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# A new effective mass Hamiltonian and associated Lamé equation: bound states

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## Abstract

A new quantum model with rational functions for the potential and effective mass is proposed in a stretchable region outside which both are constant. Starting from a generalized effective mass kinetic energy operator the matching and boundary conditions for the envelope wavefunctions are derived. It is shown that in a mapping to an auxiliary constant-mass Schrödinger picture one obtains one-period ‘associated Lamé’ well bounded by two  $\delta$ -wells or  $\delta$ -barriers depending on the values of the ordering parameter  $\beta$ . The results for bound states of this new solvable model are provided for a wide variation of the parameters.

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## 1. Introduction

Effective mass theory has been used for years in several branches of modern physics such as nuclear physics [1] or solid-state physics (see, e.g., the pioneering works [2–4]). This theory is a useful tool for studying the motion of carriers in pure crystals and also for the virtual-crystal approximation to the treatment of homogeneous alloys (where the actual one-electron potential is approximated by a periodic potential), as well as of graded mixed semiconductors (where the virtual-crystal potential is not periodic). The salient feature of this theory is that it approximates a complicated physical situation to the solution of a Schrödinger equation with position-dependent effective mass function, the so-called effective mass (EM) eigenvalue equation. The position-dependent EM is also used in the construction of pseudo-potentials, which have a significant computational advantage in quantum Monte Carlo method

[5]. Needless to emphasize that the growing interest in semiconductor physics parallel to the modern development in fabricating nanostructure technology creates a renewed attention to study the behaviour of one-dimensional EM eigenvalue equation

$$H_{EM}(x)\psi(x) \equiv [T_{EM}(x) + V(x)]\psi(x) = E\psi(x) \quad (1.1)$$

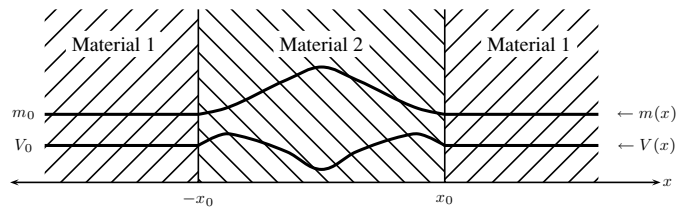
from a theoretical standpoint. In this equation  $T_{EM}(x)$  is the EM kinetic energy operator and  $\psi(x)$  is the EM wavefunction (also known as ‘envelope wavefunction’ in the literature [4–18]). It has to be mentioned that the justification of this EM approximation in the context of a realistic situation is not the purpose of the present study, rather we will concentrate on the analysis of the spectral properties of the EM eigenvalue equation (1.1). The first step is certainly to choose a suitable form of the Hermitian kinetic energy operator arising from non-commutativity of momentum operator  $p \equiv -i\hbar\partial_x$  and the effective mass operator  $m(x)$ . Different forms had been proposed in the literature, most of which may be written as a special class of the general two-parameter family proposed in [9]:

$$T_{EM}(x) = \frac{1}{4}(m^\alpha pm^\beta pm^\gamma + m^\gamma pm^\beta pm^\alpha), \quad (1.2)$$

with the constraint  $\alpha + \beta + \gamma = -1$  over the ordering parameters.

Considerable efforts were made to remove the non-uniqueness of the kinetic energy operator (1.2) or, in other words, to fix the values of the ordering parameters  $\alpha, \beta, \gamma$ . In [19] a step potential and a step mass were considered, and it was shown that  $\alpha = \gamma$  is the only physical choice for an abrupt heterojunction. Later in an attempt to fix  $\beta$ , two different conclusions were drawn, namely  $\beta = 0$  for a one-dimensional model [20] and  $\beta = -1$  for a three-dimensional model [21]. On the other hand, in a series of works [14, 22, 23], the authors concluded that  $\alpha = \gamma = 0, \beta = -1$  for an abrupt heterojunction. Among these works, [23] deserves to be mentioned separately because it presented the first example of a continuous function  $m(x)$  across the heterojunction. A new kind of kinetic energy operator was proposed [15] for strained heterostructure, which is not included in (1.2), in general, for position-dependent lattice constant. It should be mentioned that the choice  $\alpha = \gamma = 0, \beta = -1$  gives rise to the kinetic energy operator  $T_{EM} = p(1/2m)p$ , which was first proposed in [6]. Choosing the same operator some interesting pedagogical models were considered [17, 24] to show the qualitative differences in quantum mechanical observables (e.g. reflection and transmission coefficient, band-structure, etc) between EM and constant-mass case. Many other forms of kinetic energy operator have also been proposed, e.g.,  $\alpha = -1, \beta = 0$ , and  $\gamma = 0$  which gives from (1.2)  $T_{EM} = (1/4m)p^2 + p^2(1/4m)$  [25],  $\alpha = \gamma = -1/2, \beta = 0$  which yields  $T_{EM} = (1/2\sqrt{m})p^2(1/2\sqrt{m})$  [26], etc. A different variation was derived, via path-integral formalism [27], which comes from (1.2) for the following values:  $\alpha = (-\sqrt{2} + i)/3\sqrt{2}, \beta = -1/3, \gamma = \alpha^*$ . It is therefore clear that no universal choice for the ordering parameters exists in the literature of EM theory.

In recent times several authors [28–50] either started from a preferred *ad hoc* choice for  $\alpha, \beta, \gamma$  or kept them arbitrary. In both cases attention had been paid to solvability for various smooth functional forms of  $V(x)$  and  $m(x)$  by employing the existing tools like supersymmetry [29, 30, 34, 35, 40, 44–48], Lie-algebraic approach [32, 33, 35, 39], shape-invariance [43, 46], etc. The connection between solvability and the ordering parameters in equations (1.1) and (1.2) was discussed in [31]. On the full line, smooth functions (in the sense that  $m'$  and  $m''$  are also continuous) were chosen for the first time in [28], where the authors however concluded again that  $\alpha = \gamma = 0, \beta = -1$  by comparing their results with a limiting case where the potential and mass become abrupt. It may be mentioned that in several works [33–35] mass function was kept arbitrary and thus the solutions provided there were only formal. In contrast, in most cases where smooth functional forms were chosen for



**Figure 1.** A schematic representation of the model: a variable mass and a potential well in the interval  $(-x_0, x_0)$ , and outside of this interval both are constant.

