Solvable relativistic quantum dots with vibrational spectra

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Abstract

For Klein-Gordon equation a consistent physical interpretation of wave functions is reviewed as based on a proper modification of the scalar product in Hilbert space. Bound states are then studied in a deep-square-well model where spectrum is roughly equidistant and where a fine-tuning of the levels is mediated by $\mathcal{PT}$-symmetric interactions (composed of imaginary delta functions) which mimic creation/annihilation processes.
1 Klein-Gordon equation

1.1 Pseudo-Hermitian Feshbach-Villars Hamiltonian

As long as the most common relativistic Klein-Gordon (KG) operators are partial differential operators of the second order with respect to time, the time evolution of the wave functions $\Psi^{(KG)}(x,t)$ must be studied together with their first time derivatives $i \partial_t \Psi^{(KG)}(x,t)$. After the routine Fourier transformation we arrive at the Feshbach-Villars (FV, [1]) non-Hermitian eigenvalue problem

$$\hat{H}^{(FV)} |\psi\rangle = E |\psi\rangle, \quad \hat{H}^{(FV)} = \begin{pmatrix} 0 & \hat{h}^{(KG)} \\ 1 & 0 \end{pmatrix}$$

(1)

where the two wave-function components may be marked as $|D\rangle$ (="down component") and $|U\rangle$ (="up component"). For the description of the bound states in one dimension the two-by-two partitioning in (1) allows us to extract $|U\rangle = E |D\rangle$ and to replace our Klein-Gordon equation by its reduced form

$$\hat{h}^{(KG)} |D_n\rangle = \varepsilon_n |D_n\rangle, \quad n = 1, 2, \ldots$$

(2)

with squared energy $E^2$ abbreviated as $\varepsilon$ and with the “large” Hilbert space $\mathcal{H}$ of kets $|\psi\rangle$ reduced to the “smaller” Hilbert space $\mathcal{H}_{(c)}$ of the curly-ket “down” components $|D_n\rangle$ [2].

1.2 Biorthogonal bases

The “right” eigenkets $|D_n\rangle$ will not carry all information about $\hat{h}^{(KG)}$ whenever $[\hat{h}^{(KG)}] \neq [\hat{h}^{(KG)}]^\dagger$. Then, the parallel Schrödinger-type problem generates different eigenkets marked by the double curly ket symbol. The latter sequence may be re-read as the left eigenvectors of our original operator $\hat{h}^{(KG)}$, related to the same (by assumption, real) eigenvalues $\varepsilon_n \equiv \kappa_n^2$,

$$\{ \{L_n| \hat{h}^{(KG)} = \kappa_n^2 \{ \{L_n|, \quad n = 1, 2, \ldots \}$$

(3)
It is well known that the set of the bras \( \{L_n\} \) and kets \( |D_n\rangle \) is bi-orthogonal \(^2\),

\[
\{L_m|D_n\rangle\} = \begin{cases} 
0 & \text{for } m \neq n, \\
\varrho_n & \text{for } m = n,
\end{cases}
\]

and that it forms, usually, a basis in the infinite-dimensional Hilbert space \( \mathcal{H}(c) \).

Then, we may decompose the unit operator and/or derive the bi-orthogonal spectral representation of the Hamiltonian in \( \mathcal{H}(c) \),

\[
I(c) = \sum_{n=1}^{\infty} |D_n\rangle \frac{1}{\varrho_n} \{L_n|, \quad \hat{H}^{(KG)} = \sum_{n=1}^{\infty} |D_n\rangle \frac{\kappa_n^2}{\varrho_n} \{L_n|.
\]

The overlaps \( \varrho_n \) need not be all of the same sign.

