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Regularized Scarf potentials: energy band structure and supersymmetry

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Abstract

The singular one-dimensional periodic Scarf potential is regularized by means of one-parameter square well counter-terms. It is shown that the regularized spectrum converges formally to the conventional Scarf energy bands for specific values of the parameter. The behaviour of the regularizations under supersymmetric transformations is also investigated; this is a key point for the algebraic solvability of the regularized Scarf potential.

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1. Introduction

In this paper we will deal with the one-dimensional Scarf potential [1] considered as a periodic and singular potential in the framework of non-relativistic quantum mechanics. Our aim is to regularize the singularities to get a physically sensible band structure and also to study the behaviour of these regularizations under Darboux—also called supersymmetric (susy)—transformations.

The regularization of singular potentials is a problem that already arose at the early stages in the development of quantum mechanics. Some general discussions on this topic can be found in [2] and [3]. In particular, it was also considered in the original papers by Scarf [1] concerning the potential bearing his name that will here be referred to as the 'conventional' Scarf potential. In general, the process consists in substituting, inside some intervals containing the isolated singularities, the original potential by non-divergent terms. Usually it is also required that certain properties of the new system behave properly in the limit when the radius of these intervals goes to zero and, at the same time, the regularization terms are modified accordingly. A similar situation appears in effective field theories (see e.g. [4]).

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There are other approaches to regularization. For example, analytic prolongation in the complex plane has been applied to avoid singularities in the real axis, either by surrounding the singularity [1], or by moving it slightly into the imaginary axis [5]. The subject can also be presented from a more abstract point of view by removing the singular points of the real axis and imposing boundary conditions on the wavefunctions to determine domains for the relevant self-adjoint operators [6]. However, when using this method it is quite difficult to interpret the resulting solutions from a physical point of view.

Here we want to address the regularization question following the first approach keeping always in touch with physics. First, we substitute the Scarf potential V by what we will call 'ϵ-regular' potential V_ϵ differing in the intervals with radius ϵ around each singularity, as previously mentioned, with the following conditions: (i) for each ϵ we have a regular periodic potential with a band structure and discrete eigenfunctions for the band borders; (ii) in the limit $\epsilon \to 0$, we get a well-defined and nontrivial limit for such band spectrum and eigenfunctions; (iii) for any $\epsilon \neq 0$ the ϵ-regular potential V_ϵ constitutes a global aproximation to the limiting values. We will see that, after a detailed analysis, we are faced with all these possibilities: regularization cases where the limit is rather trivial; the limit exists and defines a consistent periodic quantum system but is only locally similar to that given by V_ϵ, and finally a very special case where all the requirements are satisfied.

In the final section of the paper we will investigate how this regularization process is affected by susy transformations. We will show that, if we start with a regularization of the Scarf Hamiltonian, then a suitable susy transformation automatically provides a regularization of the partner Hamiltonian. In other words, we can say that susy transformations are consistent with regularizations (another point of view, where the regularization is suggested by the susy transformation, is displayed in [7]). This consistency is crucial for the solvable character of the regularized Hamiltonian: since the Scarf potential requires a regularization to have a physical meaning, the algebraic methods that rely on supersymmetry to solve the system can only be applied if there exists a regularization scheme that is consistent with supersymmetry.

2. The Scarf potential revisited

Let us consider a particle in the presence of the one-dimensional periodic Scarf potential

$$V(x) = \frac{V_0}{\sin^2 x} \qquad V_0 \in \mathbb{R}. \tag{2.1}$$

The related Schrödinger equation $H\psi(x) = \mathcal{E}\psi(x)$ can be rewritten as

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\alpha}{\sin^2 x} - \lambda^2\right]\psi(x) = 0 \tag{2.2}$$

where $\alpha \equiv 2mV_0/\hbar^2, \lambda^2 \equiv 2m\mathcal{E}/\hbar^2 = E$ (note that λ may be a real or purely imaginary number). This potential (2.1) is π-periodic and it can be a useful idealization of a crystal lattice. It has strong singularities at $x_m = m\pi, m \in \mathbb{Z}$, in whose neighbourhood the potential has an attractive or repulsive character according to the sign of the strength V_0. We shall fix our attention primarily on the interval $(0, \pi)$, in which equation (2.2) admits two linearly independent eigenfunctions for a given eigenenergy λ^2. They can be determined by changing the independent variable to $y = \sin^2 x/2$, as well as the ψ function as $\psi(x(y)) = y^\mu(1-y)^\nu\varphi(y)$, where the parameters μ, ν are chosen in such a way that the new function $\varphi(y)$ satisfies a hypergeometric equation [8]. It is also convenient to introduce a parameter k, defined by $\alpha = k(k-1)$. Then, one arrives at the general solution

$$\psi(x) = Au(x) + Bv(x) \tag{2.3}$$

where

$$u(x) := \left(\sin\frac{x}{2}\right)^k \left(\cos\frac{x}{2}\right)^{1-k} {}_2F_1\left(\frac{1}{2}+\lambda, \frac{1}{2}-\lambda, \frac{1}{2}+k; \sin^2\frac{x}{2}\right) \tag{2.4}$$

$$v(x) := \left(\frac{\sin x}{2}\right)^{1-k} {}_2F_1\left(1+\lambda-k, 1-\lambda-k, \frac{3}{2}-k; \sin^2\frac{x}{2}\right). \tag{2.5}$$

Note the implicit dependence of u and v on λ and k. The constants A, B are arbitrary, and k is constrained by $k \neq \pm n - 1/2$, $n = 0, 1, 2, \ldots$, in order to avoid solutions with logarithmic singularities. In other words, $\alpha \in (-1/4, 3/4) \cup (3/4, 15/4) \cup \cdots$.

In order to construct physical eigenfunctions ψ, normalized in the interval $(0, \pi)$, let us analyse the behaviour of the basis (2.4)–(2.5) near the boundaries of the interval. At the left edge, $x \to 0^+$, they behave as

$$u(x) \approx \left(\frac{x}{2}\right)^k \qquad v(x) \approx \left(\frac{x}{2}\right)^{1-k}. \tag{2.6}$$

Near the right end point we can write $x = \pi - \delta$ and, by taking $\delta \to 0^+$, get $x \to \pi^-$. Thus we have the following expressions [8]:

$$u(\pi-\delta) \approx \frac{\cos(\pi\lambda)}{\cos(\pi k)}\left(\frac{\delta}{2}\right)^k + \frac{\pi\cos^{-1}(\pi k)}{\Gamma(k+\lambda)\Gamma(k-\lambda)}\left(\frac{\delta}{2}\right)^{1-k} \tag{2.7}$$

$$v(\pi-\delta) \approx -\frac{\pi\cos^{-1}(\pi k)}{\Gamma(1+\lambda-k)\Gamma(1-\lambda-k)}\left(\frac{\delta}{2}\right)^k - \frac{\cos(\pi\lambda)}{\cos(\pi k)}\left(\frac{\delta}{2}\right)^{1-k}. \tag{2.8}$$

As we can see, the analytical properties of $u(x)$ and $v(x)$ depend on the eigenvalue λ^2 and on the potential strength α by means of the parameter k. Next, we summarize the results classified in terms of k.