$m(x)$ , we note that  $m(x) \rightarrow 0$  as  $|x| \rightarrow \infty$ . One possible way of eliminating this nonphysical situation is to consider the variation of the mass in a finite region (being constant outside), which is also natural on realistic grounds. Of course, this correction will force us to obtain correct matching conditions for the model.

Quite justifiably we will use the generic kinetic energy operator (1.2) without imposing any additional constraint over the ordering parameters. One of the purposes of our present work is to show that a sensible quantum situation could be modelled by a continuous functional form for  $V(x)$  and  $m(x)$ , which are free from the above-mentioned defect of vanishing mass at infinity. A new combination of rational forms will be chosen for both functions inside a region, but outside they will be considered to be constant, that is to say, our EM Hamiltonian is asymptotically equivalent to conventional constant-mass Hamiltonian. Our other purpose is to study the properties of bound states of this model and to compare the results with the constant-mass problem. The precise model chosen in the present work for  $m(x)$  and for the potential is motivated by the following property: it allows the transformation to the auxiliary spectral problem of a conventional (constant mass) Schrödinger equation, which is solvable. In this sense this variable mass problem can also be characterized as solvable.

The structure of the paper is as follows. In section 2 we will introduce our model and derive the appropriate matching conditions. Applying these conditions the equation for the energies of the bound states will be obtained (the details of some of the issues dealt in this section will be provided in appendix, for readers' convenience). In section 3, we will map the whole problem in an auxiliary constant-mass Schrödinger picture and obtain the correct physical range of bound-state energies of our EM potential. A limiting case will be considered in section 4, where the potential becomes the well-known harmonic oscillator. In section 5, we will solve numerically the transcendental energy equation for bound states and examine the spectral properties for a wide range of the parameters. Some characteristic differences from the constant-mass case will be noted here. Section 6 will contain a description of some interesting features of bound-state wavefunctions, obtained by the analysis of the numerical results of the previous section. We will end with our conclusion in section 7.

## 2. A model Hamiltonian and the energy equation

### 2.1. The model

To start with, we will introduce a hypothetical sample shown in figure 1, consisting of two materials, which produces a variation of mass in a stretchable region  $(-x_0, x_0)$ . We are interested in this exposition to study the bound states of a particle in the presence of a local

potential  $V(x)$ :

$$V(x) = \begin{cases} f_V(x), & |x| \leq x_0, \\ f_V(x_0) \equiv V_0 = \text{constant}, & |x| > x_0, \end{cases} \quad (2.1)$$

where the function  $f_V(x)$  is chosen to be

$$f_V(x) = \frac{Ak^2}{1+x^2} + \frac{Bk^2}{1+k^2x^2} + Ck^2x^2 + D. \quad (2.2)$$

The potential function depends on three classes of parameters : (i) the ordering parameters  $\alpha, \beta, \gamma \in \mathbb{R}$  of the kinetic term (1.2), such that  $\alpha + \beta + \gamma = -1$  , (ii) the elliptic modulus parameter  $k^2 \in (0, 1)$  or the complementary modulus  $k'^2 = 1 - k^2$  and (iii) the ‘Lamé parameters’  $\mu, \nu \in \mathbb{N}$  (this terminology will be explained shortly). The four constants  $A, B, C, D$  are expressed in terms of these parameters as

$$\begin{aligned} A &= 4(1 + \beta - \eta) - \left(\mu + \frac{1}{2}\right)^2, & B &= \left(\nu + \frac{1}{2}\right)^2 - 4(1 + \beta - \eta), \\ C &= 2[8\eta - 5\beta - 6] - 2, & D &= (1 + \beta)(3k^2 + 2) - 4\eta k^2 + \frac{k^2}{4} - 1. \end{aligned} \quad (2.3)$$

In the above expressions the quantity  $\eta$  stands for  $\eta = 1 + \beta + \alpha(\alpha + \beta + 1)$ . The point  $x_0$  depends on  $k$  by  $x_0 = 1/\sqrt{k'}$  and the mass function is given by

$$m(x) = \begin{cases} f_m(x), & |x| \leq x_0, \\ f_m(x_0) \equiv m_0 = \text{constant}, & |x| > x_0, \end{cases} \quad (2.4)$$

where

$$f_m(x) = [(1+x^2)(1+k^2x^2)]^{-1}. \quad (2.5)$$

It should be stressed that the choice of this particular model is made because it not only provides a continuous mass function with physically reasonable non-vanishing limit at infinity, but also leads to well-known associated Lamé equation, as we shall show subsequently. Thus, our task now is to solve the eigenvalue equation (1.1) for the general kinetic energy operator (1.2) with the potential  $V(x)$  and mass  $m(x)$  given by (2.1)–(2.5). Choosing for our convenience the scale  $\hbar^2 = 2$ , this equation may be written as

$$\psi''(x) - \frac{m'}{m}\psi'(x) + \left[ m\{E - V(x)\} - \frac{1 + \beta}{2} \frac{m''}{m} + \eta \left(\frac{m'}{m}\right)^2 \right] \psi(x) = 0, \quad (2.6)$$

where throughout this paper prime and dot will denote derivatives with respect to  $x$  and  $z$ , respectively.

## 2.2. Matching conditions

To derive the correct matching and boundary conditions for the envelope wavefunction  $\psi(x)$ , we note that the presence of  $m''/m$  in (2.6) produces a  $\delta$ -discontinuity at the two junctions  $x = \pm x_0$ . Thus,  $\psi'$  must have a definite jump at these junctions to balance these singularities in the EM eigenvalue equation (2.6). To calculate precisely these jumps, we will express  $m(x)$  and  $V(x)$  in terms of the Heaviside  $\Theta$ -function

$$\Theta(x) = \begin{cases} 1, & x > 0, \\ 1/2, & x = 0, \\ 0, & x < 0, \end{cases} \quad [\Theta'(x) = \delta(x)] \quad (2.7)$$

as

$$m(x) = m_0 \Xi(x) + f_m(x)[1 - \Xi(x)], \quad V(x) = V_0 \Xi(x) + f_V(x)[1 - \Xi(x)], \quad (2.8)$$

where

$$\Xi(x) = \Theta(-x_+) + \Theta(x_-), \quad x_{\pm} = x \pm x_0. \tag{2.9}$$

It may be noted at once that, due to the cancellation effect,  $m'$  will not contain  $\delta$ -discontinuity. Thus, we get

$$m'(x) = f'_m(x)[1 - \Xi(x)], \quad m''(x) = f''_m(x)[1 - \Xi(x)] - f'_m(x)\Xi'(x). \tag{2.10}$$

