Analytical solution of the compressed, one-dimensional delta atom via quadratures and exact, absolutely convergent periodic-orbit expansions

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Abstract
The compressed delta atom is a one-dimensional version of the compressed hydrogen atom where the finite-range Coulomb potential is replaced by a zero-range delta function. The spectral equation of the compressed delta atom is transcendental. Nevertheless, using recently developed quadrature and absolutely convergent periodic-orbit expansion techniques, it can be solved analytically, which yields its energy levels explicitly in the form $E_n = f(n; p)$, where n is the quantum number, p is a set of parameters characterizing the atom and f, a function expressed as a quadrature or as an absolutely convergent sum over periodic orbits, is the same for all n. The compressed delta atom may serve as a template for the explicit, exact and analytical solution of other one-dimensional quantum problems with potentials consisting of a superposition of delta-function potentials and piecewise constant potentials.

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1. Introduction

Consider a gas of hydrogen atoms under a pressure exceeding tens of thousands of atmospheres. Under such extreme conditions the atoms can no longer be considered free; their atomic orbitals experience considerable compression, resulting in a reduction of their atomic volumes. The simplest model describing a hydrogen atom under such exotic conditions is the *compressed hydrogen atom*. It consists of a single hydrogen atom confined to a spherical box of radius $r_0 < \infty$. This model was first successfully employed close to 70 years ago by Michels, De Boer and Bijl [1] for the computation of the kinetic energy and the polarizability of pressurized hydrogen. Motivated by astrophysical considerations, the compressed hydrogen atom soon attracted the attention of Sommerfeld and Welker [2], who improved the mathematical theory of the ground state energy as a function of r_0. In 1946 De Groot and Ten Seldam [3] extended the mathematical work of Sommerfeld and Welker to include the first two excited states of the compressed hydrogen atom.

Apart from its relevance to the theory of highly compressed gases, the compressed hydrogen atom is also interesting from the following purely theoretical point of view. Non-relativistically, and assuming an infinite proton mass, the ground-state energy of the hydrogen atom is given by [4]

$$E_{\mathrm{H}} = -\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2,\tag{1}$$

where e is the elementary charge, ϵ_0 is the electric permittivity of the vacuum, m is the electron mass and $\hbar$ is Planck's constant. In 1954 Wigner asked the question whether the hydrogen ground-state energy, according to (1) suggestively proportional to the second power of the electron–proton coupling constant $e^2/(4\pi\epsilon_0)$, could be obtained exactly in second order perturbation theory using the unperturbed box wavefunctions of the compressed hydrogen model as the basis states and letting $r_0 \to \infty$ [5]. While the answer to this question turns out to be negative [5], 'Wigner's failure' [6] provides an excellent pedagogical example for illustrating the fine points of the convergence properties of perturbation series [5, 6].

A central point of this paper is to define what we mean by *solving* a (quantum) spectral problem. Although often considered a 'solution' (see, e.g., [7]), in the context of this paper mere reduction to its spectral equation does not qualify as a solution of a problem. In fact, the spectral equation is only the *starting point* for obtaining the solution of a spectral problem. For a problem with square-normalizable bound states only, we require a solution to be of the form

$$E_n = f(n; p), \qquad n = 1, 2, \ldots,\tag{2}$$

where E_n are the energy levels, f is a known function, n is the quantum number labelling the states and p is a set of parameters characterizing the problem. It is important to require that f in (2) is the *same* for *all n* and *all p*. Only a few physically relevant systems are solvable in the form (2). Examples are the unperturbed hydrogen atom and the harmonic oscillator. Even though spherically symmetric, and therefore effectively one-dimensional, the compressed hydrogen atom has not yet been solved in the form (2).

However, replacing the finite-range Coulomb potential with a zero-range, one-dimensional delta-function potential [6, 7] leads to the *compressed delta atom*, whose spectrum is solvable explicitly, exactly and analytically in the form (2) using recently developed periodic-orbit expansion techniques [8, 9]. With the confining walls located at $x = 0$ and $x = b > 0$, respectively, and the δ function located at $x = a$ with $0 < a < b$, the potential of the compressed delta atom is

$$V(x) = \begin{cases} \infty, & \text{for } x \leqslant 0, \\ V_\delta(E)\delta(x-a), & \text{for } 0 < x < b, \\ \infty, & \text{for } x \geqslant b, \end{cases}\tag{3}$$

where the argument E of the strength V_δ of the delta-function potential indicates a possible energy dependence (see section 5). Although mathematically simpler, the compressed delta atom preserves the main analytical feature (the main difficulty) of the compressed hydrogen problem: its spectral equation is transcendental. For this reason, neither the compressed hydrogen atom nor the compressed delta atom has ever been solved before.

The results presented in this paper may be seen in the context of periodic-orbit theory [10]. But while 'conventional' periodic-orbit theory [10] provides periodic-orbit expansions of the density of states or the spectral functions of a quantum system, the direct expansion of the spectral eigenvalues themselves into a periodic-orbit series is a new direction in quantum mechanics [9, 11]. Expansions of this type satisfy the solution requirement (2). Recently a

program has been outlined [9] of how to obtain explicit, exact and analytical periodic-orbit expansions of the type (2) for all one-dimensional quantum problems whose potentials can be represented as a sum of piecewise constant potentials and delta-function potentials. In partial fulfilment of this program a step-in-the-box potential with a non-trivial spectral equation has been solved in all energy regimes [9, 11–13]. Recently the finite quantum square well has been added to the list of problems solvable in the form (2) [14]. This paper adds one more solvable system to the still small set of explicitly solved problems: the compressed delta atom. The step-in-the-box potential, the finite square well and the compressed delta atom solved here may be used as templates to solve additional quantum systems explicitly in the form (2).

The paper is organized in the following way. Section 2 analyses the overall spectral properties of the compressed delta atom. Section 3 presents exact, explicit solution formulae of the positive-energy spectrum. The negative-energy state is investigated in section 4. If we assume that the strength of the δ function is proportional to the momentum, a scaling version of the compressed delta atom results. Section 5 shows how in the scaling case integral-free, explicit solutions of the spectrum can be constructed. Curiously, the number-theoretic properties of the placement of the δ function between the two potential walls matter. Section 6 discusses the consequences of 'rational placement', i.e., the ratio of the distances of the δ function from the two walls, respectively, is rational. The convergence properties of the explicit solution formulae are investigated in section 7. Section 8 discusses the results and section 9 summarizes and concludes the paper. Appendix A establishes a connection between the present paper and a previous publication on the solution of the finite quantum square well [14] by showing that the results presented in [14] yield the bound-state energy of an attractive δ function in the limit of an infinitely deep, but narrow well with the product of the depth and width of the well kept constant. This is an important check of a set of previously obtained explicit solution formulae whose derivation qualitatively follows the solution methods employed in this paper.

2. Organization of the spectrum

Although it is possible to construct potential functions $V_\delta(E)$ for which the compressed delta atom has a continuous spectrum (see section 8.5), in the generic case (see, e.g., sections 2 and 3 for $V_\delta(E) \equiv$ const and section 5 for $V_\delta(E) \sim \sqrt{E}$), since the delta atom is confined between two infinitely high potential walls, its spectrum is pure point and all of its physical eigenstates are square-normalizable bound states. Therefore, the aim is to compute its spectrum in the form (2). In preparation for section 3, where this goal is achieved, we derive, in section 2.1, the positive- and negative-energy spectral equations. In section 2.2 we investigate the global properties of the spectrum. In particular, we show the existence of non-overlapping root intervals containing precisely one spectral point each. This is the key for the explicit computation of the spectrum according to (2) in section 3. In section 2.3 we derive an alternative form of the spectral equations which plays a prominent role for the explicit computation of spectral points in section 3.

2.1. Spectral equations

The Schrödinger equation of the non-relativistic delta atom is

$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\psi(x), \tag{4}$$

where E is the energy and $V(x)$ is defined in (3). Using the hard-wall (Dirichlet) boundary conditions $\psi(0) = \psi(b) = 0$ together with the continuity of the wavefunction at $x = a$ and

the δ-function boundary condition $\lim_{\epsilon \to 0} \psi'(a + \epsilon) - \psi'(a - \epsilon) = 2mV_\delta \psi(a)/\hbar^2$ [4], we obtain the transcendental spectral equation

$$g(k; v, \omega) = 0, \tag{5}$$

where

$$g(k; v, \omega) = v \cos(k) - k \sin(k) - v \cos(\omega k) \tag{6}$$

with

$$k = \pm b\sqrt{2mE}/\hbar, \qquad v = mV_\delta b/\hbar^2, \qquad \omega = (2a - b)/b. \tag{7}$$

In (7) k is the dimensionless wave number, v is the dimensionless strength of the δ-function potential and $-1 < \omega < 1$ measures the asymmetry of the placement of the δ-function potential; $\omega = 0$ corresponds to symmetric placement of the δ-function potential. Since (6) is symmetric in $\omega \leftrightarrow -\omega$, we focus, without loss of generality, on $0 \leqslant \omega < 1$.

The spectral equation (5) has both real and imaginary solutions. The $k \leftrightarrow -k$ symmetry of (6) allows us, without loss of generality, to choose $k \geqslant 0$ for real solutions of (5) and $\text{Im}(k) \geqslant 0$ for imaginary solutions of (5). For $E < 0$, with $k = i\kappa$ (κ real), the real version of (5) is

$$h(\kappa; v, \omega) = 0, \tag{8}$$

where

$$h(\kappa; v, \omega) = v \cosh(\kappa) + \kappa \sinh(\kappa) - v \cosh(\omega\kappa). \tag{9}$$

For $v > 0$, (9) is positive definite. Therefore there is no non-trivial solution which corresponds to a physical bound state. Real, non-trivial solutions of (8) exist only for $v < v_c(\omega) < 0$, where

$$v_c(\omega) = \frac{2}{\omega^2 - 1} \tag{10}$$

is determined exactly with the help of a fourth-order Taylor-series expansion of (9). For $v < v_c < 0$ and $\kappa > 0$, we write (8) in the form

$$\tilde{h}(\kappa; v, \omega) = 0, \tag{11}$$

where

$$\tilde{h}(\kappa; v, \omega) = \frac{\kappa}{2|v|} \{\coth[\kappa(1 - \omega)/2] + \coth[\kappa(1 + \omega)/2]\} - 1. \tag{12}$$

Since for $x > 0$ the function $x \coth(x)$ is monotonically increasing, $\tilde{h}(\kappa; v, \omega)$ is a monotonically increasing function of κ. Since $\tilde{h}(0; v, \omega) = |v_c/v| < 1$, (11) ((8), respectively) has exactly one non-trivial solution κ_1. For $v \to v_c, \kappa_1 \to 0$.

We denote the physical solutions of (5) by $k_n(v; \omega)$, $n = 1, 2, \ldots$. For $v \geqslant v_c$, all k_n are real. For $v < v_c$, we set $k_1 = i\kappa_1$. We order the k_n such that the energies

$$E_n = \frac{\hbar^2 k_n^2(v; \omega)}{2m} \tag{13}$$

are arranged in ascending order, i.e. $E_n \leqslant E_{n+1}, n = 1, 2, \ldots$.