- *Discrete spectrum* ($3/4 < \alpha$, or $3/2 < k$). The terms $(x/2)^{1-k}$ and $(\delta/2)^{1-k}$ in (2.6)–(2.8) strongly diverge and they give rise to wavefunctions not square integrable in $(0, \pi)$. Therefore, we must take $B = 0$ and at the same time the coefficient of $(\delta/2)^{1-k}$ in (2.7) must vanish. This last condition is achieved if $k \pm \lambda = -n$ and it is responsible for a discrete spectrum:

  $$E_n = \lambda_n^2 \equiv (k+n)^2 \qquad n = 0, 1, 2, \ldots. \tag{2.9}$$

  Thus, the physical solutions are bound states given by

  $$\psi_n(x) = A_n\left[\sin\frac{x}{2}\right]^k\left[\cos\frac{x}{2}\right]^{1-k} {}_2F_1\left(\frac{1}{2}+k+n, \frac{1}{2}-k-n, \frac{1}{2}+k; \sin^2\frac{x}{2}\right). \tag{2.10}$$

  These solutions are such that

  $$\lim_{x\to\pi^-}\psi_n(x) = \lim_{x\to 0^+}\psi_n(x) = 0.$$

  We can associate them with the states of a particle in the interval $(0, \pi)$.
- *Continuous spectrum* ($-1/4 < \alpha < 3/4$, or $1/2 < k < 3/2$). For a strength α such that $-1/4 < \alpha < 3/4$, all terms in (2.6)–(2.8) are square integrable and thus, all the solutions are also square integrable in $(0, \pi)$. Of course, due to the periodicity, the same will happen with the solutions in any interval $(m\pi, (m+1)\pi)$, $m \in \mathbb{Z}$. From this set of solutions we can construct quasi-periodic functions [9], provided some rules are given to match the solutions on both sides of each singularity. The different ways to achieve this is the central problem of regularization. Once these rules are satisfactorily fixed, we can speak of the regularized Scarf potential which can be seen as a periodic potential, thus sharing the corresponding properties such as band structure, etc [1].

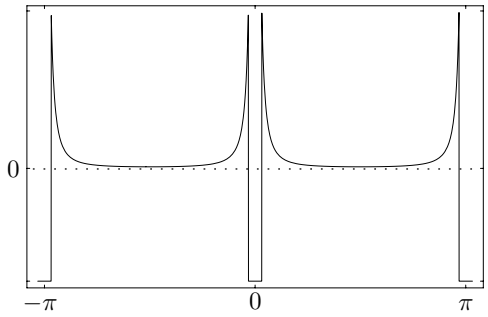


Figure 1. General aspect of the ϵ-regular Scarf potential V_ϵ for given values of ϵ, a and q.

- *Unphysical case* ($\alpha < -1/4$, or $k = 1/2 \pm \mathrm{i}d$). Replacing $k = 1/2 + \mathrm{i}d$ for instance in (2.6) we see that the behaviour of the fundamental solutions near the singularities give rise to wildly oscillating functions in the form $\psi(x) \approx Ax^{1/2}\cos(d\log x + B)$, where A, B are constants [10]. So, in this case also the general solution is square integrable and therefore we can establish connection rules in the singularities. However, in this way we are led to a spectrum which is not bounded from below [2, 11], hence we will discard this case from our dicussion.

In the neighborhood of $x_m = m\pi$, $m \in \mathbb{Z}$, the Scarf potential behaves as α/x^2. This kind of power law describes the transition between regular and singular potentials as indicated by Landau and Lifshitz [10]. In models with such singularities, one regularization scheme that has been used successfully is that of [2], which uses square well counterterms to control the singularities. In this paper, we shall use such a regularization scheme in analysing the Scarf potential in the continuous spectrum regime. We will concentrate on the repulsive region $1 < k < 3/2$, as a complement to the work of Scarf, which deals exclusively with the atractive interval, $1/2 < k < 1$.

3. Regularizing singularities

We shall substitute the initial potential (2.1) by a 'more realistic' one $V_\epsilon(x)$ (see figure 1), which we will call an ϵ-regular Scarf potential:

$$V_\epsilon(x) = \begin{cases} v_\epsilon = -\dfrac{a^2}{\epsilon^q}, & x \in (m\pi - \epsilon, m\pi + \epsilon), \quad m \in \mathbb{Z} \\ \dfrac{k(k-1)}{\sin^2 x}, & \text{otherwise.} \end{cases} \tag{3.1}$$

The cutoff range $\epsilon > 0$ is intended to be as small as one wishes, while the cutoff strength a^2 and the power law ϵ^{-q} are to be determined. We look for the potential $V_\epsilon(x)$ admitting well-defined energy bands and wavefunctions in the limit $\epsilon \to 0$. The limit of such a potential as $V_\epsilon(x)$, if it exists as a generalized function, will be called the 'regularized Scarf potential' $V_s(x)$. Now, as is well known, the monodromy matrix [12] allows us to get all the physical description of periodic potentials like (3.1). Hence, we shall proceed in the following manner: we obtain first the monodromy matrix M_ϵ, related to $V_\epsilon(x)$ for a given cutoff ϵ; then, we shall evaluate the limit $\epsilon \to 0$, just as is usual in distribution theory. The appropriate values of a and q will be obtained as an immediate result by imposing that the matrix elements of $\lim_{\epsilon\to 0} M_\epsilon$ must be well defined.

3.1. Crossing a singularity

In order to construct the monodromy matrix M_ϵ, it is necessary to obtain first the transfer matrix T_ϵ connecting the wavefunctions at both sides of the well. Hence, let us consider the general eigenfunction $\psi(x)$ for the potential (3.1), corresponding to a given eigenvalue λ^2. In a natural manner, ψ is defined in the three regions surrounding the point $x_0 = 0$ (see figure 1). Thus, by considering an appropriate basis, we have

$$\begin{aligned} \psi_1(x) &= A_1 u(-x) + B_1 v(-x), && x \leqslant -\epsilon \\ \psi_2(x) &= A_2 \sin(px) + B_2 \cos(px), && -\epsilon \leqslant x \leqslant \epsilon \\ \psi_3(x) &= A_3 u(x) + B_3 v(x), && x \geqslant \epsilon \end{aligned} \tag{3.2}$$

where $u(x)$ and $v(x)$ are given by (2.4)–(2.5), A_j, B_j, $j = 1, 2, 3$, are constants related by the matching conditions at $\pm\epsilon$ and

$$p = \sqrt{\lambda^2 - v_\epsilon} \tag{3.3}$$

is the kinetic energy inside the domain of the cutoff potential. Hence, in this basis, the action of the transference matrix T_ϵ is as follows:

$$\begin{pmatrix} A_3 \\ B_3 \end{pmatrix} = T_\epsilon \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}. \tag{3.4}$$