It is obvious that the first-order derivative term in (2.6) could be eliminated by introducing the transformed function

$$\phi(x) = \psi(x)/\sqrt{m(x)}. \tag{2.11}$$

The EM eigenvalue equation (2.6) reduces to

$$\phi''(x) = \left[ m\{V(x) - E\} + \frac{\beta}{2} \frac{m''}{m} + \left(\frac{3}{4} - \eta\right) \left(\frac{m'}{m}\right)^2 \right] \phi(x). \tag{2.12}$$

Integration of equation (2.12) with respect to  $x$  in the interval  $[x_0 - \epsilon, x_0 + \epsilon]$  yields

$$\begin{aligned} \phi'(x) \Big|_{x_0-\epsilon}^{x_0+\epsilon} &= \int_{x_0-\epsilon}^{x_0} \left[ f_m\{f_V - E\} + \frac{\beta}{2} \frac{f''_m}{f_m} + \left(\frac{3}{4} - \eta\right) \left(\frac{f'_m}{f_m}\right)^2 \right] \phi(x) \\ &\quad + m_0(V_0 - E) \int_{x_0}^{x_0+\epsilon} \phi(x) dx - \frac{\beta}{2} \int_{x_0-\epsilon}^{x_0+\epsilon} \frac{f'_m}{f_m} \delta(x_-) \phi(x) dx. \end{aligned} \tag{2.13}$$

Let us note that for our model the wavefunction  $\psi(x)$  must be continuous<sup>4</sup> on the full line, for otherwise  $\psi''(x)$  would have stronger singularity than that from the term  $m''$  in equation (2.6). It then follows from (2.11) that  $\phi(x)$  is a continuous function. Hence all integrands in (2.13) are continuous except the last term. Thus letting  $\epsilon \rightarrow 0$ , we will obtain the jump at  $x = x_0$ :

$$\Delta\phi' \Big|_{x=x_0} = -\frac{\beta}{2} \frac{f'_m(x_0)}{f_m(x_0)} \phi(x_0). \tag{2.14}$$

Proceeding similarly for the other junction  $x = -x_0$ :

$$\Delta\phi' \Big|_{x=-x_0} = \frac{\beta}{2} \frac{f'_m(-x_0)}{f_m(-x_0)} \phi(-x_0). \tag{2.15}$$

We thus derive the following conditions for the envelope wavefunction  $\psi$  and its derivative:

- a)  $\psi(x)$  is continuous,
- b)  $\Delta \left( \frac{\psi}{\sqrt{m}} \right)' \Big|_{x=\pm x_0} = \mp \frac{\beta}{2} \frac{f'_m(\pm x_0)}{f_m(\pm x_0)} \frac{\psi(\pm x_0)}{\sqrt{m(\pm x_0)}}$ ,

and for the bound-state wavefunctions

$$c) \int_{-\infty}^{\infty} |\psi_n(x)|^2 dx = 1, \quad (\text{normalizability}). \tag{2.17}$$

<sup>4</sup> The case of discontinuity in both  $V(x)$  and  $m(x)$  (e.g. potential-mass step [19] or a quantum well with mass mismatch) corresponds to discontinuity of  $\psi(x)$  [51].

### 2.3. Expressions for wavefunctions

The EM eigenvalue equation (2.12) takes the following form in the three regions:

$$\phi''(x) = \begin{cases} \kappa^2 \phi(x), & |x| > x_0 \\ [f_m(x)\{f_V(x) - E\} + \frac{\beta}{2} \frac{m''}{m} + (\frac{3}{4} - \eta)(\frac{m'}{m})^2] \phi(x), & |x| < x_0, \end{cases} \quad (2.18)$$

in which we have used the abbreviation

$$\kappa^2 = m_0(V_0 - E). \quad (2.19)$$

In this exposition we are primarily interested in bound states and thus the quantity  $\kappa$  in (2.19) will be always real and nonzero. The scattering states for which  $E \geq V_0$  will be discussed at length elsewhere. The acceptable solutions of (2.18) for  $|x| > x_0$  are

$$\phi(x) = \begin{cases} \mathcal{N}^- e^{\kappa x}, & x < -x_0 \\ \mathcal{N}^+ e^{-\kappa x}, & x > x_0, \end{cases} \quad (2.20)$$

where  $\kappa$  is taken as positive square root of (2.19) and the constants  $\mathcal{N}^\pm$  have to be determined from the conditions (a)–(c). In the intermediate region the reformulation of equation (2.18) is useful to solve the spectral problem. The crucial observation is that this equation may be transformed into the well-known associated Lamé equation [52–57],

$$\ddot{\chi}(z) - k^2 \left[ \mu(\mu + 1) \operatorname{sn}^2 z + \nu(\nu + 1) \frac{\operatorname{cn}^2 z}{\operatorname{dn}^2 z} - \frac{E}{k^2} \right] \chi(z) = 0, \quad (2.21)$$

by means of the following changes of variables:

$$x(z) = \operatorname{sn} z / \operatorname{cn} z, \quad \chi(z) = [f_m(x(z))]^{1/4} \phi(x(z)). \quad (2.22)$$

In the above equations  $\operatorname{sn} z \equiv \operatorname{sn}(z, k)$ ,  $\operatorname{cn} z \equiv \operatorname{cn}(z, k)$  and  $\operatorname{dn} z \equiv \operatorname{dn}(z, k)$  are three Jacobian elliptic functions of real modulus  $k$ . Since the parameters  $\mu, \nu$  enter in the associated Lamé potential (2.21), we will reserve the terminology ‘Lamé parameters’ for them. Note that equation (2.21) is of period  $K$  or  $2K$  according as  $\mu = \nu$  or  $\mu \neq \nu$ , where  $K(k) = \int_0^{\pi/2} d\tau / \sqrt{1 - k^2 \sin^2 \tau}$  is the complete elliptic integral of second kind. The Lamé parameters can be chosen as any integral pair, but for simplicity we will choose  $\mu = \nu = 1$ . In this context it may be emphasized that the associated Lamé equation (2.21) for  $\mu = \nu$  can be mapped via coordinate transformation  $\tilde{z} = (1 + k')z$  to ordinary Lamé equation with a different modulus parameter  $\tilde{k} = (1 - k')/(1 + k')$  and the energy variable  $\tilde{E} = -\mu(\mu + 1)\tilde{k} + E/(1 + k')^2$  through the use of the relation  $\operatorname{sn}(\tilde{z}, \tilde{k}) = (1 + k')\operatorname{sn}(z, k)\operatorname{cn}(z, k)/\operatorname{dn}(z, k)$ . However, in our auxiliary variable  $z$ , equation (2.21) represents associated Lamé equation, and for  $\mu = \nu$  it becomes  $K$ -periodic. This means that we are going to consider this equation in a single period  $(-K/2, K/2)$ .