We note that $k = 0$ ($\kappa = 0$) is always a solution of (5) ((8), respectively). However, for $k = 0$ ($\kappa = 0$), the wavefunction is identically zero and does not therefore correspond to a physical, square-normalizable state. Such a state contains no particles. Therefore we do not count the $k = 0$ ($\kappa = 0$) solution among the physical states of the system.
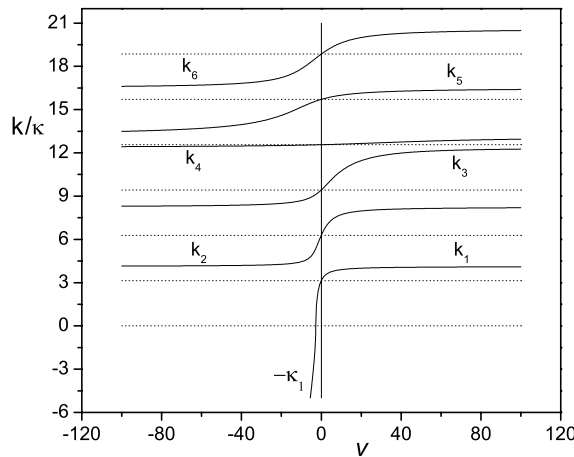
Figure 1. Spectrum of the compressed delta atom as a function of the dimensionless potential strength v for asymmetry parameter $\omega = \pi/6$. The first six levels (solid lines) are shown. The level corresponding to the negative-energy state is plotted as $-\kappa_1$. The horizontal, dotted lines, plotted at integer multiples of π, are the root separators of the spectrum. They define the root intervals to which the spectral lines are confined.

While (5) is difficult to solve for generic v and irrational ω, explicit solutions of (5) can be obtained for rational ω. For $\omega = P/Q$, where P and Q are positive, relatively prime integers, and $N = 1, 2, \ldots$,

$$k_N = \begin{cases} NQ\pi, & \text{for both } P \text{ and } Q \text{ odd,} \\ 2NQ\pi, & \text{otherwise} \end{cases} \tag{14}$$

are solutions of (5) for all v since $\sin(k_N) = 0$ and $\cos(k_N) = \cos(\omega k_N) = \pm 1$. It includes the case $\omega = 0$ if we choose $P = 0$, $Q = 1$. Physically the solutions (14) correspond to unperturbed box wavefunctions. They are exact solutions of the perturbed problem because they have a node at the position of the δ function and thus do not 'feel' the presence of the δ-function potential.

2.2. Spectral properties and root separators

Figure 1 shows the spectrum of the compressed delta atom as a function of v for $\omega = \pi/6$. The energy levels $k_n(v; \omega)$ ($\kappa_1(v; \omega)$, respectively) (full lines), labelled from the bottom up with the quantum number n, are monotonically increasing as a function of v. They never cross; they are clearly separated from each other. In particular, except at $v = 0$, the energy levels never cross the horizontal, dotted lines in figure 1 drawn at integer multiples of π. These lines separate energy levels with different n from each other. This observation, proved below, is significant. It is the key for obtaining explicit expressions for the energy levels.

For $v = 0$, the δ function in (3) is switched off and the spectrum is the one of a quantum particle in a box with infinite walls. In this case, as confirmed by figure 1, the spectrum is

$$k_n(v = 0; \omega) = n\pi, \qquad n = 1, 2, \ldots. \tag{15}$$

For fixed ω, the slope of the spectrum as a function of v is obtained by implicit differentiation of (5):

$$k'_n(v; \omega) = \frac{\partial}{\partial v} k_n(v; \omega) = \frac{\cos(k_n) - \cos(\omega k_n)}{(v + 1)\sin(k_n) + k_n \cos(k_n) - v\omega \sin(\omega k_n)}. \tag{16}$$

From (16) we obtain

$$k'_n(v = 0; \omega) = \frac{2}{n\pi} \sin^2 \left[n\pi \left(\frac{\omega + 1}{2} \right) \right]. \tag{17}$$

According to (17), $k'_n(v = 0; \omega)$ has four important properties: (i) it is $\geqslant 0$ for all n; (ii) it may be zero only for rational ω; (iii) it is quasi-random for irrational ω; (iv) it approaches zero for $n \to \infty$. The first three properties are reflected in figure 1: all energy levels plotted in figure 1 have positive slope illustrating property (i). Since $\omega = \pi/6 = 0.523\ldots$ is close to $1/2$, level $n = 4$ in figure 1, for which $\omega n\pi \approx 2\pi$, is near degenerate with the horizontal dotted line at $k = 4\pi$, illustrating property (ii). Although only a few energy levels are plotted in figure 1 there does not seem to be any apparent rule to the slopes of the energy levels at $v = 0$, illustrating property (iii).

The aim now is to establish isolating intervals $[k_n^<(v; \omega), k_n^>(v; \omega)]$ $([\kappa_1^<(v; \omega), \kappa_1^>(v; \omega)]$, respectively) in which only the state k_n (κ_1), and no other, is found. Since $k_n^{<,>}(v; \omega)$ ($\kappa_1^{<,>}(v; \omega)$, respectively) separate the different roots of (5) ((8), respectively) from each other, they are called *root separators*; the intervals $[k_n^<(v; \omega), k_n^>(v; \omega)]$ $([\kappa_1^<(v; \omega), \kappa_1^>(v; \omega)]$, respectively) are called *root intervals* [9].

Since the levels (14) are known explicitly, it is straightforward to establish root intervals for them. We will do this at the end of this section. Meanwhile we focus on energy levels different from (14). We call them *generic levels*. All levels corresponding to irrational ω, and all levels corresponding to rational ω, but not satisfying (14), fall into this category.

Consider the case $v > 0$ as a function of increasing v. At $v \approx 0$, $v > 0$, the level $k_n(v; \omega)$ is injected into the interval $(n\pi, (n+1)\pi)$, from which it can never escape, since escape means crossing the lines $k = n\pi$ or $k = (n + 1)\pi$. But this is impossible, since for a generic level k_n, $k_n = M\pi$, M integer, is not a solution of (5). For rational ω this is trivially so because of the definition of a generic level. For irrational ω it would imply that $M\omega$ is an integer, which is impossible.

We obtain the important result that for $v > 0$ a generic level $k_n(v; \omega)$ is confined to the open interval $(n\pi, (n + 1)\pi)$. Similar considerations for $v < 0$ show that for $n > 1$ the level $k_n(v; \omega)$ is confined to the open interval $((n - 1)\pi, n\pi)$. For $v_c < v < 0$, this holds for $n = 1$, too, while for $v < v_c$, as shown in figure 1, the energy level $k_1(v; \omega)$ turns into the negative-energy bound state. In summary, and in the generic case, we obtain the following root separators for the $E > 0$ spectrum:

$$k_n^<(v; \omega) = \begin{cases} n\pi & \text{for } v > 0, \\ (n - 1)\pi & \text{for } n > 1 \quad \text{and} \quad v < 0, \\ 0 & \text{for } n = 1 \quad \text{and} \quad v_c < v < 0, \end{cases}$$

$$k_n^>(v; \omega) = k_n^<(v; \omega) + \pi. \tag{18}$$

We now turn to the case $E < 0$. Since $\kappa_1 > 0$ for a non-trivial bound state, we may choose $\kappa_1^< = 0$. In order to obtain $\kappa_1^>$, we write (11) in the form

$$\kappa = \frac{2|v|}{\coth[\kappa(1 - \omega)/2] + \coth[\kappa(1 + \omega)/2]}. \tag{19}$$

With $\coth(x) > 1$ for $x > 0$ we obtain $\kappa < |v|$. Therefore, we can choose $|v|$ as the root separator $\kappa_1^>$. In summary, for $E < 0$,

$$\kappa_1^< = 0, \qquad \kappa_1^> = |v|. \tag{20}$$

As illustrated in figure 1, generic levels $k_n(v; \omega)$ are monotonically rising functions of v. We already showed above that for a generic level $k'_n(v; \omega) > 0$ for $v = 0$. Since $k'_n(v; \omega)$ is

a continuous function of v, $k'_n(v; \omega)$ may turn negative only if it first passes through zero. In order to show that this is impossible we use (5) to write (16) in the form

$$k'_n(v; \omega) = \frac{k_n \sin(k_n)}{v(v+1) \sin(k_n) + v k_n \cos(k_n) - v^2 \omega \sin(\omega k_n)}. \tag{21}$$

Since $k_n(v; \omega) > 0$, $k'_n(v; \omega) = 0$ is possible only if k_n is a multiple of π. But, as proved above, this does not happen for generic levels. Therefore we established that $k_n(v; \omega)$ is indeed a monotonically rising function of v.

So far we showed that generic $E > 0$ levels $k_n(v; \omega)$ (i) satisfy $k'_n(v; \omega) > 0$ for all v and (ii) are confined to their respective root intervals. There is only one way to reconcile (i) and (ii): $k_n(v; \omega)$ has to be asymptotically constant for $|v| \to \infty$. Writing (5) in the form $v[\cos(k) - \cos(\omega k)] = k \sin(k)$ shows that the asymptotic values of $k_n(v; \omega)$ for $|v| \to \infty$ satisfy the equation

$$\cos(k) = \cos(\omega k), \tag{22}$$

since $k_n \sin(k_n)$ is asymptotically constant and finite. Equation (22) is solved in section 8.4. Since (22) is independent of the sign of v it follows that the asymptotic value of k_n for $v \to +\infty$ is the same as the asymptotic value of k_{n+1} for $v \to -\infty$. As an interesting aside this shows that if we identify the points $v = \pm\infty$, the topology of the energy levels of the compressed delta atom is the one of a single spiral wound on the surface of a cylinder.

We now return to the problem of determining a root interval for the levels (14). Let k_n be one of the levels (14) and k_{n-1} and k_{n+1} the two neighbouring, generic levels. Because of the property, proved above, that k_{n-1} for $v \to +\infty$ has the same asymptotic value as k_n for $v \to -\infty$, and since k_n is a constant, k_{n-1} approaches the level k_n for $v \to \infty$. Moreover, since k_n is a multiple of π, k_{n-1} approaches the upper limit of its root interval for $v \to \infty$. This is not a problem for the level k_{n-1}, but it is a nuisance for determining a root interval for the level k_n. Still, a straightforward, if cumbersome, fix exists. To determine a root interval for k_n at some finite value of v, one first determines $k_{n-1}(v; \omega)$ and $k_{n+1}(v; \omega)$ using the methods outlined in sections 3–5. Then, suitable root intervals for k_n are $[(k_{n-1}(v; \omega) + k_n(v; \omega))/2, k_n + \pi]$ for $v > 0$, and $[k_n - \pi, (k_n(v; \omega) + k_{n+1}(v; \omega))/2]$ for $v < 0$. This concludes the determination of root intervals for any level $k_n(v; \omega)$ for any given values of v and ω. Since each spectral point is confined to a root interval whose end-points, for finite v, are off limits to the spectral point enclosed, the spectrum of the compressed delta atom is non-degenerate.

2.3. Alternative form of the spectral equations

For later use in sections 3 and 7 we derive here a set of spectral equations, which, for $E > 0$, are equivalent to (5).