### 2 Relativistic observables

#### 2.1 \( \Theta \)–quasi-Hermiticity

In the space \( \mathcal{H} = \mathcal{H}(c) \oplus \mathcal{H}(c) \) of the eigenstates of \( H^{(FV)} \) we have to consider the pair of conjugate equations

\[
\hat{H}^{(FV)}|n^{(\pm)}\rangle = \pm \kappa_n |n^{(\pm)}\rangle, \quad \langle\langle n^{(\pm)}|\hat{H}^{(FV)} = \pm \kappa_n \langle\langle n^{(\pm)}|.
\]

Both the left and right eigenstates have the two-component structure,

\[
|m^{(\pm)}\rangle = \begin{pmatrix} |L_m\rangle \\ \pm \kappa_m |L_m\rangle \end{pmatrix}, \quad |n^{(\pm)}\rangle = \begin{pmatrix} \pm \kappa_n |D_n\rangle \\ |D_n\rangle \end{pmatrix}
\]

and form the bi-orthogonal set in the “bigger” space \( \mathcal{H} \),

\[
\langle\langle m^{(\nu)}|n^{(\nu')}\rangle = \delta_{mn} \delta_{\nu\nu'} \mu_m^{(\nu)}, \quad \mu_m^{(\pm)} = \pm 2 \kappa_m \varrho_m, \quad \nu, \nu' = \pm 1.
\]

It is expected to be complete and useful,

\[
I = \sum_{\tau=\pm 1} \sum_{n=1}^{\infty} |n^{(\tau)}\rangle \frac{1}{\mu_n} \langle\langle n^{(\tau)}|,
\]

3
\[
H^{(FV)} = \sum_{\tau=\pm 1} \sum_{n=1}^{\infty} |n^{(\tau)}\rangle \frac{\tau \kappa_n}{\mu_n} \langle \langle n^{(\tau)} \rangle \rangle = \sum_{n=1}^{\infty} \left( |n^{(+)}\rangle \langle \langle n^{(+)} \rangle \rangle + |n^{(-)}\rangle \langle \langle n^{(-)} \rangle \rangle \right) \frac{2 \varrho_n}{\langle \langle n^{(\tau)} \rangle \rangle}. 
\]

Let us now assume that at a given \( \hat{H}^{(FV)} \), equation

\[
\left[ \hat{H}^{(FV)} \right]^\dagger = \eta \hat{H}^{(FV)} \eta^{-1} \tag{7}
\]

possesses a positive and Hermitian solution \( \eta_+ = \Theta > 0 \). Such an operator may play the role of a metric and induces the following specific scalar product in \( \mathcal{H} \),

\[
(\langle \psi_1 \rangle \otimes |\psi_2\rangle) = \langle \psi_1 | \Theta | \psi_2 \rangle = \langle \psi_1 | \psi_2 \rangle_{(\text{physical})}, \quad |\psi_1\rangle \in \mathcal{H}, \quad |\psi_2\rangle \in \mathcal{H}. \tag{8}
\]

This product generates the norm, \( ||\psi|| = \sqrt{\langle \psi | \psi \rangle_{(\text{physical})}} \). In terms of the later product and metric we may call all the operators \( A \) with the property \( A^\dagger = \Theta A \Theta^{-1} \) quasi-Hermitian and treat them as observables (see \[3\] for a deeper outline of some more sophisticated mathematical details). Indeed, we have

\[
(\langle \psi_1 \rangle \otimes |A \psi_2\rangle) \equiv (|A \psi_1\rangle \otimes |\psi_2\rangle) \tag{9}
\]

so that the probabilistic expectation values \( \langle \psi | A | \psi \rangle_{(\text{physical})} \) are mathematically unambiguously defined.

### 2.2 Explicit constructions of the metric \( \Theta \)

Let us assume non-Hermiticity of the type \( \hat{h}^{(KG)} \neq [\hat{h}^{(KG)}]^\dagger = \mathcal{P} \hat{h}^{(KG)} \mathcal{P} \) in the smaller space \( \mathcal{H}_c \) (here, \( \mathcal{P} \) is operator of parity). Then, a consistent physical meaning may still be assigned to all the relativistic bound states, provided only that in the bigger space \( \mathcal{H} \) we find a suitable physical metric \( \Theta \). For this purpose we may employ the ansatz

\[
\Theta = \sum_{\tau,\tau'=\pm 1} \sum_{m,n=1}^{\infty} \langle n^{(\tau')} \rangle \langle m^{(\tau')} \rangle M_{nm}^{(\tau\tau')} \langle \langle n^{(\tau)} \rangle \rangle, 
\]

