2 (E - E_0)^2, \tag{27}
\]

a re-scaling of eq. (26) leads to the new bound-state problem with the spectrum determined by the closed formulae

\[
E = \begin{cases} 
E_n^{(+)} = E_0 + \sqrt{E_0^2 + \frac{8n+1}{A}}, & n = 0, 1, \ldots, \\
E_n^{(-)} = E_0 - \sqrt{E_0^2 - \frac{8n+1}{A}}, & n = 0, 1, \ldots, n_{\text{max}}.
\end{cases} \tag{28}
\]
The latter two sets are finite and exist only for $AE_0^2 \geq 4$. The new levels emerge at each new $n_{\text{max}} = \text{entier}[(AE_0^2 - 4)/8]$. The message of this test is quite persuasive – the structure of the spectrum may be modified thoroughly even by a very innocent-looking energy-dependent term.

Appendix B. An artificial energy dependence originating from the model-space projections

One of the most usual approaches to the realistic Schrödinger equation is variational. Typically, people start from a suitable microscopic Hamiltonian. Such a quantum model is usually constructed on the basis of the correspondence principle. As a rule, it is energy-independent and complicated, its handling proves time-consuming and its numerical diagonalization appears distressingly slow. These difficulties force us to reduce the Hilbert space to a smaller subspace. This means that we must replace the original microscopic bound-state problem by its model-space version or reduction. As long as our attention is merely paid to the certain “most relevant” subsets of all the possible degrees of freedom, an abstract algebraic reformulation of the above statement may be based on a split of the identity operator $I$ into the projector $P$ (on the manageable subspace) and its complement $Q = I - P$. The exact and complete Schrödinger equation $H |\Psi\rangle = E |\Psi\rangle$ acquires the two-by-two partitioned form

$$P (H - E) P |\Psi\rangle + P (H - E) Q |\Psi\rangle = 0,$$

$$Q (H - E) P |\Psi\rangle + Q (H - E) Q |\Psi\rangle = 0.$$

The energy-dependence emerges when we eliminate the component $Q |\Psi\rangle$ of the wave function from the second row and insert it in the first equation. The resulting explicit form of the reduced problem,

$$P (H - E) P |\Psi\rangle + P H Q \left[ \frac{Q}{Q (H - E) Q} \right] Q H P |\Psi\rangle = 0,$$

may be understood as a projected or “effective” Schrödinger equation

$$H_{\text{eff}} |\Psi_{\text{eff}}\rangle = E |\Psi_{\text{eff}}\rangle . \tag{29}$$

The value of the energy remains unchanged while the wave function is reduced to a subspace, $|\Psi_{\text{eff}}\rangle = P |\Psi\rangle$. In general, the energy dependence appearing in the effective Hamiltonian $H_{\text{eff}}(E)$ is very complicated.

Appendix C. Partial solvability re-interpreted as an energy-dependence

For the sake of definiteness, let us pick up the two most elementary and popular QES examples, viz., the Hautot’s [19] shifted harmonic oscillator defined at
certain exceptional charges $F$ only,

\[
\left[ \frac{d^2}{dr^2} + \frac{\ell(\ell + 1)}{r^2} + \frac{F}{r} + f r + r^2 \right] \psi_{n,\ell}(r) = E_{n,\ell} \psi_{n,\ell}(r)
\]  

(30)

and the sextic oscillator of Singh et al [20] with certain exceptional “spring” constants $A$,

\[
\left[ -\frac{d^2}{dr^2} + \frac{\ell(\ell + 1)}{r^2} + A r^2 + a r^4 + r^6 \right] \phi_{n,\ell}(r) = \varepsilon_{n,\ell} \phi_{n,\ell}(r).
\]  

(31)

Both these models may be made mathematically completely equivalent via a suitable change of the variables [21] but each of them plays a slightly different role in physics. We may index their bound states in the same manner, viz., by their angular momenta $\ell$ and by the number $n$ of nodes in the wave function.

In both cases, the essence of the QES construction lies in the requirement that the Taylor series for the bound-state wave functions terminate and become proportional to a polynomial of degree $N$. In the former, Coulombic case (30) this implies that the exceptional QES energy becomes fixed and remains unique and charge-independent. Thus, the spectrum will be numbered by $N$ and coincides, incidentally, with the equidistant energies of the pure harmonic oscillator. In contrast, at each $N$ there exist as many as $N + 1$ different QES-compatible values of the charge $F = F_{(N,j)}$, with $j = 0, 1, \ldots, N$ (see [19] for details). At each energy, the admissible value of the charge becomes unique only after a particular choice of the index $j = j_0$ which may vary with the changes of the second index $N$. Thus, the QES charge may be understood as an energy-dependent quantity, $F = F_{QES}(E)$.

In the latter, sextic illustrative example (31), the roles of coupling and energy become interchanged [22]. At any angular momentum $\ell$, the main quantum number $N$ now counts the eligible couplings $A = A_N$. The related $(N+1)$—plets of the admissible energy values $\varepsilon_{n,j}$ must be generated by the specific algorithm of ref. [20]. Although the resulting overall energy-dependence pattern remains very similar, its practical aspects become less comfortable since up to the exceptional large—$\ell$ limit [23], the correspondence between $E$ and $N$ acquires an awkward numerical character at the larger $N$. 

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