Defining

$$\Phi(k; v) = \arccos\left[\frac{v}{\sqrt{v^2 + k^2}}\right], \qquad 0 \leqslant \Phi(k; v) \leqslant \pi, \tag{23}$$

we write (5) in the form

$$\cos[k + \Phi(k; v)] = \frac{v}{\sqrt{v^2 + k^2}} \cos(\omega k). \tag{24}$$

Using symmetry and 2π-periodicity of the cosine function, (24) is equivalent to the following two types of transcendental spectral equations

$$f^{(\pm)}(k; v, \omega) = 2N\pi, \qquad N = 1, 2, \dots, \tag{25}$$

where

$$f^{(\pm)}(k; v, \omega) = k + \Phi(k; v) \pm \Psi(k; v, \omega) \tag{26}$$

with

$$\Psi(k; v, \omega) = \arccos\{\cos[\Phi(k; v)]\cos(\omega k)\}, \qquad 0 \leqslant \Psi(k; v, \omega) \leqslant \pi. \tag{27}$$

The solutions of (25) are denoted by $k_N^{(\pm)}(v; \omega)$.

We establish a mapping between the index N of the spectral equations (25) and the index n, which enumerates the spectrum as a function of increasing energy as illustrated in figure 1. Because of $\Phi(k; v = 0) = \pi/2$ and $\Psi(k; v = 0, \omega) = \pi/2$, we have

$$k_N^{(+)}(v = 0; \omega) = (2N - 1)\pi, \qquad k_N^{(-)}(v = 0; \omega) = 2N\pi. \tag{28}$$

This shows that for $v = 0$ the levels $k_N^{(+)}$ represent the odd-n ladder of states, while the levels $k_N^{(-)}$ represent the even-n ladder. Accordingly, we have

$$N = \begin{cases} n/2 & \text{for } n \text{ even,} \\ (n+1)/2 & \text{for } n \text{ odd.} \end{cases} \tag{29}$$

For $n = 1$, the equivalence holds for $v > v_c$.

3. Positive-energy spectrum

This section provides explicit, exact series expansions of the energy eigenvalues of the compressed delta atom. We proceed in the following way. In section 3.1 we re-derive the spectral equation (5) via scattering quantization [15, 16] based on the scattering matrix S of the compressed delta atom and express the eigenvalues (eigenphases) of the S matrix in terms of the spectral functions (26). In section 3.2 we use the S matrix to construct the staircase function $N(k)$ of the energy levels of the compressed delta atom and use $N(k)$ to obtain an explicit solution of the energy levels in integral form. An explicit solution of the energy spectrum via periodic-orbit expansions is presented in section 3.3.

3.1. Spectral equation via S matrix

In this section we consider the quantization problem of the compressed delta atom from the scattering point of view. We define four scattering channels. They correspond, respectively, to quantum flux moving left-to-right from $x = 0$ to $x = a$ (channel 1), right-to-left from $x = a$ to $x = 0$ (channel 2), left-to-right from $x = a$ to $x = b$ (channel 3) and right-to-left from $x = b$ to $x = a$ (channel 4). Denoting by S_{jl} the amplitude for scattering from channel number l to channel number j, the scattering matrix (S matrix) of the compressed delta atom is

$$S = \begin{pmatrix} 0 & -e^{iS_I} & 0 & 0 \\ r\,e^{iS_I} & 0 & 0 & t\,e^{iS_{II}} \\ t\,e^{iS_I} & 0 & 0 & r\,e^{iS_{II}} \\ 0 & 0 & -e^{iS_{II}} & 0 \end{pmatrix}, \tag{30}$$

where

$$S_I = k(1 + \omega)/2, \qquad S_{II} = k(1 - \omega)/2 \tag{31}$$

are the classical actions of a particle moving from $x = 0$ to $x = a$ (S_I) and from $x = a$ to $x = b$ (S_{II}), respectively, and

$$r = \frac{v}{ik - v}, \qquad t = \frac{ik}{ik - v} \tag{32}$$

are the quantum reflection and transmission amplitudes for a δ-function potential [17]. Because of $r^*t + rt^* = 0$, the S-matrix (30) is unitary. Because of the unitarity of S its eigenvalues Λ_j, $j = 1, \ldots, 4$, are unimodular. They can be written in the form $\Lambda_j = \exp(i\sigma_j)$ with real phases σ_j (eigenphases of S). Although S is a 4×4 matrix, its diagonalization involves only the solution of quadratic equations since the compressed delta atom is time-reversal symmetric. Therefore S can be diagonalized analytically. We obtain

$$
\begin{aligned}
\sigma_1 &= \tfrac{1}{2} f^{(+)}(k; v, \omega), & \sigma_2 &= \sigma_1 + \pi, \\
\sigma_3 &= \tfrac{1}{2} f^{(-)}(k; v, \omega), & \sigma_4 &= \sigma_3 + \pi,
\end{aligned}
\tag{33}
$$

where $f^{(\pm)}$ in (33) are the spectral functions (26). According to (25), a spectral point is encountered whenever $f^{(+)}$ ($f^{(-)}$, respectively) is a multiple of 2π. In this case, according to (33), at least one of the eigenphases σ_j is a multiple of 2π. Since σ_1 and σ_2 (σ_3 and σ_4, respectively) always differ by π, and since (see section 2, and apart from $v = v_c$, which results in a doubly degenerate, trivial solution $k = 0$) the spectrum of the compressed delta atom is non-degenerate, a spectral point is encountered whenever exactly one of the eigenphases σ_j is a multiple of 2π.

This '2π-criterion' for the S-matrix eigenphases can also be derived as follows. The S matrix transforms incoming flux into outgoing flux. A stationary state ψ, i.e. a spectral point, is encountered whenever $S\psi = \psi$. From this we obtain $[S - 1]\psi = 0$, which, for non-trivial ψ, requires $\det[S - 1] = 0$. We obtain

$$
\det[S - 1] = \frac{2 \, e^{ik}}{v - ik} g(k; v, \omega),
\tag{34}
$$

where $g(k; v, \omega)$ is the spectral function (6). Thus, indeed, since the pre-factor in (34) is never zero, $\det[S - 1] = 0$ is equivalent with the spectral equation (5). Moreover, $\det[S - 1] = 0$ whenever one of the eigenvalues Λ_j of S is 1, i.e., whenever one of the eigenphases σ_j is a multiple of 2π. This confirms the 2π criterion.

3.2. Explicit solution by reduction to quadratures

For $E > 0$, define the staircase function

$$
N(k) = n_i(v) - 1 + \sum_{n=n_i(v)}^{\infty} \theta(k - k_n),
\tag{35}
$$

where

$$
n_i(v) = \begin{cases} 1, & \text{if } v > v_c, \\ 2, & \text{if } v < v_c \end{cases}
\tag{36}
$$

and

$$
\theta(x) = \begin{cases} 0, & \text{if } x < 0, \\ \tfrac{1}{2}, & \text{if } x = 0, \\ 1, & \text{if } x > 0 \end{cases}
\tag{37}
$$

is Heavisides's step function. The function (35) jumps by one unit whenever its argument encounters a spectral point k_n. Thus (35) counts the total number of states (including, if it exists, the negative-energy state) with $k_n \leqslant k$ and the convention that if $k = k_n$, the state k_n counts as $1/2$ of a state. The derivative of the staircase function (35) is the density of states

$$
\rho(k) = \frac{\mathrm{d}}{\mathrm{d}k} N(k) = \sum_{n=n_i(v)}^{\infty} \delta(k - k_n).
\tag{38}
$$

We define the normalized staircase function

$$\Theta_{2\pi}(x) = -\frac{1}{2} + \frac{x}{2\pi} + \frac{1}{\pi} \sum_{m=1}^{\infty} \frac{\sin(mx)}{m}. \tag{39}$$

It is zero in $(0, 2\pi)$ and jumps by one unit whenever its argument x is an integer multiple of 2π. We use (39) and the '2π-criterion' of the S-matrix eigenphases σ_j of section 3.1 to obtain an alternative expression for the staircase function

$$N(k) = \sum_{j=1}^{4} \Theta_{2\pi}(\sigma_j). \tag{40}$$

This expression can be turned into an explicit formula for $N(k)$ by inserting the S-matrix eigenphases (33) into (40). We obtain

$$N(k) = -1 + \frac{k}{\pi} + \frac{1}{\pi} \arccos\left(\frac{v}{\sqrt{v^2 + k^2}}\right) + \frac{2}{\pi} \sum_{m=1}^{\infty} \frac{1}{m} \left\{ \sin(mk) T_m\left(\frac{v}{\sqrt{v^2 + k^2}}\right) \right.$$
$$\left. + \frac{k}{\sqrt{v^2 + k^2}} \cos(mk) U_{m-1}\left(\frac{v}{\sqrt{v^2 + k^2}}\right) \right\} T_m\left(\frac{v}{\sqrt{v^2 + k^2}} \cos(\omega k)\right), \tag{41}$$

where

$$T_n(x) = \sum_{m=0}^{[n/2]} \Gamma_{nm} x^{n-2m}, \qquad \Gamma_{nm} = (-1)^m \frac{n(n-m-1)!}{m!(n-2m)!} 2^{n-2m-1} \tag{42}$$

and

$$U_n(x) = \sum_{m=0}^{[n/2]} \Upsilon_{nm} x^{n-2m}, \qquad \Upsilon_{nm} = (-1)^m \frac{(n-m)!}{m!(n-2m)!} 2^{n-2m} \tag{43}$$

are Chebyshev's polynomials of the first and second kinds, respectively [18]. The symbol $[x]$ in (42) and (43) denotes the integer part of x, i.e., $[x]$ is the largest integer $\leqslant x$. Since the spectral point k_n, and only k_n, is located between the root separators $k_n^<$ and $k_n^>$, we compute k_n with the help of the density of states (38):

$$k_n = \int_{k_n^<}^{k_n^>} k\rho(k)\, dk. \tag{44}$$

A partial integration yields

$$k_n = nk_n^> - (n-1)k_n^< - \int_{k_n^<}^{k_n^>} N(k)\, dk. \tag{45}$$

Thus the problem of computing k_n is reduced to a quadrature. Since all the quantities on the right-hand side of (45) are known, k_n is now known explicitly.

Some of the integrals in (45) can be done analytically. We obtain

$$k_n = (n+1)k_n^> - nk_n^< - \frac{1}{2\pi}\left[(k_n^>)^2 - (k_n^<)^2\right] - \frac{1}{\pi}\left[\varphi(k_n^>; v) - \varphi(k_n^<; v)\right]$$
$$- \frac{2}{\pi} \sum_{m=1}^{\infty} \frac{1}{m} \int_{k_n^<}^{k_n^>} \left\{ \sin(mk) T_m\left(\frac{v}{\sqrt{v^2 + k^2}}\right) \right.$$
$$\left. + \frac{k}{\sqrt{v^2 + k^2}} \cos(mk) U_{m-1}\left(\frac{v}{\sqrt{v^2 + k^2}}\right) \right\} T_m\left(\frac{v}{\sqrt{v^2 + k^2}} \cos(\omega k)\right) dk, \tag{46}$$

where

$$\varphi(k; v) = k \arccos\left(\frac{v}{\sqrt{v^2 + k^2}}\right) - \frac{v}{2}\ln(v^2 + k^2), \quad k > 0. \tag{47}$$

The result (46) solves the problem of obtaining an explicit, exact and analytical expression for the spectral points k_n in the form $k_n = f(n; v, \omega)$, where f is the same for all n. The result (46) is not the only way of computing k_n. In the following section we go one step further and derive an exact periodic-orbit expansion for the spectral points k_n. Apart from presenting an alternative expression for k_n, it adds physical insight to the solution formulae, since each term in the expansions has a direct physical interpretation.

3.3. Binary necklaces

In this section we derive an exact formula for k_n which is based on classical periodic orbits. These orbits can be enumerated and manipulated with the help of symbolic dynamics [10] and the theory of binary necklaces [8, 19].