At this stage it is worth mentioning that the region  $(-x_0, x_0)$  of material 2 must be so chosen that it may be stretched as large as we please, but it will be always finite (it must be surrounded by material 1). On the other hand, it cannot be shrunk to a point due to the presence of material 2 (see figure 1). For this reason we need to exclude the points  $z = \pm K$  from the domain of equation (2.21), as it can be easily verified from transformation (2.22) that these points lead to  $x = \pm\infty$ . For definiteness we have chosen the interval  $z \in (-K/2, K/2)$  which just corresponds to  $x \in (-x_0, x_0)$ , where  $x_0 = 1/\sqrt{k'}$ . Let us remark about two well-known limits  $k \rightarrow 1$  and  $0$ , which are usually considered for elliptic functions. Note that as  $k \rightarrow 1$ , the complementary modulus  $k' \rightarrow 0$  and consequently  $x_0$  goes to infinity. Thus  $k \rightarrow 1$  limit is not allowed in our model. But the other limit  $k \rightarrow 0$  may be considered as it allows the shrinking of the region  $(-x_0, x_0)$  up to a finite interval  $(-1, 1)$ . The general solutions of equation (2.21) for arbitrary energy  $E$ , which we need, were obtained only recently

in [57, 58]. Here we will not describe the method of obtaining these solutions, but for readers' convenience, we have included a self-contained brief introduction about elliptic functions in appendix. The two linearly independent solutions<sup>5</sup> of (2.21) are (for three exceptional cases see below)

$$\chi_{1,2}(z) = \frac{\prod_{i=1}^2 \sigma(z - iK' \pm a_i)}{\sigma(z - iK' + \omega_1)\sigma(z - iK')} \exp[(z - iK')\{\zeta(\omega_1) \mp \zeta(a_1) \mp \zeta(a_2)\}], \quad (2.23)$$

where  $a_i(E)$  are to be determined from the equation  $\wp(a_i) = c_i$ ,  $c_i$  being zeros of the following quadratic equation (see equations (4)–(5) in [57]):

$$c^2 + (E - 4 + e_1)c + (3e_1 - e_2 - 2e_1e_3 - e_1E) = 0. \quad (2.24)$$

Here,  $e_i$  are always real ( $e_1 > e_2 > e_3$ ) defined by  $\wp(\omega_i) = e_i$ ,  $\omega_1$  and  $\omega_3$  are half-periods of Weierstrass elliptic function  $\wp(z)$  (see appendix for more details). For the numerical convenience, here we have chosen the scale  $e_1 - e_3 = 1$  so that  $\omega_1 = K$ ,  $\omega_3 = iK'$ ,  $\omega_2 = \omega_1 + \omega_3$ ,  $K'(k) = K(k')$ . Thus, the solution in the intermediate region takes the form

$$\chi(z) = d_1\chi_1(z) + d_2\chi_2(z). \quad (2.25)$$

The constants  $d_1, d_2$  have to be fixed from the conditions (a)–(c). Before proceeding to do that, we would like to point out that for special values of  $E = E^{(j)}$ ,  $j = 0, 1, 2$  both solutions  $\chi_1(z)$  and  $\chi_2(z)$  become identical and coincide to periodic (or anti-periodic) band-edge solutions  $\chi^{(j)}$ . The explicit expressions for these solutions [53] and corresponding values of  $a_i$  in (2.24) are

$$\begin{aligned} \chi^{(0)} &= \operatorname{dn} z + k'/\operatorname{dn} z, & E^{(0)} &= 2 + k^2 - 2k', & a_1 &= -a_2 = \omega_1/2, \\ \chi^{(1)} &= \operatorname{dn} z - k'/\operatorname{dn} z, & E^{(1)} &= 2 + k^2 + 2k', & a_1 &= -a_2 = -\omega_3 + \omega_1/2, \\ \chi^{(2)} &= \operatorname{sn} z \operatorname{cn} z / \operatorname{dn} z, & E^{(2)} &= 4, & a_1 &= \omega_3, \quad a_2 = \omega_2. \end{aligned} \quad (2.26)$$

Thus, for  $E = E^{(j)}$  the two linearly independent solutions of associated Lamé equation (2.21) may be given as

$$\chi_1(z) = \chi^{(j)}(z), \quad \chi_2(z) = \chi_1(z) \int^z \frac{d\tau}{[\chi_1(\tau)]^2}. \quad (2.27)$$

It should be emphasized that in our model the situation is different from that of periodic associated Lamé equation [53, 55] because equation (2.21) is considered in only one period  $(-K/2, K/2)$ . We will show later that the discrete energy levels of our EM Hamiltonian lie inside the allowed bands of constant-mass periodic associated Lamé Hamiltonian, and corresponding wavefunctions  $\psi(x)$  are obtained from (2.20) and (2.23).