Near the matching points, $-\epsilon$ and ϵ, the behaviour of $\psi(x)$ when $\epsilon \approx 0$ is given by

$$\begin{aligned} \psi_1(x) &\approx A_1(-x)^k + B_1(-x)^{1-k}, && x \lessapprox -\epsilon \\ \psi_3(x) &\approx A_3 x^k + B_3 x^{1-k}, && x > \epsilon \end{aligned} \tag{3.5}$$

while the kinetic term (3.3) behaves as

$$p \approx a\epsilon^{-\frac{q}{2}} \qquad \epsilon \gtrapprox 0. \tag{3.6}$$

Taking into account (3.2) and (3.5), one easily obtains the expression for the elements t_{ij} of the matrix T_ϵ when $\epsilon \gtrapprox 0$:

$$-(2k-1)t_{11} = \cos(2p\epsilon) + (\epsilon p + k(k-1)\epsilon^{-1}p^{-1})\sin(2p\epsilon) \tag{3.7}$$

$$(2k-1)\epsilon^{2k}t_{12} = 2(k-1)\epsilon\cos(2p\epsilon) + (-p\epsilon^2 - (k-1)^2 p^{-1})\sin(2p\epsilon) \tag{3.8}$$

$$(2k-1)\epsilon^{2-2k}t_{21} = 2k\epsilon\cos(2p\epsilon) + (\epsilon^2 p - k^2 p^{-1})\sin(2p\epsilon) \tag{3.9}$$

$$(2k-1)t_{22} = -(2k-1)t_{11}. \tag{3.10}$$

As $1 < k < 3/2$, the matrix elements t_{ij} will have a finite limit when $\epsilon \to 0$ if $q = 2$ and the cutoff strength a satisfies any of the following periodic conditions:

$$\text{Type I}: \quad k = 1 + a\tan a \tag{3.11}$$

$$\text{Type II}: \quad k = 1 - a\cot a. \tag{3.12}$$

Hence, we have respectively

$$\text{Type I}: \quad \lim_{\epsilon\to 0} T_\epsilon = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \tag{3.13}$$

$$\text{Type II}: \quad \lim_{\epsilon\to 0} T_\epsilon = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3.14}$$

In each case, the leading orders of the independent solutions are transformed by T_ϵ as follows:

$$\text{Type I}: \quad (-x)^k \to -x^k, \qquad (-x)^{1-k} \to (-x)^{1-k} \tag{3.15}$$

$$\text{Type II}: \quad (-x)^k \to x^k, \qquad (-x)^{1-k} \to -(-x)^{1-k}. \tag{3.16}$$

The regularization of type I allows us to recover the results for the free particle potential as a particular case by taking simply $k = 1$. Type II, on the other hand, produces an additional change of global phase $e^{i\pi}$.

3.2. The monodromy matrix

Let us recall here some basic results about the Schrödinger equation in a π-periodic potential such as $V_\epsilon(x)$ (3.1),

$$H_\epsilon \psi = \lambda^2 \psi. \tag{3.17}$$

As the translation operator L, defined by $L\psi(x) = \psi(x+\pi)$, commutes with H_ϵ, then inside each two-dimensional λ-eigenspace (3.17) we can also find at least one L-eigenfunction such that

$$L\psi(x) = \psi(x+\pi) = \mu\psi(x) = e^{i\sigma\pi}\psi(x). \tag{3.18}$$

These are the Bloch functions. Only the Bloch functions with $|\mu| \leqslant 1$ are suitable bounded generalized eigenfunctions from a physical point of view. The corresponding λ-eigenvalues constitute the alowed energy bands, and the real parameter σ is then called the crystal momentum in solid state physics [12]. The other Bloch functions are not bounded either when $x \to +\infty$ or when $x \to -\infty$, and the respective values of λ belong to the forbidden bands.

Usually relation (3.18) is expressed with the help of a basis of λ-eigenfunctions $\{\xi(x), \chi(x)\}$ such that $\xi(0) = 0, \xi'(0) = 1$ and $\chi(0) = 0, \chi'(0) = 1$. In this basis the operator L is represented by the matrix M with the elements m_{ij},

$$\begin{aligned} L\xi(0) &= \xi(\pi) = m_{11}\xi(0) + m_{12}\chi(0) \\ L\chi(0) &= \chi(\pi) = m_{21}\xi(0) + m_{22}\chi(0). \end{aligned} \tag{3.19}$$

It is obtained that $m_{11} = \xi(\pi), m_{12} = \chi(\pi), m_{21} = \xi'(\pi), m_{22} = \chi'(\pi)$.

In our case, in order to include the singular points, we will work with the interval $[\epsilon, \pi + \epsilon]$, and instead of the standard basis defined above, here we adopt the more natural basis $\{u(x), v(x)\}$. The corresponding matrix (3.19) under these assumptions will be called (with a certain abuse of langage) the monodromy matrix M_ϵ [12] for the ϵ-regular potential. Next, we will evaluate the limit $\epsilon \to 0$ of this matrix.

Thus, M_ϵ can be decomposed as the product of T_ϵ with a new matrix N_ϵ, which connects $\psi(\epsilon)$ (in the basis $\{u(x), v(x)\}$) with $\psi(\pi - \epsilon)$ (in the basis $\{u(\pi - x), v(\pi - x)\}$). Schematically,

$$N_\epsilon : \psi(\epsilon) \mapsto \psi(\pi - \epsilon) \tag{3.20}$$

$$T_\epsilon : \psi(\pi - \epsilon) \mapsto \psi(\pi + \epsilon) \tag{3.21}$$

$$M_\epsilon = T_\epsilon N_\epsilon : \psi(\epsilon) \mapsto \psi(\pi + \epsilon). \tag{3.22}$$

Indeed, N_ϵ is such that $\operatorname{tr} N_\epsilon = 0, \det N_\epsilon = -1$, and it produces but a change of basis which is independent of ϵ (see equations (2.7), (2.8)). The explicit form of this matrix is

$$N_\epsilon = \frac{1}{\cos(\pi k)} \begin{pmatrix} \cos(\pi\lambda) & -\dfrac{\pi}{\Gamma(1+\lambda-k)\Gamma(1-\lambda-k)} \\ \dfrac{\pi}{\Gamma(k+\lambda)\Gamma(k-\lambda)} & -\cos(\pi\lambda) \end{pmatrix}. \tag{3.23}$$

The matrix T_ϵ, on the other hand, embraces the previously defined conditions of regularization (3.11)–(3.12) and, in general, depends on two parameters ρ and θ, which are either both real or both pure imaginary numbers, and which can be determined by the cutoff ϵ and the eigenvalue λ^2:

$$T_\epsilon = \begin{pmatrix} \cos\theta & \rho\sin\theta \\ \dfrac{\sin\theta}{\rho} & -\cos\theta \end{pmatrix}. \tag{3.24}$$