A symbolic dynamics for the compressed delta atom is obtained if we label the left-hand and right-hand potential walls with the symbols $\mathcal{L}$ and $\mathcal{R}$, respectively. This way any orbit, Newtonian or non-Newtonian [20], bouncing between the two walls, or between the walls and the δ-function potential, can be coded with binary words [9, 12, 13]. An example is the word $w = \mathcal{L}\mathcal{L}\mathcal{R}$. It corresponds to a classical trajectory originating somewhere between the left-hand wall and the δ-function potential with a velocity directed toward the left-hand potential wall, bouncing off the left-hand potential wall (symbol $\mathcal{L}$), then bouncing off the δ-function (no symbol necessary) and heading back to the left-hand potential wall, bouncing off this wall (symbol $\mathcal{L}$), then transmitting through the δ-function potential (no symbol necessary), bouncing off the right-hand wall (symbol $\mathcal{R}$), and after a second transmission through the δ-function potential completing its journey by joining up with its starting point. Apparently, compared to the verbal description of the history of this trajectory, the symbolic description is very concise. On the other hand, as indicated by the phrase '...originating somewhere between ...', the symbolic description does not convey all the information on the history of a classical trajectory. In the case of periodic orbits, however, and only these are needed for the explicit formulae below, the start- and end-points of a classical trajectory are irrelevant, and the symbolic description conveys all we need to know about a particular classical orbit.

A word w is turned into a necklace $\hat{w}$ with the help of the 'hat function' $\hat{\ }$. Words and necklaces are different. Words are linear strings of symbols, with a beginning and an end, while necklaces are symbol strings that are interpreted cyclically. In fact this is where the word 'necklace' comes from—by imagining the symbols arranged in a circle like pearls in a necklace. We use words to describe trajectories that have a beginning and an end; we use necklaces to describe periodic orbits without beginning or end. To illustrate, while $w_1 = \mathcal{R}\mathcal{L}\mathcal{L}$ and $w_2 = \mathcal{L}\mathcal{R}\mathcal{L}$ are two different words, turning them into necklaces, they are equal, i.e., $w_1 \neq w_2$, but $\hat{w}_1 = \hat{w}_2$. Although, in general, necklaces may contain an arbitrary number of different symbols, the two symbols $\mathcal{L}$ and $\mathcal{R}$ suffice for the purposes of this paper. Necklaces constructed from two symbols are called binary necklaces.

Next, we define functions that take words or necklaces as arguments. An example of a word function is $l(w)$. It counts the number of symbols in w. Its necklace analogue is the necklace function $\hat{l}(\hat{w})$, which returns the number of symbols in $\hat{w}$. Apparently $l(w) = \hat{l}(\hat{w})$. We also define the necklace functions $\hat{n}_\mathcal{L}(\hat{w})$ and $\hat{n}_\mathcal{R}(\hat{w})$, which count the number of symbols $\mathcal{L}$ and $\mathcal{R}$ in $\hat{w}$, respectively. Apparently we have $\hat{l}(\hat{w}) = \hat{n}_\mathcal{L}(\hat{w}) + \hat{n}_\mathcal{R}(\hat{w})$. In addition to the

necklace functions $\hat{l}$, $\hat{n}_{\mathcal{L}}$ and $\hat{n}_{\mathcal{R}}$, we define the following two necklace functions, which will turn out to be useful later:

$$\hat{\alpha}(\hat{w}) = \hat{n}_{\mathcal{LL}}(\hat{w}) + \hat{n}_{\mathcal{RR}}(\hat{w}), \qquad \hat{\beta}(\hat{w}) = \hat{n}_{\mathcal{LR}}(\hat{w}) + \hat{n}_{\mathcal{RL}}(\hat{w}), \qquad (48)$$

where $\hat{n}_{\mathcal{LL}}$, $\hat{n}_{\mathcal{LR}}$, $\hat{n}_{\mathcal{RL}}$ and $\hat{n}_{\mathcal{RR}}$ count the number of $\mathcal{LL}$, $\mathcal{LR}$, $\mathcal{RL}$ and $\mathcal{RR}$ pairs in $\hat{w}$, respectively. We have to be careful to keep in mind that necklaces are defined cyclically. If, e.g., $\hat{w} = \mathcal{RR}$ then $\hat{n}_{\mathcal{RR}}(\hat{w}) = 2$, although the word $w = \mathcal{RR}$ contains only one $\mathcal{RR}$ pair. But recalling that a necklace is a word 'wrapped around', with symbols arranged in a circle, it becomes clear that $\hat{n}_{\mathcal{RR}}(\hat{w}) = 2$, not 1.

In order to derive a periodic-orbit expansion for the spectral points k_n, our first goal is the derivation of a periodic-orbit expansion of the staircase function (35). Again we start with (40), but proceed in such a way as to obtain an explicit expression of $N(k)$ in terms of the S matrix itself

$$N(k) = -1 + \frac{k}{\pi} + \frac{1}{\pi} \arccos\left(\frac{v}{\sqrt{v^2 + k^2}}\right) + \frac{1}{\pi} \sum_{j=1}^{4} \sum_{m=1}^{\infty} \frac{\sin(m\sigma_j)}{m}$$

$$= -1 + \frac{k}{\pi} + \frac{1}{\pi} \arccos\left(\frac{v}{\sqrt{v^2 + k^2}}\right) + \frac{1}{2\pi} \operatorname{Im} \operatorname{Tr} \sum_{m=1}^{\infty} \frac{1}{m} S^{2m}(k), \qquad (49)$$

where we used the fact that $\operatorname{Tr} S^{2m+1} = 0$ for all m. Writing out the first few traces of the even powers of S, with S defined in (30), shows that

$$\operatorname{Tr} S^{2m} = 2(-1)^m \sum_{w, l(w)=m} r^{\hat{\alpha}(\hat{w})} t^{\hat{\beta}(\hat{w})} e^{2i\hat{\sigma}(\hat{w})k}, \qquad (50)$$

where

$$\hat{\sigma}(\hat{w}) = \left(\frac{1+\omega}{2}\right) \hat{n}_{\mathcal{L}}(\hat{w}) + \left(\frac{1-\omega}{2}\right) \hat{n}_{\mathcal{R}}(\hat{w}). \qquad (51)$$

Note that the sum in (50) is over the 2^m *words* that can be formed with m symbols $\mathcal{L}$, $\mathcal{R}$, but that these words are turned into binary *necklaces* by the functions $\hat{\alpha}$, $\hat{\beta}$ and $\hat{\sigma}$ occurring in the exponents of (50).

Since any word w can be broken up into $\nu \geqslant 1$ repetitions of its shortest building block w_p (which may be w itself, in which case $\nu = 1$), and since (50) is invariant under cyclic permutations of the symbols in w, we can write (50) in the form

$$\operatorname{Tr} S^{2m} = 2 \sum_{\hat{w}_p} \sum_{\nu \hat{l}(\hat{w}_p)=m} \hat{l}(\hat{w}_p) [(-1)^{\hat{l}(\hat{w}_p)} r^{\hat{\alpha}(\hat{w}_p)} t^{\hat{\beta}(\hat{w}_p)}]^{\nu} e^{2i\nu\hat{\sigma}(\hat{w}_p)k}, \qquad (52)$$

where the sum is over all primitive binary necklaces $\hat{w}_p$, i.e., necklaces that cannot be broken down into repetitions of shorter binary necklaces. We use (52) to obtain a periodic-orbit expansion of the staircase function (35). With $m = \nu\hat{l}(\hat{w}_p)$ we obtain from (49)

$$N(k) = -1 + \frac{k}{\pi} + \frac{1}{\pi} \arccos\left(\frac{v}{\sqrt{v^2 + k^2}}\right)$$

$$+ \frac{1}{\pi} \operatorname{Im} \sum_{m=1}^{\infty} \sum_{\hat{w}_p} \sum_{\nu \hat{l}(\hat{w}_p)=m} \frac{1}{\nu} [(-1)^{\hat{l}(\hat{w}_p)} r^{\hat{\alpha}(\hat{w}_p)} t^{\hat{\beta}(\hat{w}_p)}]^{\nu} e^{2i\nu\hat{\sigma}(\hat{w}_p)k}. \qquad (53)$$

Using (53) in (45) we obtain an exact, explicit periodic-orbit expansion of the spectral points k_n of the compressed delta atom

$$k_n = (n+1)k_n^> - nk_n^< - \frac{1}{2\pi}\left[\left(k_n^>\right)^2 - \left(k_n^<\right)^2\right] - \frac{1}{\pi}\left[\varphi\left(k_n^>; v\right) - \varphi\left(k_n^<; v\right)\right]$$

$$- \frac{1}{\pi}\,\mathrm{Im}\sum_{m=1}^{\infty}\sum_{\hat{w}_p}\sum_{\nu\hat{l}(\hat{w}_p)=m}\frac{1}{\nu}\int_{k_n^<}^{k_n^>}[(-1)^{\hat{l}(\hat{w}_p)}r^{\hat{\alpha}(\hat{w}_p)}t^{\hat{\beta}(\hat{w}_p)}]^{\nu}\,\mathrm{e}^{2\mathrm{i}\nu\hat{\sigma}(\hat{w}_p)k}\,\mathrm{d}k. \qquad (54)$$

Each term in the necklace sum of (54) has a direct physical interpretation. We see this in the following way. Each necklace $\hat{w}_p$ corresponds to a classical periodic orbit. Thus, each $\mathcal{LL}$ or $\mathcal{RR}$ pair in (54) can be interpreted physically as a reflection off the δ-function potential. In the same way each $\mathcal{LR}$ or $\mathcal{RL}$ pair in (54) corresponds to a transmission through the δ-function potential. Since $\hat{\alpha}(\hat{w}_p)$ is the sum of all $\mathcal{LL}$ and $\mathcal{RR}$ pairs in $\hat{w}_p$, it corresponds physically to the total number of reflections off the δ-function potential. Similarly $\hat{\beta}(\hat{w}_p)$ counts the total number of transmissions. Since each reflection off the walls of the potential at $x = 0, b$ contributes a phase factor -1, the term in square brackets under the integral sign in (54) corresponds physically to the total reflection and transmission amplitude of the classical periodic orbit represented by $\hat{w}_p$. The exponential term is an action-dependent phase factor akin to the one that appears in Gutzwiller's trace formula [10] or Feynman's path integral [21]. Thus (54) solves the problem of obtaining a physical series expansion of k_n in the spirit of (2).