#### 2.4. Energy equation for bound states

The continuity condition and slope-discontinuity requirement (2.16) can be expressed in a single pair of equations

$$\mathcal{N}^\pm m_0^{\frac{1}{4}} e^{-\kappa/\sqrt{k'}} = d_1 \chi_1^\pm + d_2 \chi_2^\pm, \quad (2.28)$$

$$\mathcal{N}^\pm (\beta\sqrt{k'} + \kappa) e^{-\kappa/\sqrt{k'}} = d_1 \left( \mp m_0^{\frac{1}{4}} \dot{\chi}_1^\pm - \frac{\sqrt{k'}}{2} m_0^{-\frac{1}{4}} \chi_1^\pm \right) + d_2 \left( \mp m_0^{\frac{1}{4}} \dot{\chi}_2^\pm - \frac{\sqrt{k'}}{2} m_0^{-\frac{1}{4}} \chi_2^\pm \right), \quad (2.29)$$

<sup>5</sup> The notations for the Lamé parameters  $\mu, \nu$  in [57, 58] are  $m, \ell$ .



where we have used the abbreviations

$$\chi_i^\pm = \chi_i(\pm K/2), \quad \dot{\chi}_i^\pm = \dot{\chi}_i(\pm K/2), \quad i = 1, 2. \quad (2.30)$$

Eliminating  $\mathcal{N}^\pm$  from (2.28)–(2.29), we obtain a homogeneous linear system for  $d_1, d_2$ :

$$\begin{aligned} d_1[2m_0^{1/4}\dot{\chi}_1^+ + m_0^{-1/4}\mathcal{B}\chi_1^+] + d_2[2m_0^{1/4}\dot{\chi}_2^+ + m_0^{-1/4}\mathcal{B}\chi_2^+] &= 0, \\ d_1[2m_0^{1/4}\dot{\chi}_1^- - m_0^{-1/4}\mathcal{B}\chi_1^-] + d_2[2m_0^{1/4}\dot{\chi}_2^- - m_0^{-1/4}\mathcal{B}\chi_2^-] &= 0, \end{aligned}$$

where the quantity  $\mathcal{B}$  reads

$$\mathcal{B} = (2\beta + 1)\sqrt{k'} + 2\kappa. \quad (2.31)$$

Demanding for non-trivial solutions of  $d_1, d_2$  from the previous system of equations, we have obtained our energy equation in the following form:

$$4m_0(T_2^- - T_2^+) + 2\sqrt{m_0}\mathcal{B}(\dot{T}_1^- + \dot{T}_1^+) + \mathcal{B}^2(T_1^+ - T_1^-) = 0, \quad (2.32)$$

where

$$T_1^\pm = \chi_1^\pm \chi_2^\mp, \quad \dot{T}_1^\pm = \dot{\chi}_1^\pm \chi_2^\mp - \chi_1^\pm \dot{\chi}_2^\mp, \quad T_2^\pm = \dot{\chi}_1^\pm \dot{\chi}_2^\mp. \quad (2.33)$$

In particular for  $E \neq E^{(j)}$ ,  $j = 0, 1, 2$ , the energy equation (2.32) may be further simplified by inserting the expressions for  $\dot{\chi}_i^\pm$  from equation (2.23) (see appendix) and then the energy equation reduces to the form

$$[4m_0A_-^2 - 4\mathcal{B}\sqrt{m_0}A_- + \mathcal{B}^2]T_1^- - [4m_0A_+^2 + 4\mathcal{B}\sqrt{m_0}A_+ + \mathcal{B}^2]T_1^+ = 0, \quad (2.34)$$

where  $A_\pm$  are given by

$$A_\pm = \pm \frac{1}{2} \left[ \sum_{i=1}^2 \frac{\wp\left(\frac{\omega_1}{2} + \omega_3\right) \mp \wp(a_i)}{\wp\left(\frac{\omega_1}{2} + \omega_3\right) - \wp(a_i)} - \frac{\wp\left(\frac{\omega_1}{2} + \omega_3\right)}{\wp\left(\frac{\omega_1}{2} + \omega_3\right) - e_1} \right] \quad (2.35)$$

Hence, similar to the well-known textbook example of the finite square well potential, we have to deal with the transcendental energy equations (2.32) and (2.34). It is clear from the structure of equation (2.34) that for  $T_1^- = T_1^+$ , some roots will be given by the equation  $A_- - A_+ = 0$ . But one may note from (2.35) that this equation will be true if and only if  $\sum \wp(a_i) = 0$ . The latter condition is, however, satisfied only for band-edge energies  $E = E^{(j)}$ , mentioned in equation (2.26). This clearly implies that the roots  $E = E^{(j)}$  of (2.34) have to be discarded, because for these values the correct energy equation is (2.32), where  $\chi_i$  s are given by (2.26) and (2.27). It may be mentioned that we have checked numerically for different values of the potential parameters that the energy equation (2.32) is not satisfied for  $E = E^{(j)}$ . This means that for those cases the band-edge energies of periodic associated Lamé Hamiltonian are not roots of the energy equation for bound states of our EM Hamiltonian. Thus, we will solve numerically equation (2.34) for  $E$ , and the roots, if they exist, may lie in principle inside the allowed and forbidden bands. However, the numerical results could be well handled if we have, *a priori*, some analytical insight from the theory. To achieve this insight we have to fall back upon the auxiliary constant-mass Schrödinger equation of which we know very well the structure of the spectrum. In the following section, we will obtain an image of our EM model in this conventional Schrödinger language.

### 3. Auxiliary constant-mass equation

Our purpose is to extend (2.21) onto the whole  $z$ -axis in the form

$$-\ddot{\chi}(z) + \tilde{V}(z)\chi(z) = E\chi(z), \quad (3.1)$$

which can be viewed as a constant-mass Schrödinger equation for a single particle of unit mass (according to our chosen scale  $\hbar^2 = 2$ ). Of course, equation (3.1) plays the role of auxiliary equation, and our aim is to extract general information about its spectral properties, which could be used as a guide in our numerical procedure for physical model (1.1). The observation here is that this can be achieved by extending transformations (2.22) to the entire  $z$ -axis:

$$z = \int^x \sqrt{m(\tau)} \, d\tau, \quad \chi(z) = [m(x(z))]^{-1/4} \psi(x(z)). \tag{3.2}$$