The eigenvalues of the monodromy matrix M_ϵ are given by the characteristic polynomial $P(\mu) = \mu^2 - D\mu + \det M_\epsilon = 0$, where $\det M_\epsilon = \det(T_\epsilon N_\epsilon) = 1$ and $D = D(\lambda) \equiv \operatorname{tr} M_\epsilon$:

$$D = \frac{2\cos(\pi\lambda)\cos\theta}{\cos(\pi k)} + \left[\frac{\rho}{\Gamma(k+\lambda)\Gamma(k-\lambda)} - \frac{1}{\rho\Gamma(1+\lambda-k)\Gamma(1-\lambda-k)}\right]\frac{\pi\sin\theta}{\cos(\pi k)}. \tag{3.25}$$

Hence, the eigenvalues of M_ϵ are given by

$$\mu_\pm = \frac{D}{2} \pm \sqrt{\frac{D^2}{4} - 1}. \tag{3.26}$$

If $|D| > 2$, then (3.26) leads to real values of $\mu_\pm$ such that $|\mu_\pm| \neq 1$, which correspond to eigenvalues in a forbiden band. If $|D| \leqslant 2$, then $\mu_\pm$ are complex numbers of modulus 1

$$\mu_-^* = \mu_+ = \mathrm{e}^{\mathrm{i}\sigma\pi}, \qquad \sigma \in \mathbb{R}, \tag{3.27}$$

which, in turn, correspond to eigenvalues λ^2 inside an allowed energy band. In particular, $\lambda(\mu)$-values with $\mu_\pm$ both equal to $+1$ or -1, correspond to the edges of the Brillouin zones.

4. Band structure

4.1. Energy bands of the regularized Scarf potential

We have already mentioned that the regularized Scarf potential V_s is obtained as $\lim_{\epsilon\to 0} V_\epsilon$ in a certain sense. Let us analyse the involved energy bands. First, note that the matrix N_ϵ in (3.23) is independent of ϵ, while $\lim_{\epsilon\to 0} T_\epsilon$ for type I regularization gives the matrix (3.13) or equivalently (3.24) with $\theta = \pi$ (for type II this limit is (3.14) or (3.24) with $\theta = 0$.) For each of these cases we get

$$\operatorname{tr} M_s = \pm\frac{2\cos(\pi\lambda)}{\cos(\pi k)}. \tag{4.1}$$

Therefore, for both types, condition $D = \operatorname{tr} M_s = \pm 2$ is reached by the values $\lambda = k + \ell$, $\ell \in \mathbb{Z}$, which in turn defines the energy band edges:

$$E_\ell = \lambda_\ell^2 = (k+\ell)^2, \quad \ell \in \mathbb{Z}. \tag{4.2}$$

It is easy to see that if $k \in (1, 3/2)$, then $E_{-1} < E_{-2} < E_0 < E_{-3} < E_1 < E_{-4} \cdots$, and the allowed energy bands are delimited as follows:

$$[E_{-1}, E_{-2}], [E_0, E_{-3}], [E_1, E_{-4}], \ldots, [E_{n-1}, E_{-2-n}], \ldots. \tag{4.3}$$

The eigenfunctions in $[0, \pi]$ corresponding to the band borders are of two kinds: either $\lambda = k + n, n \in \mathbb{Z}^+$, with $\psi_\lambda(x) \propto u(x, \lambda, k)$, or $\lambda = k - n, n \in \mathbb{N}$, with $\psi_\lambda(x) \propto v(x, \lambda, k)$, where we have made explicit the dependence of u and v on λ and k. To construct the solutions in other intervals, one has to make a symmetric or antisymmetric periodic extension depending on the type of regularization considered (see relations (3.15) and (3.16)). Finally, note that the energy bands obtained in this section for the regularized Scarf potential with $k \in (1, 3/2)$ coincide with those already known for the conventional Scarf potential for $k \in (1/2, 1)$.

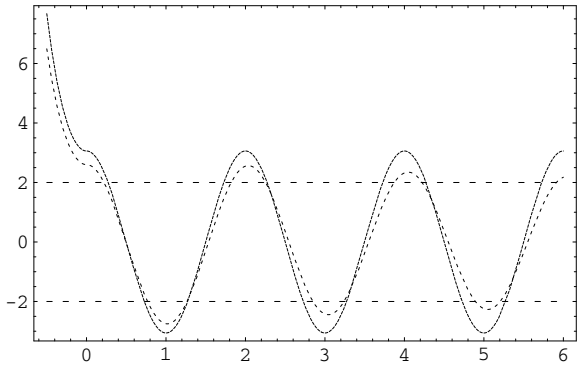


Figure 2. The trace of the monodromy matrix for the regularized Scarf potential (solid curve) and for the ϵ-regular Scarf potential with $\epsilon = 0.1$, $a = 0.5 \in \mathcal{A}_0^{\mathrm{I}}$ (dashed curve).

4.2. Bands of the ϵ-regular potentials $V_\epsilon(x)$

Now we will discuss the energy bands of the potential $V_\epsilon(x)$. We will concentrate mainly on the regularizations satisfying equations (3.11)–(3.12). Since they are transcendental equations, some numerical approximations will be necessary (however, there are also analytical expressions for the multiple solutions, see [4]). We will show the way in which our (numerical) solutions approximate to those obtained by Scarf with arbitrary precision.

Starting with type I, for a given value of $k \in (1, 3/2)$, the condition $k = 1 + a \tan a$ in (3.11) has infinite solutions for $a \geqslant 0$, one in each interval $((n - 1/2)\pi, (n + 1/2)\pi)$, $n = 0, 1, \ldots$. If k covers its whole range, $k \in (1, 3/2)$, then a takes values on some sub-intervals, let us call them $\mathcal{A}_n^{\mathrm{I}} \subset ((n - 1/2)\pi, (n + 1/2)\pi)$.

On the other hand, once k is fixed, the equation $k = 1 - a \cot a$ for type II regularizations also leads to multiple solutions for a, one in each interval $(n\pi, (n + 1)\pi)$, $n = 0, 1 \ldots$. Again, if we cover the whole interval $k \in (1, 3/2)$, then a is restricted to some sub-intervals $\mathcal{A}_n^{\mathrm{II}} \subset (n\pi, (n + 1)\pi)$.

As we shall see, only the solutions of $a \in \mathcal{A}_0^{\mathrm{I}}$ will give rise in the limit $\epsilon \to 0$ to a sensible physical Hamiltonian, bounded from below. The other solutions lead, besides the Scarf positive energy bands, to infinite negative energies in the limit $\epsilon \to 0$ and therefore are not fully satisfactory. For other values not satisfying either of the two equations (3.11)–(3.12), the spectrum degenerates into discrete values in the limit $\epsilon \to 0$, as will be discussed later.

4.2.1. Type I regularizations. Let us consider equation (3.11) and, once k is fixed, let us take the solution in the first sub-interval: $a \in \mathcal{A}_0^{\mathrm{I}} = (0, a_0)$, where a numerical calculation gives $a_0 = 0.653\,271$. The energy band structure is adequately described by a plot of the trace of the monodromy matrix, as represented in figure 2 by a dashed line (in this plot the results for the Scarf potential are also included as a solid line). There, we can appreciate a good qualitative approach between both spectra, especially in the energy range of the lowest allowed bands. For smaller values of ϵ, a much better approximation is obtained for a wider range of energies.