4. Negative-energy state

As discussed in section 2.1, a negative-energy solution κ_1 of (8) exists only for $v < v_c$, where v_c is defined in (10). Evaluating $\tilde{h}(\kappa; v, \omega)$, defined in (12), at the root separators (20), and using $|v| > |v_c|$ for a non-trivial κ_1 to exist, we obtain $\tilde{h}(\kappa_1^<; v, \omega) < 0$ and $\tilde{h}(\kappa_1^>; v, \omega) > 0$. In addition, using the fact, proved in section 2.1, that $\tilde{h}(\kappa; v, \omega)$ is a monotonically increasing function of κ, we obtain $|\tilde{h}(\kappa; v, \omega)| < 2\pi$ in the entire root interval $\kappa_1^< = 0 \leqslant \kappa \leqslant \kappa_1^> = |v|$. Therefore, since $\tilde{h}(\kappa_1; v, \omega) = 0$, we may choose the following explicit form of the $E < 0$ staircase function,

$$N(\kappa) = \Theta_{2\pi}[\tilde{h}(\kappa; v, \omega)] + 1 = \frac{1}{2} + \frac{\tilde{h}(\kappa; v, \omega)}{2\pi} + \frac{1}{\pi}\sum_{m=1}^{\infty}\frac{1}{m}\sin[m\tilde{h}(\kappa; v, \omega)]. \qquad (55)$$

This result can now be used to obtain κ_1 explicitly via quadrature

$$\kappa_1 = \int_0^{|v|}\kappa\rho(\kappa)\,\mathrm{d}\kappa = |v| - \int_0^{|v|}N(\kappa)\,\mathrm{d}\kappa. \qquad (56)$$

5. The scaling case

A potential strength linearly dependent on the momentum,

$$v = \eta k, \qquad (57)$$

where η is a (positive, or negative) constant, defines the *scaling, compressed delta atom*. A possible experimental realization of the scaling, compressed delta atom is discussed in section 8.1.

5.1. Spectral equations and structure of the scaling spectrum

In the scaling case the $E > 0$ spectral equation is

$$g_s(k; \eta, \omega) = 0, \qquad (58)$$

where the spectral function g_s, obtained from (6), is given by

$$g_s(k; \eta, \omega) = \eta \cos(k) - \sin(k) - \eta \cos(\omega k). \tag{59}$$

For the computation of the spectrum of special cases in section 6 it is convenient to rewrite (58) (with (59)) according to

$$-2\eta \sin\left[\left(\frac{1+\omega}{2}\right)k\right] \sin\left[\left(\frac{1-\omega}{2}\right)k\right] = \sin(k) \tag{60}$$

or, if $\sin[k(1-\omega)/2)] \sin[k(1+\omega)/2] \neq 0$,

$$\cot\left[\left(\frac{1+\omega}{2}\right)k\right] + \cot\left[\left(\frac{1-\omega}{2}\right)k\right] = -2\eta. \tag{61}$$

In the case $E < 0$ the spectral equation is

$$h_s(\kappa; \eta, \omega) = 0, \tag{62}$$

where $h_s(\kappa; \eta, \omega)$, obtained from (8) with $v = \eta\kappa$, is

$$h_s(\kappa; \eta, \omega) = \eta \cosh(\kappa) + \sinh(\kappa) - \eta \cosh(\omega\kappa). \tag{63}$$

Using trigonometric formulae for the hyper functions we write (63) in the form

$$-2\eta \sinh\left[\left(\frac{1+\omega}{2}\right)\kappa\right] \sinh\left[\left(\frac{1-\omega}{2}\right)\kappa\right] = \sinh(\kappa). \tag{64}$$

Writing the right-hand side of (64) in the form $\sinh[(1+\omega)\kappa/2 + (1-\omega)\kappa/2]$ and using the appropriate sum formula for hyper functions, (64) is transformed into

$$\coth\left[\left(\frac{1+\omega}{2}\right)\kappa\right] + \coth\left[\left(\frac{1-\omega}{2}\right)\kappa\right] = -2\eta. \tag{65}$$

A possible negative-energy state is a non-trivial solution of (65) with $\kappa > 0$. Since $0 \leqslant \omega < 1$, the arguments of the coth functions in (65) are positive, which implies that both coth functions are larger than 1. This implies the necessary condition

$$\eta < -1 \tag{66}$$

for a non-trivial solution of (65) to exist.

In the scaled case a non-trivial k_1 exists for all η. Therefore, we adopt a labelling scheme that differs slightly from the scheme used in the non-scaling case: we use the label '0' for the negative-energy state and, therefore, κ_0 for the real solution of (62).

5.2. Root separators

For $E > 0$, the root separators in the scaling case are the same as the root separators in the non-scaling case. This is immediately obvious since $k_n(\eta)$ can be obtained from $k_n(v)$ via a smooth transformation of the arguments. Thus, since $k_n(v)$ is confined to the root intervals (18), so is $k_n(\eta)$. The only difference occurs for $k_1(\eta)$, which now is defined for all η. Thus one set of root separators of (58) is

$$k_n^<(\eta) = \begin{cases} n\pi & \text{for } \eta > 0, \\ (n-1)\pi & \text{for } \eta < 0, \end{cases} \qquad k_n^>(\eta) = k_n^<(\eta) + \pi. \tag{67}$$

An equally valid set of root separators of (58) is obtained as follows. Writing (58) in the form

$$\cos[k + \Phi(\eta)] = \beta(\eta) \cos(\omega k), \qquad \beta(\eta) = \frac{\eta}{\sqrt{1 + \eta^2}},$$

$$\Phi(\eta) = \arccos[\beta(\eta)] = \arctan(1/\eta), \tag{68}$$

we obtain the root separators

$$k_n^<(\eta) = n\pi - \Phi(\eta), \qquad k_n^>(\eta) = k_n^<(\eta) + \pi, \qquad n = 1, 2, \ldots. \qquad (69)$$

While the set (67) of root separators is characterized by simplicity and has advantages for obtaining concise quadrature and periodic-orbit expansions, the set (69) is valid for both positive and negative η and for both generic and non-generic levels.

We turn now to the case $E < 0$. Since $\kappa > 0$, we choose $\kappa_0^< = 0$. A root separator $\kappa_0^>$ may be obtained from (65) according to the following reasoning. For small enough κ and $\omega > 0$, the left-hand side of (65) is larger than $2|\eta|$. If we require

$$\coth\left[(1 - \omega)\kappa_0^>/2\right] = |\eta|, \qquad (70)$$

and since coth is a monotonically decreasing function for positive arguments, it is guaranteed that for $\omega > 0$ the left-hand side of (65) is smaller than $2|\eta|$ and that $\kappa_0^< < \kappa_0 < \kappa_0^>$. From (70) we obtain

$$\kappa_0^> = \frac{1}{1 - \omega} \ln\left(\frac{\eta - 1}{\eta + 1}\right), \qquad \eta < -1, \quad \omega > 0. \qquad (71)$$

The case $\omega = 0$ is solved in section 6.1; no root separators are required in this case.

5.3. Explicit, integral-free solution formulae

We derive an exact, integral-free formula for the solutions $k_n^{(s)}$ of the transcendental spectral equation (59) in the following way. In the scaling case, the staircase function (41) is

$$N(k) = -1 + \frac{k}{\pi} + \frac{\Phi}{\pi} + \frac{2}{\pi} \sum_{m=1}^{\infty} \frac{1}{m} \left\{ \sin(mk) T_m(\beta) + \frac{\beta}{\eta} \cos(mk) U_{m-1}(\beta) \right\} T_m[\beta \cos(\omega k)], \qquad (72)$$

where we used β and Φ defined in (68). We use expression (72) in (45) to obtain an integral-free expression for the spectral points $k_n^{(s)}$:

$$k_n^{(s)} = \frac{1}{2\pi}\left[\left(k_n^>\right)^2 - \left(k_n^<\right)^2\right] - \frac{2}{\pi} \sum_{m=1}^{\infty} \frac{1}{m} \left\{ T_m(\beta) S_m\left(k_n^<, k_n^>; \beta, \omega\right) \right.$$
$$\left. + \frac{\beta}{\eta} U_{m-1}(\beta) C_m\left(k_n^<, k_n^>; \beta, \omega\right) \right\}, \qquad (73)$$

where $k_n^<$ and $k_n^>$ are the root separators defined in (69), the functions $C_m(a, b; \beta, \omega)$ and $S_m(a, b; \beta, \omega)$ are defined as

$$C_m(a, b; \beta, \omega) = \int_a^b \cos(mk) T_m[\beta \cos(\omega k)] \, dk$$
$$= \sum_{\mu=0}^{[m/2]} \Gamma_{m\mu} \beta^{m-2\mu} [c_{m,m-2\mu}(b; \omega) - c_{m,m-2\mu}(a; \omega)] \qquad (74)$$

and

$$S_m(a, b; \beta, \omega) = \int_a^b \sin(mk) T_m[\beta \cos(\omega k)] \, dk$$
$$= \sum_{\mu=0}^{[m/2]} \Gamma_{m\mu} \beta^{m-2\mu} [s_{m,m-2\mu}(b; \omega) - s_{m,m-2\mu}(a; \omega)] \qquad (75)$$

with

$$c_{mv}(k; \omega) = \int \cos(mk) \cos^v(\omega k) \, dk$$

$$= \frac{1}{2^v} \sum_{\mu=0}^{v} \binom{v}{\mu} \begin{cases} k, & \text{if } m + v\omega - 2\mu\omega = 0, \\ \dfrac{\sin[(m + v\omega - 2\mu\omega)k]}{m + v\omega - 2\mu\omega}, & \text{if } m + v\omega - 2\mu\omega \neq 0 \end{cases} \tag{76}$$

and

$$s_{mv}(k; \omega) = \int \sin(mk) \cos^v(\omega k) \, dk$$

$$= \frac{1}{2^v} \sum_{\mu=0}^{v} \binom{v}{\mu} \begin{cases} 0, & \text{if } m + v\omega - 2\mu\omega = 0, \\ \dfrac{-\cos[(m + v\omega - 2\mu\omega)k]}{m + v\omega - 2\mu\omega}, & \text{if } m + v\omega - 2\mu\omega \neq 0. \end{cases} \tag{77}$$

In the scaling case the reflection and transmission amplitudes (32) are constants given by

$$r = \frac{\eta}{i - \eta}, \qquad t = \frac{i}{i - \eta}. \tag{78}$$

Therefore, the integrals in (54) can be performed analytically. We obtain the following exact, integral-free periodic-orbit expansions:

$$k_n^{(s)} = (n + 1)k_n^> - nk_n^< - \frac{1}{2\pi} \left[(k_n^>)^2 - (k_n^<)^2 \right] - \frac{1}{\pi} (k_n^> - k_n^<) \Phi(\eta)$$

$$- \frac{1}{\pi} \text{Im} \sum_{m=1}^{\infty} \sum_{\hat{w}_p} \sum_{v\hat{l}(\hat{w}_p)=m} \frac{1}{2iv^2\hat{\sigma}(\hat{w}_p)} [(-1)^{\hat{l}(\hat{w}_p)} r^{\hat{\alpha}(\hat{w}_p)} t^{\hat{\beta}(\hat{w}_p)}]^v$$

$$\times \left[e^{2iv\hat{\sigma}(\hat{w}_p)k_n^>} - e^{2iv\hat{\sigma}(\hat{w}_p)k_n^<} \right]. \tag{79}$$

In many cases the periodic-orbit expansion (79) simplifies considerably. For generic levels and $\eta > 0$, e.g., (79) reduces to

$$k_n^{(s)} = n\pi + \frac{\pi}{2} - \Phi(\eta) - \frac{1}{\pi} \text{Im} \sum_{m=1}^{\infty} \sum_{\hat{w}_p} \sum_{v\hat{l}(\hat{w}_p)=m} \frac{1}{\hat{\sigma}(\hat{w}_p)v^2}$$

$$\times [(-1)^{\hat{l}(\hat{w}_p)} r^{\hat{\alpha}(\hat{w}_p)} t^{\hat{\beta}(\hat{w}_p)}]^v \, e^{i(2n+1)v\pi\hat{\sigma}(\hat{w}_p)} \sin[v\pi\hat{\sigma}(\hat{w}_p)], \tag{80}$$

where we used the root separators (67).