But there are two subtle points which should be taken into account to obtain the correct expression for the Schrödinger potential  $\tilde{V}(z)$ . In the first place, since  $m(x)$  is continuous, the new coordinate  $z(x)$  should also be continuous. It will then follow from (3.2) that the constant-mass wavefunction  $\chi(z)$  is also continuous function of  $z$ . One can achieve this by exploiting the arbitrariness in the indefinite integral in (3.2). Indeed the explicit relation between  $z$  and  $x$  is

$$x(z) = \begin{cases} (z - \lambda_-)/\sqrt{m_0}, & -\infty < z < -K/2, \\ \text{sn } z/\text{cn } z, & -K/2 < z < K/2, \\ (z - \lambda_+)/\sqrt{m_0}, & K/2 < z < \infty, \end{cases} \tag{3.3}$$

where  $\lambda_{\pm} = \pm(K/2 - \sqrt{m_0}x_0)$ . The second point is even more fundamental concerning the nature of  $m'$  and  $m''$  in the whole region  $x \in \mathbb{R}$ . We have mentioned in subsection 2.2 that due to the cancellation effect  $m'$  will contain  $\Theta$ -discontinuity and consequently  $m''$  will produce  $\delta$ -discontinuity at the two junctions  $x = \pm x_0$ . Noting that  $\delta(bx) = \delta(x)/|b|$ , the Schrödinger potential  $\tilde{V}(z)$  may be expressed in the following form:

$$\tilde{V}(z) = V_0 \tilde{\Xi}(z) + \tilde{f}_V(z) [1 - \tilde{\Xi}(z)] + \left(\beta + \frac{1}{2}\right) (1 + k') [\delta(z_+) + \delta(z_-)], \tag{3.4}$$

where

$$\tilde{f}_V(z) = 2k^2 \left[ \text{sn}^2 z + \frac{\text{cn}^2 z}{\text{dn}^2 z} \right], \quad \tilde{\Xi}(z) = \Theta(-z_+) + \Theta(z_-), \quad z_{\pm} = z \pm K/2. \tag{3.5}$$

The point to be noted here is the  $\beta$  dependence of the shape of  $\tilde{V}(z)$  at the two junctions  $z = \pm K/2$ . It should be kept in mind that although the auxiliary constant-mass Schrödinger wavefunction  $\chi(z)$  is continuous, its derivative is not. In this sense the auxiliary Schrödinger equation (3.1) is not exactly in conventional form. One may check readily from the matching condition (2.16) that

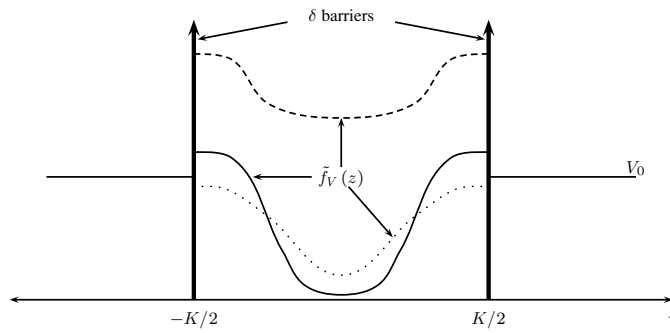
$$\Delta[\dot{\chi}(z)]|_{z=\pm K/2} = \left(\beta + \frac{1}{2}\right) (1 + k') \chi^{\pm}. \tag{3.6}$$

To understand the correct range of  $E$  for bound states, we will consider separately three cases:  $\beta > -1/2$ ,  $\beta = -1/2$  and  $\beta < -1/2$ .

*Case 1:*  $\beta > -1/2$ . In this case there will be a well, determined by one-period associated Lamé potential  $\tilde{f}_V(z)$  in the region  $(-K/2, K/2)$ , bounded by two  $\delta$ -barriers, and outside this region a constant potential  $V_0$ . Three possible situations may arise (see figure 2). Clearly there may be bound states in the range  $(\tilde{f}_V)_{\min} < E < V_0$  if and only if  $(\tilde{f}_V)_{\min} < V_0$ .

*Case 2:*  $\beta = -1/2$ . In this case the  $\delta$ -barrier will disappear and for bound states the conclusion is the same as before.

*Case 3:*  $\beta < -1/2$ . In this situation the shape of the associated Lamé well provides no restrictions from below on the bound-state energies due to the presence of two  $\delta$ -wells at the



**Figure 2.** Three possible positions of the constant-mass Schrödinger potential  $\tilde{V}(z)$  are shown for  $\beta > -1/2$ . For  $\beta = -1/2$   $\delta$ -barriers disappear, and for  $\beta < -1/2$  there are two  $\delta$ -wells at the junctions.

two junctions  $z = \pm K/2$ . We thus conclude that the bound states may exist in the range  $-\infty < E < V_0$ .

In the following section we will consider the limit  $k \rightarrow 0$  and will write the explicit energy equation for this limit. Before concluding this section it may be mentioned that in the  $k \rightarrow 0$  limit,  $\tilde{f}_V(z) \equiv 0$  and  $\tilde{V}(z)$  reduces to

$$\tilde{V}(z) \rightarrow V_0 \tilde{\Xi}(z) + (2\beta + 1)[\delta(z_+) + \delta(z_-)], \tag{3.7}$$

where  $z_{\pm} \rightarrow z \pm \pi/4$ . Thus, for  $\beta \geq -1/2$ , (cases 1 and 2 above) bound states may exist in the range  $0 < E < V_0$  and for  $\beta < -1/2$  the possible range is  $-\infty < E < V_0$ .

#### 4. A limiting case : $k \rightarrow 0$

It is well known that the Jacobian elliptic functions degenerate into trigonometric and hyperbolic functions in  $k \rightarrow 0$  and  $k \rightarrow 1$  limits. We have already pointed out that  $k \rightarrow 1$  limit is prohibited<sup>6</sup> in our model, as this limit corresponds to the nonphysical situation of vanishing mass for large  $|x|$ . In the  $k \rightarrow 0$  limit, the intermediate region shrinks up to the interval  $(-1, 1)$  inside which the harmonic oscillator well  $V(x)$  and the mass function  $m(x)$  are

$$V(x) = \begin{cases} Cx^2 + D, & |x| \leq 1 \\ V_0, & |x| \geq 1, \end{cases} \quad m(x) = \begin{cases} (1+x^2)^{-2}, & |x| \leq 1 \\ 1/4, & |x| \geq 1. \end{cases} \tag{4.1}$$

In the two infinite regions  $-\infty < x < -1$  and  $1 < x < \infty$ , the solutions will be given by (2.11) and (2.20), where  $\kappa$ ,  $m_0$  and  $V_0$  take the limiting forms

$$\kappa \rightarrow \sqrt{V_0 - E}/2, \quad m_0 \rightarrow 1/4, \quad V_0 \rightarrow 5 + 8[\beta + 2\alpha(\alpha + \beta + 1)]. \tag{4.2}$$

In the intermediate region, we have obtained the free-particle equation

$$-\ddot{\chi}(z) = E\chi(z), \quad z \in (-\pi/4, \pi/4), \tag{4.3}$$

where transformations (2.22) now reduce to

$$x = \tan z, \quad \chi(z) = (\sec z)\psi(x(z)). \tag{4.4}$$

<sup>6</sup> But this limit becomes interesting if different boundary conditions are adopted [59].