the backward insertion of which in (7) gives the condition

\[
\tau \kappa_n M_{nm}^{(\tau\tau')} = M_{nm}^{(\tau\tau')} \tau' \kappa_m
\]
with the set of solutions $M_{nm}^{(r \tau \ell)} = \omega_n^{(r)} \delta_{mn} \delta_{(r \tau \ell)}$ numbered by the free parameters $\omega^{(\pm)}$. The Hermiticity and positivity constraints restrict the freedom of the choice of both the optional sequences $\omega^{(\pm)}$ to the real and positive values, $\omega_n^{(\pm)} > 0$. Vice versa, any choice of the latter two sequences defines an eligible operator of the metric

$$\Theta = \Theta_{\omega^{(\pm)}} = \sum_{\tau = \pm 1} \sum_{n = 1}^{\infty} |n^{(\tau)}\rangle \langle n^{(\tau)}| \omega_n^{(\tau)}.$$  \hspace{1cm} (10)

Its inverse

$$\Theta^{-1} = \sum_{\tau = \pm 1} \sum_{n = 1}^{\infty} |n^{(\tau)}\rangle \frac{1}{\omega_n^{(\tau)}|\mu_n^{(\tau)}|^2} \langle n^{(\tau)}|$$ \hspace{1cm} (11)

is similar. In terms of the metric $\Theta$, the formal bound-state wave functions re-acquire the standard probabilistic interpretation.

3 Models with complex point interactions

In a way inspired by the success of several non-relativistic studies of $\mathcal{PT}$—symmetric models with point interactions [4] and by the encouraging experience we made in our paper [5] we shall combine the infinitely deep square-well real part of the potential $[V(x) = \infty$ for all $x \notin (-1, 1)]$ with the following purely imaginary delta-function formula for its remaining part,

$$V(x) = \sum_{\ell=1}^{L} [i \xi_\ell \delta (x - a_\ell) - i \xi_\ell \delta (x + a_\ell)], \quad x \in (-1, 1),$$ \hspace{1cm} (12)

at real couplings $\xi_\ell$ and ordered points $0 < a_1 < a_2 < \ldots < a_{L-1} < a_L < 1$.

3.1 Wave functions

The key advantage of our $V(x)$ in (12) is that the $\mathcal{PT}$—symmetrically normalized coordinate representants $\psi(x) = \psi^*(-x)$ of $|D\rangle$ in eq. (2) remains piecewise trigono-
metric. At each real and positive bound-state energy \( \varepsilon = \kappa^2 \) we shall have

\[
\psi(x) = \begin{cases}
\psi^{(\ell)}_L(x) = (\alpha_\ell - i \beta_\ell) \sin \kappa(1 + x), & x \in (-1, -a_\ell), \\
\psi^{(\ell+1)}_L(x) = (\alpha_\ell + i \beta_\ell) \sin \kappa(a_\ell + 1 + x), & x \in (-a_\ell + 1, -a_\ell), \\
\psi^{(0)}_C(x) = \mu \cos \kappa x + i \nu \sin \kappa x, & x \in (-a_1, a_1), \\
\psi^{(1)}_R(a_1) = \psi^{(0)}_C(a_1), \\
\psi^{(\ell+1)}_R(a_{\ell+1}) = \psi^{(\ell)}_R(a_{\ell+1}), & \ell = 1, 2, \ldots, \mathcal{L} - 1,
\end{cases}
\]  

(13)

Its differentiation as well as continuity conditions

\[
\psi^{(\ell)}_L(-a_\ell) = \psi^{(\ell)}_L(-a_\ell), \quad \ell = \mathcal{L}, \mathcal{L} - 1, \ldots, 2, \\
\psi^{(0)}_C(-a_1) = \psi^{(1)}_C(-a_1), \\
\psi^{(1)}_R(a_1) = \psi^{(0)}_C(a_1), \\
\psi^{(\ell+1)}_R(a_{\ell+1}) = \psi^{(\ell)}_R(a_{\ell+1}), & \ell = 1, 2, \ldots, \mathcal{L} - 1,
\]