6. Rational ω

In sections 3–5 we presented a complete solution of the spectral problem of the compressed (scaling) delta atom using quadratures and periodic-orbit expansions. In some cases, in particular for rational ω, spectral solutions may be obtained independently using different solution methods. For instance, for any rational ω, a subset of the spectrum is immediately known according to (14). Computation of a spectrum via both a periodic-orbit expansion and a different, independent method offers the possibility to derive as yet unknown combinatorial identities [8] or to compute the value of infinite sums (see section 6.1).

A host of alternative, independent spectral solutions, e.g., is provided in the scaling case for some rational ω values (see, e.g., sections 6.1–6.3). In these cases the entire spectrum of the scaling, compressed delta atom can be computed and expressed explicitly in terms of radicals. The reason is the following. While even in the scaling case irrational ω produce

transcendental spectral equations, rational ω produce spectral equations that may be expressed as polynomial equations. The cases $\omega = 0, 1/3, 1/2$, e.g., lead to polynomial equations of orders one, two and three, respectively. The complete spectra for these three cases are worked out explicitly in sections 6.1–6.3, respectively. Not explicitly worked out in this paper are the cases $\omega = 1/5, 3/5$. They lead to quartic polynomial equations, which, if desired, may be solved by radicals, too [22].

6.1. $\omega = 0$

From (61) together with (14) the complete $E > 0$, $\omega = 0$ spectrum is

$$k_N^{(1)} = (2N - 1)\pi + 2\arctan(\eta),$$

$$k_N^{(2)} = 2N\pi, \qquad N = 1, 2, \ldots.$$
(81)

With (65) we obtain for the $E < 0$ solution

$$\kappa_0 = \ln\left(\frac{\eta - 1}{\eta + 1}\right), \qquad \eta < -1.$$
(82)

Alternatively we may express $k_N^{(1,2)}$ with the help of quadrature formulae. For $E > 0$, $\omega = 0$, the staircase function (72) is

$$N(k) = -1 + \frac{k}{\pi} + \frac{\Phi}{\pi} + \frac{2}{\pi} \sum_{m=1}^{\infty} \frac{1}{m} \left[\sin(mk)T_m(\beta) + \frac{\beta}{\eta} \cos(mk)U_{m-1}(\beta) \right] T_m(\beta).$$
(83)

For $0 < \eta < \infty$, the level $k_1^{(1)}$ is found in the root interval $[\pi, 2\pi]$. Since we are going to use this root interval as an integration interval, it does not matter that $k_1^{(2)}$ coincides with the upper edge of the root interval. With (45) we obtain

$$k_1^{(1)} = 2\pi - \int_{\pi}^{2\pi} N(k) \, dk.$$
(84)

Equating (81) and (84) we obtain the following sum rule for Chebyshev polynomials:

$$\sum_{m=1}^{\infty} \frac{1}{(2m-1)^2} T_{2m-1}^2(x) = \frac{\pi}{4} \arctan\left(\frac{x^2}{1-x^2}\right)^{1/2}, \qquad |x| \leqslant 1.$$
(85)

This result illustrates how a combination of quadrature solutions and an independent solution can be used to compute infinite sums, in this case a sum rule for Chebyshev polynomials.

6.2. $\omega = 1/3$

Using $\omega = 1/3$ in (61) and substituting $x = \cot(k/3)$ we obtain the quadratic equation

$$3x^2 + 4\eta x - 1 = 0$$
(86)

with the two solutions

$$x_{1,2} = -\tfrac{2}{3}\eta \pm \tfrac{1}{3}\sqrt{4\eta^2 + 3}.$$
(87)

Transforming back to k and supplementing the resulting two solutions with (14) we obtain the complete $E > 0$ spectrum

$$k_N^{(1)} = 3\arccos\left(\frac{1}{2\sqrt{1+\eta^2}}\sqrt{2\eta^2 + 1 - \eta\sqrt{4\eta^2 + 3}}\right) + 3N\pi,$$

$$k_N^{(2)} = 3\arccos\left(\frac{-1}{2\sqrt{1+\eta^2}}\sqrt{2\eta^2 + 1 + \eta\sqrt{4\eta^2 + 3}}\right) + 3N\pi,$$
(88)

$$k_N^{(3)} = 3\pi + 3N\pi, \qquad N = 0, 1, 2, \ldots.$$

We now turn to the case $E < 0$. Starting from (65) with $\omega = 1/3$ and $x = \coth(\kappa/3)$ we obtain the quadratic equation

$$3x^2 + 4x\eta + 1 = 0. \tag{89}$$

Solving this equation and using the root that leads to real, positive κ we obtain

$$\kappa_0 = 3\operatorname{arccosh}\left(\frac{1}{2\sqrt{\eta^2 - 1}}\sqrt{2\eta^2 - 1 - \eta\sqrt{4\eta^2 - 3}}\right), \qquad \eta < -1, \tag{90}$$

where ([23], formula 4.6.21)

$$\operatorname{arccosh}(x) = \ln\left(x + \sqrt{x^2 - 1}\right). \tag{91}$$

6.3. $\omega = 1/2$

This case is more difficult than the case $\omega = 1/3$, since it involves the solution of a polynomial equation of order three. We treat the case $E > 0$ first. Substituting $x = \cot(k/4)$ the spectral equation (61) for $\omega = 1/2$ is transformed into the cubic equation

$$x^3 + \tfrac{3}{2}\eta x^2 - x - \tfrac{1}{2}\eta = 0. \tag{92}$$

The roots of (92) are [22]

$$x_1 = -2r\cos\left(\frac{\varphi}{3}\right) - \frac{\eta}{2}, \qquad x_2 = 2r\cos\left(\frac{\pi}{3} + \frac{\varphi}{3}\right) - \frac{\eta}{2}, \qquad x_3 = 2r\cos\left(\frac{\pi}{3} - \frac{\varphi}{3}\right) - \frac{\eta}{2}, \tag{93}$$

where

$$q = \frac{1}{8}\eta^3, \qquad r = \operatorname{sign}(q)\left(\frac{4 + 3\eta^2}{12}\right)^{1/2}, \qquad \cos(\varphi) = q/r^3. \tag{94}$$

From (94) together with (14) we obtain the complete $E > 0$ spectrum

$$k_N^{(j)} = 4\operatorname{arccot}(x_j) + 4N\pi, \qquad k_N^{(4)} = 4\pi + 4N\pi, \qquad j = 1, 2, 3, \quad N = 0, 1, 2, \ldots. \tag{95}$$

For $E < 0$, we substitute $x = \coth(\kappa/4)$, which turns (65) into

$$x^3 + \tfrac{3}{2}\eta x^2 + x + \tfrac{1}{2}\eta = 0. \tag{96}$$

Defining

$$p = \frac{4 - 3\eta^2}{12}, \qquad r = -\sqrt{|p|}, \qquad \tan(\psi) = [\tan(\varphi/2)]^{1/3},$$

$$\varphi = \begin{cases} \arctan(r^3/q), & \text{for } p > 0, \\ \arcsin(r^3/q), & \text{for } p < 0, \end{cases} \tag{97}$$

where q is defined in (94), the real solution of (96) is [22]

$$\xi = \begin{cases} -2r\cot(2\psi) - \eta/2, & \text{for } p > 0, \\ (1 + 2^{1/3})/\sqrt{3}, & \text{for } p = 0, \\ -[2r/\sin(2\psi)] - \eta/2, & \text{for } p < 0. \end{cases} \tag{98}$$

With ξ defined in (98) we obtain for $E < 0$

$$\kappa_1 = 2\ln\left(\frac{\xi + 1}{\xi - 1}\right). \tag{99}$$

7. Convergence

Since the periodic-orbit expansions (46), (54), (73) and (79) are derived via integration from a piecewise constant (staircase) function, they converge. In this section we show even more: the expansions (46), (54), (73) and (79) converge *absolutely*. The purpose of this section is to provide the necessary proofs.

We start by proving that (46) is absolutely convergent. To this end, we observe that the integral in (46) can be cast into trigonometric form according to

$$
\begin{aligned}
I_{nm}(v, \omega) &= \int_{k_n^<}^{k_n^>} \left\{ \sin(mk) T_m \left(\frac{v}{\sqrt{v^2 + k^2}} \right) + \frac{k}{\sqrt{v^2 + k^2}} \cos(mk) U_{m-1} \left(\frac{v}{\sqrt{v^2 + k^2}} \right) \right\} \\
&\quad \times T_m \left(\frac{v}{\sqrt{v^2 + k^2}} \cos(\omega k) \right) \mathrm{d}k \\
&= \frac{1}{2} \int_{k_n^<}^{k_n^>} \{ \sin[m f^{(+)}(k; v, \omega)] + \sin[m f^{(-)}(k; v, \omega)] \} \, \mathrm{d}k,
\end{aligned}
\tag{100}
$$

where $f^{(\pm)}(k; v, \omega)$ are the spectral functions (26). For fixed integration limits it is straightforward to prove

$$
\int_a^b \sin[m f(x)] \, \mathrm{d}x \sim \begin{cases} 1/m, & \text{if } f'(x) \neq 0 \text{ in } [a, b] \\ 1/\sqrt{m}, & \text{if } f'(x) \text{ has simple zeros in } [a, b] \end{cases}
\tag{101}
$$

for large m and for any smooth function $f(x)$. Since the derivatives $\partial f^{(\pm)}(k; v, \omega)/\partial k$ of the spectral functions (26) have at most simple zeros, the absolute value of the integral (100) can be estimated as

$$
|I_{nm}(v, \omega)| < \gamma_n(v, \omega)/\sqrt{m},
\tag{102}
$$

where the positive constant $\gamma_n(v, \omega)$ may depend on n, v and ω, but does not depend on m. With this result we can estimate the sum in (46) as

$$
\left| \sum_{m=1}^{\infty} \frac{1}{m} I_{nm}(v, \omega) \right| \leqslant \sum_{m=1}^{\infty} \frac{1}{m} |I_{nm}(v, \omega)| < \gamma_n(v, \omega) \sum_{m=1}^{\infty} \frac{1}{m^{3/2}} = \gamma_n(v, \omega) \zeta(3/2),
\tag{103}
$$

where $\zeta(x)$ is Riemann's zeta function [18]. Equation (103) shows that the sum in (46) converges. But (103) shows even more: sum over the absolute values of the individual terms of the sum, $\sum_{m=1}^{\infty} |I_{nm}(v, \omega)/m|$, is finite, too. This shows that the m-sum in (46) is absolutely convergent. Since the periodic-orbit terms in the m-sum of (54) sum up to the corresponding m-terms in (46), the m-sum in (54) converges absolutely, too.