Thus, the envelope wavefunction of (1.1) for  $k \rightarrow 0$  acquires the form

$$\psi(x) = \begin{cases} \mathcal{N}^- e^{\kappa x}/2, & x < -1, \\ \frac{d_1 e^{i\sqrt{E} \tan^{-1}(x)} + d_2 e^{-i\sqrt{E} \tan^{-1}(x)}}{\sqrt{1+x^2}}, & |x| < 1, \\ \mathcal{N}^+ e^{-\kappa x}/2, & x > 1. \end{cases} \tag{4.5}$$

As before, imposing the matching conditions, we obtain homogeneous linear systems for  $d_1, d_2$

$$\begin{aligned} d_1 e^{i\sqrt{E}\pi/4}[\mathcal{B} + i\sqrt{E}] + d_2 e^{-i\sqrt{E}\pi/4}[\mathcal{B} - i\sqrt{E}] &= 0, \\ d_1 e^{-i\sqrt{E}\pi/4}[\mathcal{B} - i\sqrt{E}] + d_2 e^{i\sqrt{E}\pi/4}[\mathcal{B} + i\sqrt{E}] &= 0. \end{aligned}$$

Thus the energy equation for bound states ( $E < V_0$ ) in the  $k \rightarrow 0$  limit is as follows:

$$(\mathcal{B}^2 - E) \sin\left(\frac{\pi}{2}\sqrt{E}\right) + 2\mathcal{B}\sqrt{E} \cos\left(\frac{\pi}{2}\sqrt{E}\right) = 0, \tag{4.6}$$

where  $\mathcal{B}$  is given by (2.31) for  $k' \rightarrow 1$ . One may note at once that  $E = 0$  is a trivial root of equation (4.6), but it must be rejected, because the solution  $\psi(x)$  for the intermediate region  $(-1, 1)$ , given in (4.5), is valid for  $E \neq 0$ . Indeed, for  $E = 0$  one may rewrite the solution as

$$\psi(x) = \frac{1}{\sqrt{1+x^2}}[d_1 \tan^{-1} x + d_2], \quad -1 < x < 1, \tag{4.7}$$

the expressions in two semi-infinite regions being the same as in (4.5). In this case the matching conditions give the following constraints for the existence of zero energy root:

$$V_0 = (2\beta + 1)^2, \quad \beta < -\frac{1}{2}, \quad \text{or} \quad V_0 = \left[2\beta + 1 + \frac{4}{\pi}\right]^2, \quad \beta < -\left(\frac{1}{2} + \frac{2}{\pi}\right), \tag{4.8}$$

and correspondingly in (4.7) either  $d_1 = 0$  or  $d_2 = 0$ . We have checked that constraints (4.8) are not satisfied for different cases, so that zero energy state does not exist for them.

### 5. Numerical results for bound states

In this section we will solve numerically the energy equations (2.34) (and (4.6) for  $k \rightarrow 0$  limit) in the range  $\tilde{V}_{\min} < E < V_0$ , where  $\tilde{V}_{\min}$  denotes the minimum of auxiliary potential  $\tilde{V}(z)$  given by (3.4) (and (3.7)). It may be mentioned that the energy equations depend on two classes of parameters : (i) ordering parameters  $\alpha, \beta, \gamma$  connected by  $\alpha + \beta + \gamma = -1$  and (ii) elliptic modulus  $k^2 (0 \leq k^2 < 1)$  or the complementary modulus  $k'^2 = 1 - k^2$ . Thus we have examined the roots of the energy equations for bound states as a function of both these two classes of parameters. Our strategy is to vary these parameters in such a way that it will cover some of the special forms of kinetic energy operator (1.2) mentioned in the introduction.

#### 5.1. One-parameter family of kinetic energy operator for $\alpha = \gamma$

In this case kinetic energy operator (1.2) reduces to

$$T_{EM}(x) = \frac{1}{2}(m^\alpha p m^\beta p m^\gamma), \quad 2\alpha + \beta = -1. \tag{5.1}$$

We will first obtain  $E$  as a function of  $k^2 \in [0, 1)$  for the two values of  $\beta$ :  $\beta = -1$  and  $\beta = 0$ .

*Case  $\beta = -1$ .* For the choice  $\beta = -1$ , the kinetic energy operator (5.1) takes the following form:

$$T_{EM}(x) = \frac{1}{2} \left( p \frac{1}{m} p \right). \tag{5.2}$$

**Table 1.** The bound-state energies are calculated for  $\beta \in [-2, 2]$  and  $\alpha = \gamma, k^2 = 0$  along with  $V_0, V_{\min}$  ( $x_0 = 1$ ). The bound states are observed only in the range  $[-0.4, -0.1]$ .

$\beta$	$V_{\min}$	$V_0$	$E$
-0.10	0.80	0.96	0.94
-0.20	0.60	0.84	0.81
-0.30	0.40	0.64	0.62
-0.40	0.20	0.36	0.35

Although in this case the upper and lower limits for bound states are

$$V_0 = \frac{9k^2(1-k')}{4(1+k')} - (1+2k') + \frac{k^2}{4}, \quad (5.3)$$

and  $\tilde{V}_{\min} = -\infty$ , since  $\beta < -1/2$  (see equation (3.4)), no bound states are obtained in this range.

Case  $\beta = 0$ . This choice of  $\beta$  corresponds to the kinetic energy operator

$$T_{EM}(x) = \frac{1}{2} \left( \frac{1}{\sqrt{m}} p^2 \frac{1}{\sqrt{m}} \right). \quad (5.4)$$

Here, the range is

$$V_0 = \frac{5k^2(1-k')}{4(1+k')} + 1 + \frac{k^2}{4}, \quad \tilde{V}_{\min} = 2k^2. \quad (5.5)$$

In the interval  $(\tilde{V}_{\min}, V_0)$  there exist no bound states for  $k^2 \in [0, 1)$ .