In general, the eigenfunctions corresponding to the band edges are of two classes. The cosine-type solutions are defined in the interval $(-\epsilon, \pi + \epsilon)$ as follows:

$$\psi_c^{\pm}(x;\epsilon) = \begin{cases} \cos(px) & -\epsilon < x \leqslant \epsilon \\ Au(x) + Bv(x) & \epsilon \leqslant x \leqslant \pi - \epsilon \\ \pm\cos(p(x - \pi)) & \pi - \epsilon \leqslant x < \pi + \epsilon. \end{cases} \tag{4.4}$$

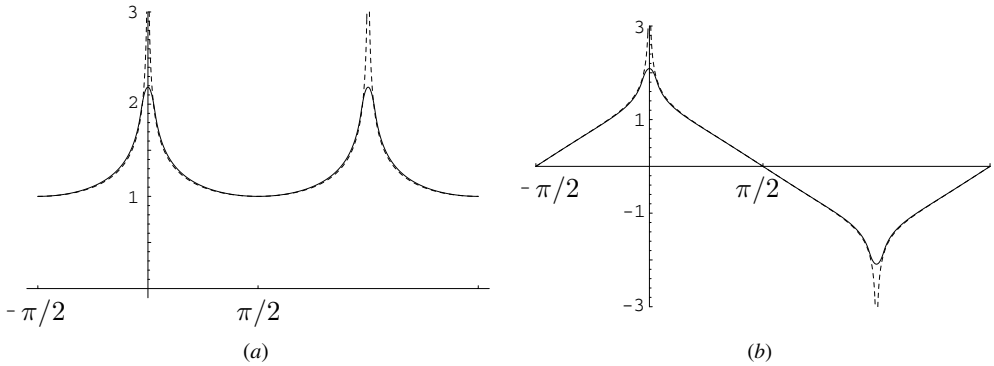


Figure 3. The lower (*a*) and first excited (*b*) energy band edge eigenfunctions of the Scarf potential (dashed curves) and the ϵ-regular one V_ϵ (solid lines) for $\epsilon = 0.1$, $a = 0.5$.

The energy quantization is obtained from the (anti) periodic condition

$$-p\tan(p\epsilon) = \left[\frac{u'(\epsilon) \mp u'(\pi-\epsilon)}{u(\epsilon) \pm u(\pi-\epsilon)}\right] = \left[\frac{v'(\epsilon) \mp v'(\pi-\epsilon)}{v(\epsilon) \pm v(\pi-\epsilon)}\right] \tag{4.5}$$

and the coefficients A, B are obtained from these values of p plus some Wronskians

$$A = \left.\frac{W(\cos(px), v(x))}{W(u,v)}\right|_{x=\epsilon} \qquad B = \left.\frac{W(u(x), \cos(px))}{W(u,v)}\right|_{x=\epsilon}. \tag{4.6}$$

These solutions soften the divergences of certain eigenfunctions for V_s such as the one shown in figure 3. The ϵ-regular solutions also explain the origin of divergent solutions in the Scarf potential: there are deep regularization wells at the singularity points which give rise to such a behaviour.

The sinus-type solutions for V_ϵ are defined by

$$\psi_s^{\pm}(x;\epsilon) = \begin{cases} \sin(px) & -\epsilon < x \leqslant \epsilon \\ Cu(x) + Dv(x) & \epsilon \leqslant x \leqslant \pi - \epsilon \\ \pm\sin(p(x-\pi)) & \pi - \epsilon \leqslant x < \pi + \epsilon \end{cases} \tag{4.7}$$

where the discrete p values are obtained from

$$p\cot(p\epsilon) = \left[\frac{u'(\epsilon) \pm u'(\pi-\epsilon)}{u(\epsilon) \mp u(\pi-\epsilon)}\right] = \left[\frac{v'(\epsilon) \pm v'(\pi-\epsilon)}{v(\epsilon) \mp v(\pi-\epsilon)}\right] \tag{4.8}$$

and the coefficients are computed with the help of the expressions

$$C = \left.\frac{W(\sin(px), v(x))}{W(u,v)}\right|_{x=\epsilon} \qquad D = \left.\frac{W(u(x), \sin(px))}{W(u,v)}\right|_{x=\epsilon}. \tag{4.9}$$

This class of solutions is quite close to that of Scarf in the whole real line since they vanish at the singular points.

Now let us consider the solution of (3.11) in the second subinterval $a \in \mathcal{A}_1^{\mathrm{I}} = (a_1, a_2)$, where $a_1 = \pi$ and a numerical computation gives $a_2 = 3.292\,31$. In figure 4 we have represented the trace of the corresponding monodromy matrix M_ϵ, for some specific values of the parameters. As we can see, the non-negative allowed energies also constitute a good approximation to the conventional Scarf energy bands, but there are two additional very narrow negative allowed bands which are absent in the Scarf case. Note that, for an arbitrary cutoff $\epsilon \neq 0$ and $a \in \mathcal{A}_1^{\mathrm{I}}$, the negative allowed energies admit bounded eigenfunctions and the

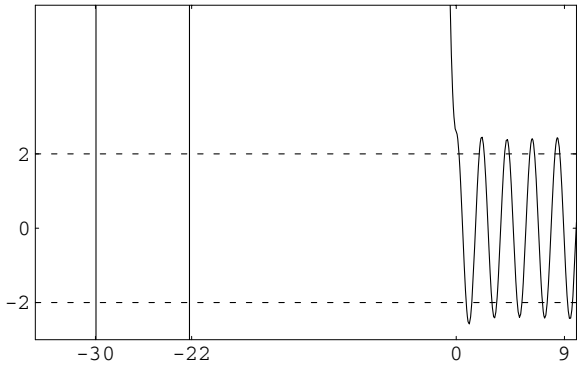


Figure 4. The monodromy matrix trace for the ϵ-regular Scarf potential V_ϵ, with $a = 3.226$ and $\epsilon = 0.1$. A couple of negative narrow allowed bands of energy may also be seen.

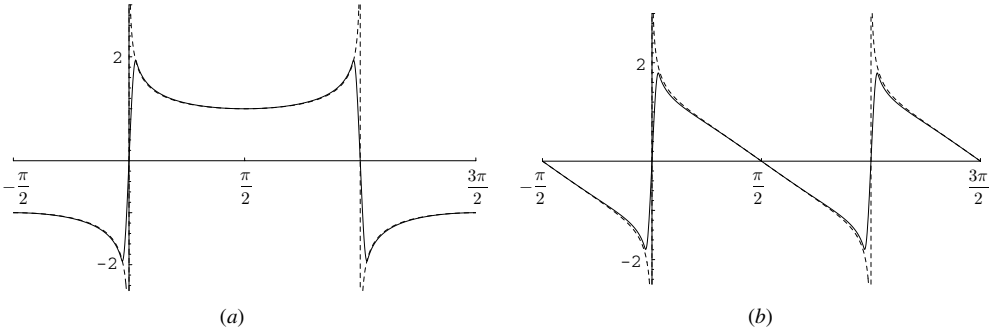


Figure 5. The lower (*a*) and first excited (*b*) band-edge eigenfunctions in the positive energy sector of the Scarf potential (dashed curves) and the ϵ-regular one V_ϵ (solid lines) for $\epsilon = 0.1$, $a = 1.727$.

potential V_ϵ represents an admissible physical situation. The limiting case $V_s = \lim_{\to 0} V_\epsilon$, in contrast, is far from being physically sound and is not a 'realistic' potential: although its positive energy bands converge to those of Scarf, the negative ones go to minus infinity, which gives rise to unstable systems (or to Hamiltonians not bounded from below). The same can be said about other type I bands for $a \in \mathcal{A}^{\mathrm{I}}_{n\neq 0}$.