We now prove the absolute convergence of (73). Defining

$$
D_n^{(M)} = \pi \left| k_n^{(s)} - k_{n,M}^{(s)} \right|,
\tag{104}
$$

where $k_{n,M}^{(s)}$ is an approximation to $k_n^{(s)}$ obtained by including the first M terms in the m sum of (73), we obtain

$$
D_n^{(M)} = \left| \sum_{m=M+1}^{\infty} \frac{1}{m} \int_{k_n^<}^{k_n^>} \{ \sin[m F^{(+)}(k; \eta, \omega)] + \sin[m F^{(-)}(k; \eta, \omega)] \} \, \mathrm{d}k \right|,
\tag{105}
$$

where

$$
F^{(\pm)}(k; \eta, \omega) = k + \arccos[\beta(\eta)] \pm \arccos[\beta(\eta) \cos(\omega k)]
\tag{106}
$$

are the scaled versions of the spectral functions (26). Because of the simple structure of $F^{(\pm)}(k; \eta, \omega)$ defined in (106), it is straightforward to prove that $\partial F^{(-)}(k; \eta, \omega)/\partial k > 0$ for

all k and $\partial F^{(+)}(k; \eta, \omega)/\partial k$ has at most a countable number of simple zeros. This shows that $D_n^{(M)} < \tilde{\gamma}_n(\eta, \omega)/\sqrt{M}$, where $\tilde{\gamma}_n(\eta, \omega) > 0$ is a constant which may depend only on n, η and ω, but is independent of M. This implies $D_n^{(M)} \to 0$ for $M \to \infty$. Therefore (73) converges. Apparently, since each term in the m-sum of (105) $\sim 1/m^{3/2}$, the convergence behaviour of $D_n^{(M)}$ is unchanged if we sum over the absolute values of the m-terms. This means that (73) is absolutely convergent. Since, up to a global, m-independent constant, each m-term in (79) is the same as the corresponding term in (73), (79) converges absolutely, too.

One might be tempted to replace $\Sigma_1 = \sum_{m=1}^{\infty} \sum_{\hat{w}_p} \sum_{v\hat{l}(\hat{w}_p)=m}$ by $\Sigma_2 = \sum_{\hat{w}_p} \sum_{v=1}^{\infty}$ in the periodic-orbit expansions (53), (54), (79) and (80). But while Σ_1 is absolutely convergent (we proved it above), Σ_2, in general, is not. Therefore, according to Riemann's reordering theorem, it is not guaranteed that Σ_2 converges to the same result as Σ_1. Thus, in general, the replacement $\Sigma_1 \to \Sigma_2$ is not allowed.

So far we proved that the periodic-orbit expansions converge. But do they converge to the correct spectral values? The answer is yes. Qualitatively the reason is the following. Since the quadrature formulae and the periodic-orbit expansions are equivalent, and since the periodic-orbit expansions converge absolutely, the quadrature formulae and the periodic-orbit expansions converge to the same spectral values. But since the quadrature formulae, by construction, converge to the correct spectral values, the periodic-orbit expansions do so, too. More formal proofs can be adapted from the proofs presented in [9, 13, 24]. Thus, in summary, the periodic-orbit expansions (46), (54), (73) and (79) converge absolutely to the correct spectral eigenvalues.

8. Discussion

Delta-function potentials provide basic model systems in physics and chemistry. In nuclear physics, e.g., Skyrme and Gogny potentials are constructed with the help of delta functions and lead to energy functionals that reproduce the binding energies of atomic nuclei with surprising accuracy over the entire nuclear chart of stable and unstable nuclei [25]. In quantum chemistry the nature of atomic and molecular binding is most effectively demonstrated with the help of delta-function potentials [26]. In atomic physics a 'kicked delta atom' has been used to study time-dependent ionization processes [27]. The compressed delta atom is another well-known model system that has been used to illustrate important points about perturbation theory [6]; it is discussed in text books (see, e.g., [28], problem 5 on page 164; [29], problems 13.3 on page 300 and 13.4 on page 301). We use the compressed delta atom as an illustrative, physical system to demonstrate how to solve transcendental spectral equations in order to obtain the spectral points explicitly, exactly and analytically via quadratures and periodic-orbit expansions. The solution of the compressed delta atom may be used as a blue print for the solution of many other quantum systems with transcendental spectral equations.

8.1. Experimental realization

Ten years ago it has been suggested to realize scaling quantum systems as microwave cavities with dielectric inserts [30]. These microwave systems have the same spectral equations as their quantum analogues. Several quasi two-dimensional microwave experiments with dielectric inserts have already been performed successfully [20, 31–33].

A quasi one-dimensional set-up for a scaling step potential has been suggested recently in [12, 13]. Using a thin dielectric insert, the experimental set-up described in [12, 13] may be used to implement the scaling, one-dimensional delta atom experimentally.

8.2. Consistency checks

All analytical results reported in this paper were spot-checked numerically for consistency and accuracy. Figure 1, e.g., was produced two ways: (i) directly via (46) and (56), respectively; and (ii) via numerical solution of (5) and (8), respectively. The resulting figures are identical on the scale of figure 1. The periodic-orbit expansions (52)–(54), (79), (80) were checked numerically by including prime binary necklaces with code lengths $\hat{l}(\hat{w}_p) \leqslant 15$.

The special case $v = 0$ of (46) provides an example of an analytical consistency check. For $v = 0$, we expect $k_n = n\pi$. Using $T_{2n+1}(0) = U_{2n+1}(0) = 0$, $T_{2n}(0) = U_{2n}(0) = (-1)^n$ [18] and the root separators $k_n^< = (n - 1/2)\pi$, $k_n^> = (n + 1/2)\pi$, the spectrum $k_n = n\pi$ is indeed obtained. Unfortunately this test does not check the m-sum in (46) which happens to be zero in this case. However, using the asymmetric root separators $k_n^< = (n - 1/4)\pi$, $k_n^> = (n + 1/2)\pi$, the m-sum in (46) is non-zero and we obtain

$$k_n = n\pi + \frac{\pi}{32} - \frac{3}{8\pi} \sum_{m=1}^{\infty} (-1)^{m+1} \frac{1}{m^2} = n\pi, \tag{107}$$

where we used ([18], formula 0.2341)

$$\sum_{m=1}^{\infty} (-1)^{m+1} \frac{1}{m^2} = \frac{\pi^2}{12}. \tag{108}$$

8.3. Mathematical aspects

From the mathematical point of view the methods discussed in this paper define procedures for the explicit, exact and analytical computation of the zeros of almost-periodic functions [34]. It has been shown earlier [9] that our methods can be used to compute the roots of all trigonometric equations of the form

$$\sum_{n=1}^{N} A_n \cos(\omega_n x + \varphi_n) = 0, \tag{109}$$

where N is finite and A_n, ω_n and φ_n are real constants. The spectral equation (58) is of this form, and many others may be generated from the scaling, compressed delta atom by changing the boundary conditions at $x = 0, b$ to Dirichlet at $x = 0$ and Neumann at $x = b$ (or vice versa) or Neumann at both $x = 0$ and $x = b$ or to general Balian–Bloch boundary conditions of mixed type [10]. All of these different boundary conditions lead to spectral equations of the form (109) which can be solved exactly, explicitly and analytically by the methods described in [9] and in this paper.

For the compressed delta atom it is relatively straightforward to obtain the root separators $k_n^<$ and $k_n^>$ (see section 2.2). In general the root separators satisfy transcendental equations which have to be solved in a preliminary step before they can be used to solve for the spectrum. However, in many cases these root separator equations are themselves of the type (109). In this case the solution techniques described in this paper and in [9] may be applied first for finding the root separators and then for finding the spectrum. Details of this multi-step, but well-defined procedure are described in [9].

Periodic orbits should not be confused with binary necklaces. They are two separate entities with distinct meanings. The term 'periodic orbit' refers to a closed physical trajectory that a classical particle traces in phase space. A periodic orbit has physical attributes, such as, e.g., stability, classical action and traversal time. We use 'binary necklaces' to label and enumerate periodic orbits.

8.4. Explicit solution of the asymptote equation

Let us denote by k_n, $k_n < k_{n+1}$, $n = 1, 2, \ldots$ the ordered set of solutions of (22). Because of the simple structure of (22) we find immediately two types of solutions

$$k_N^{(\pm)} = \frac{2\pi}{1 \pm \omega} N, \qquad N = 1, 2, \ldots \tag{110}$$

and we might be tempted to use (110) to construct k_n. This, however, cannot be done in a straightforward way since, in general, $k_N^{(+)}$ and $k_N^{(-)}$ interlace in a complicated way with no regular pattern. However, since (22) is of the form (109), we can apply the methods outlined in this paper to obtain an explicit, exact solution of (22) in the form $k_n = \ldots$. We present the solution for irrational ω.

First we construct the staircase function. It is given by

$$N(k) = \Theta_{2\pi}[(1 - \omega)k] + \Theta_{2\pi}[(1 + \omega)k] = -1 + \frac{k}{\pi} + \frac{2}{\pi} \sum_{m=1}^{\infty} \frac{1}{m} \sin(mk) \cos(m\omega k). \tag{111}$$

We use the staircase (111) in (45) together with the root separators $k_n^< = n\pi$ and $k_n^> = (n + 1)\pi$ to obtain

$$k_n = n\pi + \frac{\pi}{2} + \frac{1}{\pi} \left\{ \frac{1}{1 - \omega} \left[\Omega\big(\xi_{n+1}^{(-)}\big) - \Omega\big(\xi_n^{(-)}\big) \right] + \frac{1}{1 + \omega} \left[\Omega\big(\xi_{n+1}^{(+)}\big) - \Omega\big(\xi_n^{(+)}\big) \right] \right\}, \tag{112}$$

where

$$\xi_n^{(\pm)} = n\pi(1 \pm \omega) \bmod 2\pi \tag{113}$$

and ([18], formula 1.4433)

$$\Omega(x) = \sum_{m=1}^{\infty} \frac{1}{m^2} \cos(mx) = \frac{\pi^2}{6} - \frac{\pi x}{2} + \frac{x^2}{4}, \qquad 0 \leqslant x \leqslant 2\pi. \tag{114}$$

While $k_N^{(\pm)}$ of (110) satisfy (22), the advantage of (112) is that it also solves the 'interlacing problem', i.e., it provides the solutions of (22) correctly in ascending order.

8.5. Continuum of bound states

In the limit $a, b \to \infty$, $\omega = $ const, we obtain a quantum particle in the field of a free delta function without confining walls. The attractive, scaling case for $E < 0$ is of particular interest. In this case, after shifting the origin to the position of the δ function, the potential is $V(x) = V_0 K \delta(x)$, where $V_0 < 0$ is a constant and $K = \sqrt{2m|E|}/\hbar$. The spectral equation is

$$K \left(1 - \frac{m|V_0|}{\hbar^2} \right) = 0. \tag{115}$$

This equation is solved either by $K = 0$, which leads to an unphysical state, or by satisfying the *consistency condition*

$$\frac{m|V_0|}{\hbar^2} = 1. \tag{116}$$

If the consistency condition (116) is met, there is a continuum of normalizable, bound states, i.e., there is a normalizable, bound state at any $E < 0$. This is a useful pedagogical example to illustrate that the condition of normalizable wavefunctions does not automatically guarantee a discrete, countable spectrum.

We note that

$$v(k) = \frac{k \sin(k)}{\cos(k) - \cos(\omega k)} \tag{117}$$

leads to a continuous spectrum of the compressed delta atom, since with this $v(k)$ the spectral equation (5) (except at the singularities) is identically fulfilled for any k. The energy dependence (117) of v is not as exotic as it seems and may be realized, at least locally in k, with a suitable, frequency-dependent dielectric in a set-up similar to the one described in section 8.1.