(14)

enter the definition of the action of the delta functions,

\[
\begin{align*}
\left[\psi^{(\ell-1)}_L(-a_\ell)\right]' - \left[\psi^{(\ell)}_L(-a_\ell)\right]' &= -i \xi \psi^{(\ell)}_L(-a_\ell), & \ell = \mathcal{L}, \mathcal{L} - 1, \ldots, 2, \\
\left[\psi^{(0)}_C(-a_1)\right]' - \left[\psi^{(1)}_C(-a_1)\right]' &= -i \xi_1 \psi^{(0)}_C(-a_1), \\
\left[\psi^{(1)}_R(a_1)\right]' - \left[\psi^{(0)}_C(a_1)\right]' &= i \xi_1 \psi^{(0)}_C(a_1), \\
\left[\psi^{(\ell+1)}_R(a_{\ell+1})\right]' - \left[\psi^{(\ell)}_R(a_{\ell+1})\right]' &= i \xi_{\ell+1} \psi^{(\ell)}_R(a_{\ell+1}), & \ell = 1, 2, \ldots, \mathcal{L} - 1,
\end{align*}
\]

(15)

After the insertion of the ansatz (13), the set of formulae (14) and (15) may be read as a homogeneous linear algebraic system of \( 4\mathcal{L} \) equations for the \( 4\mathcal{L} \) unknown wavefunction coefficients \( \alpha_\ell, \beta_\ell, \ldots, \nu \). The secular determinant \( \mathcal{D}(\kappa) \) of this system must vanish so that the not too complicated transcendental equation

\[
\mathcal{D}(\kappa) = 0
\]

(16)

determines finally the set of the bound-state roots \( \kappa = \kappa_n \) at \( n = 1, 2, \ldots \).

### 3.2 Energies at the simplest choice of \( \mathcal{L} = 1 \)

At \( \mathcal{L} = 1 \), potential (12) degenerates to the most elementary double-well model with the single coupling \( \xi_1 = \xi \) and one displacement \( a_1 = a \). Out of the related eight
real constraints (14) and (15) only four are independent and define the four real coefficients \( \alpha_1 = \alpha, \beta_1 = \beta \) and \( \mu \) and \( \nu \) as an eigenvector of a four-by-four matrix with the secular determinant

\[
D(\kappa) = -\frac{1}{2} \left\{ \sin 2\kappa + \frac{\xi^2}{\kappa^2} \sin 2\kappa a \cdot \sin^2[\kappa(1-a)] \right\}.
\]  

(17)

Numerically, the first term would give us the well-known square-well spectrum at \( \xi = 0 \), the completeness of which is controlled by the Sturm-Liouville oscillation theory [7]. As long as all the roots \( \kappa_n = \kappa_n(\xi) \) are smooth and real functions of \( \xi \) at the smallest couplings, \( \kappa_n(\xi) \approx n\pi/2 + \mathcal{O}(\xi^2/n) \), our explicit construction confirms the general mathematical prediction [8] that the influence of the non-Hermiticity will be most pronounced at the lowest part of the spectrum.

3.3 The next choice of \( \mathcal{L} = 2 \)

In the quadruple-well potential with \( \mathcal{L} = 2 \) we may shorten \( a_1 = a, a_2 = b \) and drop the two redundant subscripts in \( \gamma_1 = \gamma, \delta_1 = \delta \). In the eight-dimensional matrix of the system the elimination of four unknowns is either trivial \[ \gamma = \alpha_2 \sin \kappa(1-b), \delta = \beta_2 \sin \kappa(1-b) \] or easy \[ \alpha_1 = \alpha_1(\alpha_2, \beta_2), \beta_1 = \beta_1(\alpha_2, \beta_2) \]. We end up with a four-by-four matrix problem and with the secular determinant

\[
\mathcal{D}(\kappa) = \mathcal{D}(0)(\kappa) + \mathcal{D}(\xi_1)(\kappa) + \mathcal{D}(\xi_2)(\kappa) + \mathcal{D}(\xi_1\xi_2)(\kappa),
\]  