4.2.2. Type II regularizations. A similar discussion is valid for the solutions of type II in equation (3.12). The first band $\mathcal{A}^{\mathrm{II}}_0$ supplies a good approximation for the spectrum, as well as for the eigenfunctions of the (conventional) Scarf potential. However, since $\mathcal{A}^{\mathrm{II}}_0$ contains bigger values of a than those of $\mathcal{A}^{\mathrm{I}}_0$, we have two consequences: (i) a change of sign, with respect to the type I solutions, appears when crossing every well of width 2ϵ (compare figure 5 with figure 3). This change of sign has no effect on the band structure in the limit $\epsilon \to 0$ in the positive energy sector. (ii) There is an additional band, in the far negative energy sector, whose edge eigenfunctions are represented in figure 6. This band, in the limit $\epsilon \to 0$, goes to $-\infty$, and at the same time becomes thinner and thinner. For the regularizations corresponding to other solutions $\mathcal{A}^{\mathrm{II}}_{n\neq 0}$ we have a similar situation, with an odd number of negative extra bands. As discussed in the previous subsection, these type II solutions give rise only to a partial approximation to the (conventional) Scarf spectrum.

Finally, we would like to highlight the important role played by the solutions of equation (3.11)–(3.12), since the energy band structure is quite sensible to the cutoff

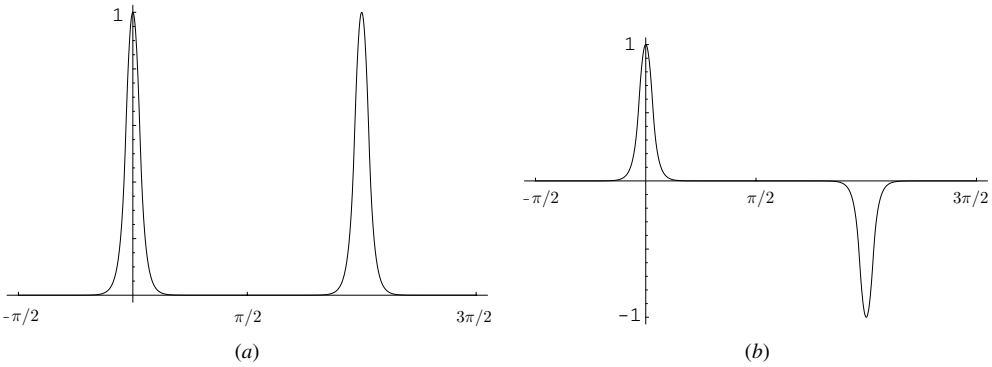


Figure 6. Lower (a) and upper (b) eigenfunctions of type II regularization corresponding to the band edges in the negative sector, $\epsilon = 0.1$, $a = 1.727$.

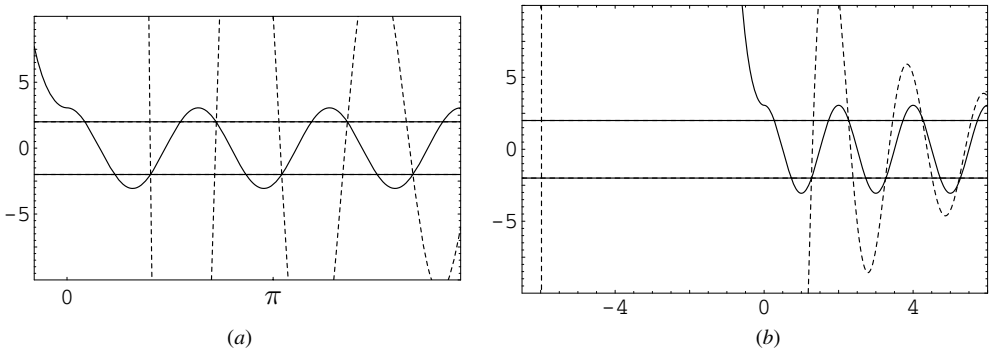


Figure 7. The solid curves correspond to the monodromy matrix of the regularized Scarf potential for $a = 0.5$, already considered in figure 2. The dashed lines correspond to $\epsilon = 0.1$ for a well more shallow than $a = 0.5$ (a), and for a deeper well (b).

strength a^2. Figure 7 shows the trace corresponding to the values of a slightly above or below the solution $a = 0.5$ of (3.11), as shown in figure 2. It is clearly seen that the bands are thinner and, in the limit $\epsilon \to 0$, they give rise to discrete solutions in the levels corresponding to the u eigenfunctions. Thus, only for the specific values of a included in the type I and II solutions, does the band spectrum not collapse into a punctual spectrum, converging to the Scarf one.

5. *k*-susy regularized Scarf partners

Susy quantum mechanics allows us to build from an initial Hamiltonian H a susy partner $\widetilde{H}$, both of them sharing many properties. Our aim in this section is to see whether these preserved properties include the regularizations, and then try to get some consequences. We will start with the regularized periodic Scarf system H_s (that is, including the rules to cross the singularities), with the band structure and eigenfunctions characterized in section 4.1. The regularization is provided by the family of ϵ-regular periodic potentials V_ϵ following the conditions of section 4.2. In this section we will use this regularization family in the sense defined in the introduction that can be stated as follows: for any given (quasi-periodic) eigensolution ψ of H_s, e.g., $H_s\psi = \lambda\psi$, such that $\psi(x+\pi) = \mathrm{e}^{\mathrm{i}\sigma}\psi(x)$, we can choose a

family of eigensolutions $H_\epsilon\psi_\epsilon = \lambda_\epsilon\psi_\epsilon$, of the same periodic type, $\psi_\epsilon(x+\pi) = \mathrm{e}^{\mathrm{i}\sigma}\psi_\epsilon(x)$, such that when $\epsilon \to 0$, then $\lambda_\epsilon \to \lambda$ and $\psi_\epsilon \to \psi$ (the limit is taken at each point, except at the singularities). In practice, we will work with the eigenfunctions of the discrete spectrum ($\mathrm{e}^{\mathrm{i}\sigma} = \pm 1$), so that the above conditions have already been described in detail in section 4.2.