8.6. Closed-form solutions

The spectral solutions presented in this paper are of the form (2). Are they 'closed-form solutions'? There are various definitions of the term 'closed-form solution' in the mathematical literature. According to the most restrictive definition, a solution is 'closed form' only if it can be expressed with finitely many elementary functions and contains only a finite number of arithmetical operations. Clearly there is a problem with this 'definition', since the set of 'elementary functions' is not well defined. To illustrate, let us look at the formula for the critical temperature T_c for Bose–Einstein condensation of an ideal gas of spin-zero Bose particles of mass m at density ρ [35]:

$$T_c = \frac{2\pi\hbar^2}{mk}\left[\frac{\rho}{\zeta(3/2)}\right]^{2/3},$$
(118)

where k is Boltzmann's constant and $\zeta(x)$ is Riemann's zeta function [23]. As physicists we would like to think of (118) as a closed-form expression for T_c. But since $\zeta(x)$ is not ordinarily included in the set of 'elementary functions', and moreover known only via its infinite series expansion [23], expression (118) would not be 'closed form' according to the strictest definition. Clearly we need a definition of 'closed form' better suited in the physics context. If we relax the strictest definition slightly to admit well-defined, convergent, infinite series as parts of the solution, equations (73), (79) and (80) are integral-free, closed-form solutions of the spectrum of the scaling, compressed delta atom.

Let us remark in this context that even the trigonometric functions $\sin(x)$ and $\cos(x)$, which just about anybody would include in the set of 'elementary functions', are transcendental functions most conveniently defined via their infinite series representations. In this light, rather than a mere convenience, inclusion of well-defined infinite series in the definition of 'closed-form solutions' appears to be a compelling necessity to achieve logical consistency of the definition.

8.7. Numerical versus analytical solutions

There is a fundamental difference between numerical and analytical solutions. While numerically we may only obtain approximate results for selected spectral points, analytical solutions, such as (73), (79) or (80) represent the *exact* solution of the *entire* spectrum in a *single* formula. No doubt, therefore, conceptually, analytical solutions are much more powerful than numerical results. Nevertheless there is an interesting symbiosis between numerical and analytical techniques when it comes to computing high-accuracy results for selected spectral points. Suppose we would like to compute $k_n(v; \omega)$ for given v, ω and $n = 7153\,713\,357$. Although for the computation of specific, selected energy levels numerical methods are much faster and more convenient to apply than, e.g., a periodic-orbit expansion, numerical methods are helpless when it comes to targeting a specific state, in this case state number n, when n is large. A purely numerical method would first have to establish, numerically, an interval in which to find state number n. But, in order to assure correct labelling, such an interval can be established only by computing all the other $n-1$ states with $k_j < k_n$, $j = 1, \ldots, n-1$ as well.

A time-consuming task for sufficiently large n. Here is where a combination of analytical and numerical techniques is successful. The analytical methods provide the exact root interval $[k_n^<, k_n^>]$ in which to find k_n, and, in addition, a low-accuracy starting value $k_n^{(start)}$ inside the root interval by summing, e.g., the first few periodic orbits. Thus the difference between analytical and numerical methods may be characterized concisely as follows. While numerical methods are sharp, specialized tools, analytical solutions are an intellectual advance.

9. Summary and conclusions

The compressed delta atom may be interpreted as a linear quantum graph with two bonds and three vertices, i.e. a two-pronged star graph [9, 11, 15, 16]. In [9] it was shown that all quantum graphs are explicitly solvable. However, the proof provided in [9] is a proof of principle. Each quantum graph provides its own ideosyncratic problems. For instance, it is often not straightforward to obtain the root separators of the spectrum. Therefore, actual worked solutions are still rare.

Following the program outlined in [9], this paper provides explicit spectral solutions of the compressed delta atom via quadratures and periodic-orbit expansions. Four qualitatively different cases—scaling and non-scaling, $E > 0$ and $E < 0$—are considered. Apart from the step-in-a-box potential [9, 11–13] and the finite square-well potential [14] the compressed delta atom is only the third physical system that has been solved explicitly using the methods of [9].

While it is interesting to know that the compressed delta atom can be solved explicitly, the main thrust of this paper is not on solving an isolated problem, but to illustrate the power of a recently suggested solution technique and to provide a template for the solution of other one-dimensional and quasi-one-dimensional (quantum graph) problems. It should, e.g., be possible to compute explicit solutions of Anderson localizing systems consisting of trains of delta functions with random potential strengths. In addition, with explicit solutions at hand, it should be possible to obtain deeper, analytical insight into the spectral statistics of (dressed) quantum graphs and Anderson localizing systems.

Acknowledgment

Appendix. Delta-limit of the finite square-well potential

Recently the finite square well was solved explicitly in [14]. We confirm here that the explicit formula for the ground-state energy of the finite square well (formula (24) in [14]) gives the correct binding energy of a δ function in the limit of vanishing width of the well. It is worth presenting the proof in this appendix since the derivations contain pitfalls such as non-commuting double limits ($v_0 \to 0, m \to \infty$) which lead to non-uniformly convergent sums.

In [14] the depth of the square well is denoted by $V_0 > 0$ and its width is $2a$. It becomes an attractive δ-function potential in the limit of $a \to 0$ keeping $V_\delta = -2aV_0$ constant. We call this limit the delta limit. The energy levels of the well in [14] are counted from the bottom of the well. Therefore, in the delta limit, we expect

$$\left(\xi_0^{(+)}\right)^2 = \frac{2ma^2}{\hbar^2}(V_0 + E_\delta) = v_0^2\left(1 - v_0^2\right), \tag{A.1}$$

where $E_\delta < 0$ is the binding energy of the δ function, $\xi_0^{(+)}$, as defined in [14], is the dimensionless wavenumber of the finite square well's ground state and $v_0 = \sqrt{ma|V_\delta|}/\hbar$ is the dimensionless potential depth, respectively. Apparently, $v_0 \to 0$ in the delta limit. Therefore, in the delta limit, we expect

$$\xi_0^{(+)} = v_0 - \tfrac{1}{2}v_0^3 \tag{A.2}$$

up to third order in v_0.

We show now that $\xi_0^{(+)}$, as stated explicitly in (24) of [14], equals (A.2) up to third order in v_0. This is all we have to show in order to prove that (24) of [14] yields the correct delta limit, since the contributions of the higher powers of v_0 are zero when (A.2) is used to compute E_δ.

According to (20) of [14], we have $b_0^{(+)} = v_0$. This turns (24) of [14] into

$$\xi_0^{(+)} = -\frac{v_0^2}{2\pi} + \frac{v_0}{2} + \frac{v_0}{\pi} - \frac{v_0}{\pi}g(v_0), \tag{A.3}$$

where

$$g(v_0) = \sum_{m=1}^{\infty} \frac{1}{m} f_m(v_0) \tag{A.4}$$

and

$$f_m(v_0) = \int_0^1 \sin[2mv_0\xi - 2m\arccos(\xi)]\,d\xi. \tag{A.5}$$

We obtain

$$g(v_0 = 0) = 2\sum_{m=1}^{\infty}(-1)^m \frac{1}{4m^2 - 1} = 1 - \frac{\pi}{2},$$

$$g'(v_0 = 0) = -\sum_{m=1}^{\infty}\frac{1}{4m^2 - 1} = -\frac{1}{2}, \tag{A.6}$$

$$g''(v_0 = 0) = 32\sum_{m=1}^{\infty}(-1)^m \frac{m^2}{(4m^2 - 9)(4m^2 - 1)} = \pi.$$

We note that $g(v_0 = 0)$ and $g'(v_0 = 0)$ can be obtained from term-by-term differentiation of (A.4). The series

$$h(v_0) = \sum_{m=1}^{\infty} f_m''(v_0)/m, \tag{A.7}$$

however, is not uniformly convergent in the vicinity of $v_0 = 0$. In fact we have

$$\lim_{v_0 \to 0} h(v_0) = \pi = 2h(v_0 = 0). \tag{A.8}$$

This has been incorporated in the third equation of (A.6). With (A.6) we obtain up to second order

$$g(v_0) = 1 - \frac{\pi}{2} - \frac{1}{2}v_0 + \frac{\pi}{2}v_0^2. \tag{A.9}$$

Using (A.9) in (A.3) yields (A.2). This shows that (24) of [14] has the correct delta limit.

References

[1]   Michels A, De Boer J and Bijl A 1937 *Physica* **4** 981
[2]   Sommerfeld A and Welker H 1938 *Ann. Phys.* **32** 56
[3]   De Groot S R and Ten Seldam C A 1946 *Physica* **12** 669
[4]   Griffiths D J 1995 *Introduction to Quantum Mechanics* (Upper Saddle River, NJ: Prentice-Hall)
[5]   Wigner E P 1954 *Phys. Rev.* **94** 77
[6]   Epstein S T 1960 *Am. J. Phys.* **28** 495
[7]   Lapidus I R 1989 *Am. J. Phys.* **57** 281
[8]   Blümel R and Dabaghian Yu 2001 *J. Math. Phys.* **42** 5832
[9]   Dabaghian Yu and Blümel R 2004 *Phys. Rev.* E **70** 046206
[10] Gutzwiller M C 1990 *Chaos in Classical and Quantum Mechanics* (New York: Springer)
[11] Blümel R, Dabaghian Yu and Jensen R V 2002 *Phys. Rev. Lett.* **88** 044101
[12] Bhullar A S, Blümel R and Koch P M 2005 *J. Phys. A: Math. Gen.* **38** L563
[13] Bhullar A S, Blümel R and Koch P M 2006 *Phys. Rev.* E **73** 016211
[14] Blümel R 2005 *J. Phys. A: Math. Gen.* **38** L673
[15] Kottos T and Smilansky U 1997 *Phys. Rev. Lett.* **79** 4794
[16] Kottos T and Smilansky U 1999 *Ann. Phys., NY* **274** 76
[17] Flügge S 1971 *Practical Quantum Mechanics I* (New York: Springer)
[18] Gradshteyn I S and Ryzhik I M 1994 *Table of Integrals, Series, and Products* (Boston, MA: Academic)
[19] Riordan J 1958 *An Introduction to Combinatorial Analysis* (New York: Wiley)
[20] Sirko L, Koch P M and Blümel R 1997 *Phys. Rev. Lett.* **78** 2940
[21] Feynman R P 1948 *Rev. Mod. Phys.* **20** 367
[22] Netz H 1975 *Formeln der Mathematik* (München: Carl Hanser Verlag)
[23] Abramowitz M and Stegun I A 1972 *Handbook of Mathematical Functions* (New York: Dover)
[24] Blümel R 2006 *Eur. J. Phys.* **27** L1
[25] Ring P and Schuck P 1980 *The Nuclear Many-Body Problem* (New York: Springer)
[26] Goodrich F C 1972 *A Primer of Quantum Chemistry* (New York: Wiley-Interscience)
[27] Blümel R and Meir R 1985 *J. Phys. B: At. Mol. Phys.* **18** 2835
[28] Sposito G 1970 *An Introduction to Quantum Physics* (New York: Wiley)
[29] Morrison M A, Estle Th L and Lane N F 1976 *Quantum States of Atoms, Molecules, and Solids* (Englewood
        Cliffs, NJ: Prentice-Hall)
[30] Prange R E, Ott E, Antonsen T M Jr, Georgeot B and Blümel R 1996 *Phys. Rev.* E **53** 207
[31] Schäfer R, Kuhl U, Barth M and Stöckmann H-J 2001 *Found. Phys.* **31** 475
[32] Vaa C, Koch P M and Blümel R 2003 *Phys. Rev. Lett.* **90** 194102
[33] Vaa C, Koch P M and Blümel R 2005 *Phys. Rev.* E **72** 056211
[34] Besicovitch A S 1954 *Almost Periodic Functions* (New York: Dover)
[35] Feynman R P 1992 *Statistical Mechanics* (Redwood City, CA: Addison-Wesley)