(18)

\[
\mathcal{D}(0)(\kappa) = -\frac{1}{2} \sin 2\kappa, \quad \mathcal{D}(\xi_j)(\kappa) = -\frac{\xi_j^2}{2\kappa^2} \sin 2\kappa a_j \cdot \sin^2[\kappa(1-a_j)], \quad j = 1, 2,
\]

\[
\mathcal{D}(\xi_1\xi_2)(\kappa) = -\left\{ \frac{\xi_1\xi_2}{\kappa^2} \sin 2\kappa a + \frac{\xi_1^2\xi_2^2}{\kappa^4} \sin^2[\kappa(b-a)] \right\} \sin^2[\kappa(1-b)].
\]

This secular determinant correctly degenerates to the previous \( \mathcal{L} = 1 \) formula in both the independent limits of \( \xi_1 \to 0 \) and \( \xi_2 \to 0 \).
3.4  Simplifications at the rational $a_j$

Let us return to the secular eq. (17) with $L = 1$ and choose $a = 1/2$. This leads to a factorization of $\mathcal{D}(\kappa)$ and to the pair of the eigenvalue conditions

$$\cos \kappa_{2m-1} = \frac{\xi^2}{\xi^2 - 4\kappa_{2m-1}^2}, \quad \sin \kappa_{2m} = 0, \quad m = 1, 2, \ldots$$

(19)

with the second series of equations being exactly solvable, $\kappa_{2m} = m\pi$.

At the next choice of $a = 1/3$ we factorize eq. (17) in the similar manner and get the series of the $\xi$–dependent roots specified by the implicit definitions

$$\cos \frac{4}{3} \kappa_p = \frac{\xi^2 + 2\kappa_p^2}{\xi^2 - 4\kappa_p^2}, \quad p = 1, 2, 4, 5, 7, 8, 10, \ldots$$

(20)

complemented by the closed formula for all the skipped roots of the factor $\sin 2\kappa/3$ which remain $\xi$–independent and read $\kappa_{3m} = 3m\pi/2$ with $m = 1, 2, \ldots$. The regularity of such a pattern of the $\xi$–independent roots is easily prolonged to the decreasing sequence of $a$ with $\kappa_{4m} = 2m\pi$ at $a = 1/4$ and all $m = 1, 2, \ldots$, etc.

The less elementary composite choice of $a = 2/3$ may be observed to give the same factor as at $a = 1/3$ and, hence, the same $\xi$–independent series of the roots $\kappa_{3m} = 3m\pi/2$ with $m = 1, 2, \ldots$. The implicit formula for the remaining roots is a slightly more complicated quadratic equation in the trigonometric unknown $X = \cos 2\kappa/3$,

$$\left(4\kappa^2 - \xi^2\right) X^2 + \xi^2 X - \kappa^2 = 0.$$  

(21)

Its trigonometric part $X$ may be eliminated in the form resembling eq. (20).

One of the important consequences of the existence of the elementary formulae for the rational $a$ is that they allow us to perform an elementary analysis of the qualitative features of the $n$–th root $\kappa_n$ during the growth of the strength $\xi$ of the non-Hermiticity. During such an analysis one discovers that these levels are either “robust” (marked by a superscript, $\kappa_n^{(R)}$, and remaining real for all $\xi$) or “fragile” (such a $\kappa_n^{(F)}$ will merge with another $\kappa_m^{(F)}$ at a “critical” $\xi_{n,m}^{(C)}$ while the pair will
complexify beyond this “exceptional” [9] point). For illustration let us display this pattern in the three simplest spectra,

\[
\begin{align*}
&\kappa_1^{(F)}, \kappa_2^{(R)}, \kappa_3^{(F)}, \kappa_4^{(R)}, \kappa_5^{(F)}, \kappa_6^{(R)}, \ldots, \quad a = 1/2 \\
&\kappa_1^{(F)}, \kappa_2^{(F)}, \kappa_3^{(R)}, \kappa_4^{(F)}, \kappa_5^{(F)}, \kappa_6^{(R)}, \ldots, \quad a = 1/3 \\
&\kappa_1^{(F)}, \kappa_2^{(F)}, \kappa_3^{(R)}, \kappa_4^{(R)}, \kappa_5^{(F)}, \kappa_6^{(F)}, \kappa_7^{(F)}, \kappa_8^{(R)}, \kappa_9^{(R)}, \kappa_{10}^{(R)}, \kappa_{11}^{(F)}, \ldots, \quad a = 1/4.
\end{align*}
\]

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