Let us start with 1-susy transformations. For a fixed ϵ-regular periodic potential V_ϵ, its 1-susy partner $\widetilde{V}_\epsilon$ is given by

$$\widetilde{V}_\epsilon(x) = V_\epsilon(x) - 2\beta'_\epsilon(x), \tag{5.1}$$

where the superpotential $\beta_\epsilon(x)$ is defined in terms of an eigenfunction $H_\epsilon\psi_\epsilon = \lambda_\epsilon\psi_\epsilon$ (known as a transformation function), through a logaritmic derivative: $\beta_\epsilon(x) = \psi'_\epsilon(x)/\psi_\epsilon(x)$. If we also want $\widetilde{V}_\epsilon(x)$ to be real, periodic and without singularities, we must take a *good* transformation function, i.e., $\lambda_\epsilon \in \left(-\infty, E^0_\epsilon\right]$, where E^0_ϵ is the ground energy, and $\psi_\epsilon(x)$ is a (quasi) periodic eigenfunction without nodes [13, 14]. In this way we arrive at a regular periodic system $\widetilde{H}_\epsilon$, whose band structure is the same as that of H_ϵ. The quasi-periodic eigenfunctions $\widetilde{\phi}_\epsilon(x)$ of $\widetilde{H}_\epsilon$ are obtained from those $\phi_\epsilon(x)$ of H_ϵ corresponding to the same eigenenergy by means of the usual intertwining relationship

$$\widetilde{\phi}_\epsilon(x) = \phi'_\epsilon(x) + \beta_\epsilon(x)\phi_\epsilon(x) = \frac{W(\phi_\epsilon(x), \psi_\epsilon(x))}{\psi_\epsilon(x)} \tag{5.2}$$

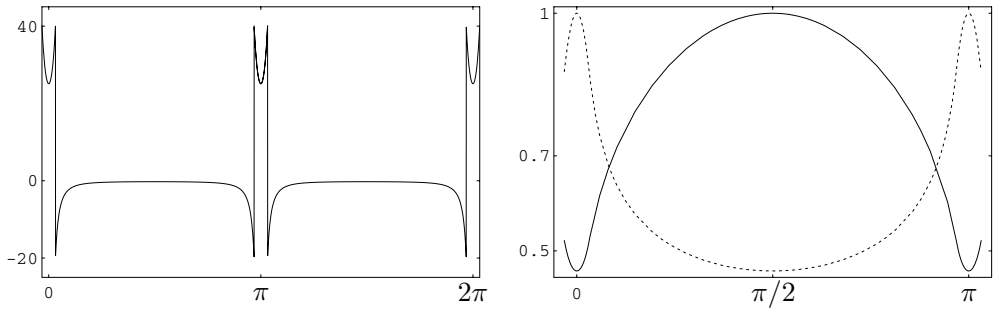
where $W(\cdot,\cdot)$ stands for the Wronskian of the involved functions. There is just one exception to the rule (5.2): if the transformation function is chosen to be the ground state ψ^0_ϵ, then the corresponding partner ground state is given by $\widetilde{\psi}^0_\epsilon = 1/\psi^0_\epsilon$.

The same formulae are useful to construct the 1-susy partner Scarf Hamiltonian $\widetilde{H}_s$ from H_s just by using a transformation function ψ, such that $\psi_\epsilon \to \psi$. Then, we have a number of properties that we enumerate below.

(1) If the transformation functions ψ are *good* (as defined above), the 1-susy partner Scarf potentials $\widetilde{V}_s$ will be periodic with the singularities at the same points as V_s. Furthermore, if for $x \approx 0$ the initial singularities are of the type $k(k-1)/x^2$, those of $\widetilde{V}_s$ will behave as $(k-1)(k-2)/x^2$. Therefore, when $1 < k < 3/2$, the initial potential is repulsive around the singularities while the partner potential is attractive at these points. In particular, if we choose as transformation function the ground state ψ^0, then $\widetilde{V}_s = (k-1)(k-2)/\sin^2 x$.
(2) If the Hamiltonian $\widetilde{H}_s$ is endowed with the same matching conditions at the singular points as those established for the regularized H_s, then H_s and $\widetilde{H}_s$ will have the same band structure. The (quasi) periodic eigensolutions of $\widetilde{H}_s$ are obtained by the 1-susy transformation (5.2) and automatically satisfy these boundary conditions. The corresponding eigenfunctions for the same eigenvalue in the discrete spectrum have opposite character, i.e., if ψ_n is either of type u (vanishing at the singular points) or v (diverging at the singularities), then $\widetilde{\psi}_n$ will be either of type v or u, respectively.
(3) The regular partner potentials $\widetilde{V}_\epsilon$ constitute a regularization for $\widetilde{V}_s$ in the same sense that the potentials V_ϵ were with respect to V_s. We can see in figure 8 that if the regularization terms around the singularities were negative in the potentials V_ϵ, they become positive for the partner potentials $\widetilde{V}_\epsilon$, as they should.

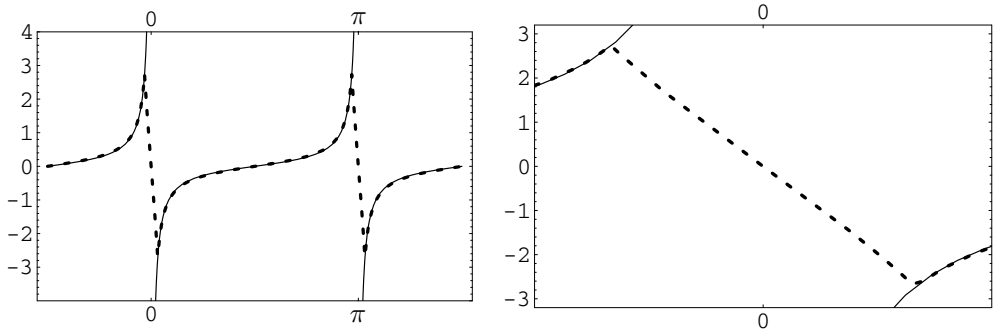
In figure 8(*a*) we have plotted the aspect of the 1-susy partner $\widetilde{V}_\epsilon(x)$ of our ϵ-regular potential (3.1), and figure 8(*b*) represents the ground states for both potentials $\widetilde{V}_\epsilon(x)$ and $V_\epsilon(x)$. Figure 9 shows the superpotential $\beta(x)$ of the Scarf system H_s using the transformation function ψ^0, together with the ϵ-regular superpotential $\beta_\epsilon(x)$ corresponding to ϕ^0_ϵ.

On the other hand, the second-order susy partners of H_ϵ make use of two of its eigenfunctions $\left\{\psi^1_\epsilon, \psi^2_\epsilon\right\}$. In order to end with a periodic nonsingular potential these transformation functions must be chosen quasi-periodic, belonging to the same forbidden



(*a*) (*b*)

Figure 8. (*a*) The 1-susy partner $\widetilde{V}_\epsilon(x)$ of the ϵ-regular Scarf potential $V_\epsilon(x)$ for $\epsilon = 0.1$ and $a = 0.5$ (compare with figure 1). (*b*) The lower-band edge energy eigenfunction (continuous curve) of the ϵ-regular potential (3.1) and its 1-susy partner for the same values of the parameters as in (*a*).



(*a*) (*b*)

Figure 9. The superpotential $\beta(x)$ for the ground state ψ^0 of H_s (solid line) versus the ϵ-regular superpotential $\beta_\epsilon(x)$ for the ground state ϕ_ϵ^0 of H_ϵ (dashed line) with $\epsilon = 0.1$ and $a = 0.5$. The figure on the right displays a detail of the regularization.

band, and with a nonvanishing Wronskian. The simplest choice is to take the two border edge eigenfunctions of any finite (forbidden) band, for instance the jth one: $\{\psi_\epsilon(x;\varepsilon_j), \psi_\epsilon(x;\varepsilon_{j'})\}$, where ε_j and $\varepsilon_{j'}$ are respectively the eigenenergies [13]. The construction of the second-order susy partner $\widetilde{V}_\epsilon(x)$ of $V_\epsilon(x)$ requires a calculation with the Wronskians:

$$\widetilde{V}_\epsilon(x;\varepsilon_j,\varepsilon_{j'}) = V_\epsilon(x) - 2\frac{\mathrm{d}^2 W(\psi_\epsilon(x;\varepsilon_1), \psi_\epsilon(x;\varepsilon_2))}{\mathrm{d}x^2}. \tag{5.3}$$

All the new potentials $\widetilde{V}_\epsilon(x;\varepsilon_j,\varepsilon_{j'})$ constructed in this way are isospectral with the initial one $V_\epsilon(x)$. The partner eigenfunctions are computed in the usual way:

$$\widetilde{\phi}_\epsilon(x) = \frac{W(\phi_\epsilon(x), \psi_\epsilon(x;\varepsilon_j), \psi_\epsilon(x;\varepsilon_{j'}))}{W(\psi_\epsilon(x;\varepsilon_j), \psi_\epsilon(x;\varepsilon_{j'}))}. \tag{5.4}$$

The results for the first example in (5.3) are shown in figure 10(*a*). A typical function of this new potential is depicted in figure 10(*b*) as well as its susy partner.

We can act in the same way with the Scarf potential to get its 2-susy partner $\widetilde{V}_s(x;\varepsilon_j,\varepsilon_{j'})$. Then we arrive at similar conclusions with respect to the behaviour of regularizations under 2-susy transformations that we summarize in the following points:

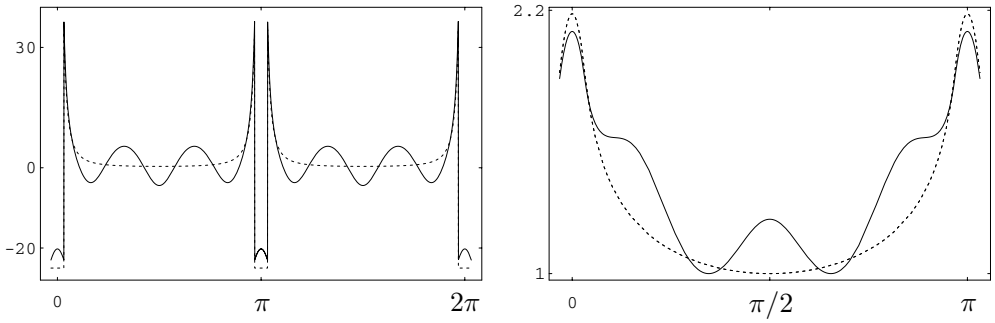


Figure 10. (*a*) The 2-susy partner (continuous curve) $\widetilde{V}_\epsilon(x;\varepsilon_1,\varepsilon_{1'})$ of the ϵ-regular Scarf potential $V_\epsilon(x)$ for $\epsilon = 0.1$ and $a = 0.5$ (compare with figure 8). (*b*) The lower band edge energy eigenfunction (dashed curve) of the ϵ-regular potential (3.1) and its 2-susy partner for the same values of the parameters as in (*a*).

(1) The potentials V_s and $\widetilde{V}_\epsilon(x;\varepsilon_j,\varepsilon_{j'})$ have singularities with the same coefficients, i.e., the leading term around the singular points is $k(k-1)/x^2$ as $x \to 0$.
(2) If $\widetilde{H}_s$ is supplied with the same boundary conditions at the singular points as H_s, then both Hamiltonians will share the same spectrum. The corresponding eigenfunctions will have the same character (diverging or vanishing) at the singular points.
(3) The family $\widetilde{V}_\epsilon(x;\varepsilon_j,\varepsilon_{j'})$ constitutes a regularization to $\widetilde{V}_s(x;\varepsilon_j,\varepsilon_{j'})$ in the same sense as V_ϵ does for V_s.

As a general conclusion of this section we can say that it is possible to make n-susy transformations which are compatible with the regularization prescriptions. Even more, these transformations supply a variety of regularization terms for the singularities starting from a known one. In fact, the consistency of susy transformations and regularized Scarf Hamiltonians is the reason why the *regularized* Scarf potential can be considered as a periodic solvable potential [15], and therefore the usual agebraic methods can be applied to get the spectrum. However, it seems that such a detail is completely forgotten in the literature dealing with the Scarf potential as a periodic potential.

6. Concluding remarks

In this work we have dealt with the general problem of regularization of singular potentials with a periodic character. So, we have focused our attention on the conditions on a class of regular potentials V_ϵ, which replaces the singularities by square wells, such that in a certain limit the band structure of the conventional Scarf potential originates. If the singularities are given in terms of $k \in (1, 3/2)$ as $k(k-1)/\sin^2 x$, then the well's intensity given by the coefficient $-a^2$ is opposite in sign and, in order to reproduce the Scarf bands, these intensities must satisfy the relation (3.11) $k = 1 + a\tan a$ (and take the lowest solution for a).

Thus, one can look at the periodic potentials as systems giving rise to a sort of resonant effect, coming from the interrelation beween the wavefunction of the particle and the period of the potential. These resonant effects show that in certain energy regions the periodic potential reproduces the exponential decay of a forbiden character corresponding to a particle whose total energy is below the energy potential, or that in other regions such perodicity imitates the transparency similar to a particle inside the continuous spectrum. Only for very special conditions (supplied by relation (3.11)) the family V_ϵ, as $\epsilon \to 0$, keeps the transparent bands

finite, but otherwise they lead in the limit $\epsilon \to 0$ to wide forbidden zones separated only by discrete levels.

We have also shown that the matching rules of the regularized Scarf potentials are preserved under *n*-susy transformations. This is the reason why the usual algebraic methods can be applied to solve correctly the spectrum of the regularized periodic Scarf potential, or for any of its isospectral *n*-susy partners. In other words, just because of this consistency, the regularized periodic Scarf potential can be considered inside the class of (algebraically) solvable potentials.

There is a number of open problems that need further clarification; for example, the importance of shape in regularizations, the equivalence of regularizations and the formal manipulation of distribution terms in the regularizations, just to mention only a few. Work is in progress on some of these problems.

Acknowledgments

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