Next we will study the bound-state energies as a function of  $\beta \in [-2, 2]$  for the two cases:  $k^2 = 0$  and  $k^2 = 0.5$ .

Case  $k^2 = 0$ . The upper limit  $V_0$  has a parabolic dependence on  $\beta$ , given by

$$V_0 = 1 - 4\beta^2, \quad (5.6)$$

and the lower limit is

$$\tilde{V}_{\min} = \begin{cases} 0, & -\frac{1}{2} \leq \beta \leq 2, \\ -\infty, & -2 \leq \beta < -\frac{1}{2}. \end{cases} \quad (5.7)$$

Our numerical calculation shows the existence of one bound state near the top of the well for  $-0.4 \leq \beta \leq -0.1$  (see table 1).

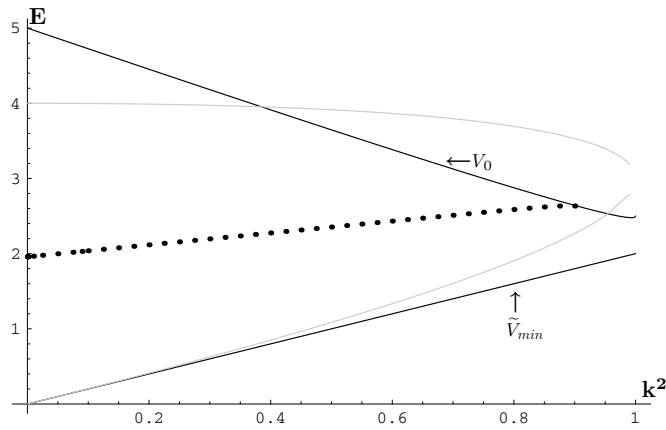
Case  $k^2 = 0.5$ . In this case also the upper limit  $V_0$  has a parabolic dependence on  $\beta$ , given by

$$V_0 = \frac{69 - 29\sqrt{2}}{20} - \frac{5}{4} \left( \beta - \frac{2\sqrt{2} - 1}{5} \right)^2, \quad (5.8)$$

while the lower limit is given by

$$\tilde{V}_{\min} = \begin{cases} 1, & -\frac{1}{2} \leq \beta \leq 2, \\ -\infty, & -2 \leq \beta < -\frac{1}{2}. \end{cases} \quad (5.9)$$

No bound states exist in this range.



**Figure 3.** Bound-state energies as a function of  $k^2$  are shown by dots for the case  $\alpha = -1, \beta = \gamma = 0$ . The lower and upper gray curves represent first two band-edge energies  $E^{(j)}, j = 0, 1$  for the corresponding constant-mass periodic associated Lamé potential.

**Table 2.** Bound-state energies are provided for  $k^2 \in [0, 1)$  where  $\alpha = -1, \beta = \gamma = 0$ . The point  $x_0$  and  $V_0, V_{\min}$  for  $V(x)$  are shown in each case. Bound states start to appear from  $k^2 \leq 0.90$ .

$k^2$	$x_0$	$V_{\min}$	$V_0$	$E$
0.90	1.78	0.32	2.64	2.63
0.80	1.50	0.40	2.88	2.59
0.70	1.35	0.48	3.13	2.51
0.60	1.26	0.55	3.38	2.43
0.50	1.19	0.62	3.65	2.35
0.40	1.14	0.70	3.91	2.28
0.30	1.09	0.78	4.18	2.20
0.20	1.06	0.85	4.45	2.12
0.10	1.03	0.92	4.73	2.04
0.00	1.00	1.00	5.00	1.96

5.2. Two-parameter family of kinetic energy operator for  $\alpha \neq \gamma$

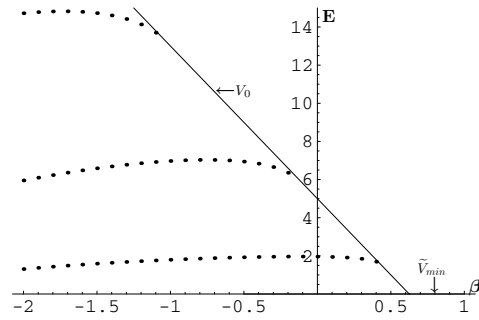
We will find  $E$  as a function of  $k^2$  for  $\alpha = -1, \beta = 0$  which yields following kinetic energy operator:

$$T_{EM}(x) = \frac{1}{4} \left[ \frac{1}{m} p^2 + p^2 \frac{1}{m} \right]. \tag{5.10}$$

The bounds are given by

$$V_0 = \frac{3k^2(1 - 2k')}{2(1 + k')} + 4k' + 1, \quad \tilde{V}_{\min} = 2k^2. \tag{5.11}$$

We have obtained one bound state of the potential (see table 2) for  $0 \leq k^2 \leq 0.90$ . The effective mass potential  $V(x)$  maintains the shape of the well for all  $k$ , and in particular for  $k = 0$  it becomes well-known harmonic oscillator inside the interval  $(-x_0, x_0)$ , the minima being at  $x = 1$ . It is interesting to observe that the bound state exists inside the first allowed band of periodic constant-mass associated Lamé potential (see figure 3).



**Figure 4.** Bound-state energies (dots) as a function of  $\beta$  for  $\alpha \neq \gamma$ ,  $\alpha = -1$ ,  $k^2 = 0$ .

**Table 3.** The bound-state energies as a function of  $\beta \in [-2, 2]$  for  $\alpha = -1 \neq \gamma$ ,  $k^2 = 0$  are given with  $V_{\min}$  and  $V_0$  ( $x_0 = 1$ ). The asterisk in  $\beta$  indicates that  $V(x)$  is a constant potential.

$\beta$	$V_{\min}$	$V_0$	$E$
0.40*	1.80	1.80	1.69
0.20	1.40	3.40	1.91
0.00	1.00	5.00	1.96
-0.20	0.60	6.60	1.96; 6.36
-0.40	-0.20	8.20	1.94; 6.83
-0.60	-0.20	9.80	1.91; 7.00
-0.80	-0.60	11.40	1.86; 7.03
-1.00	-1.00	13.00	1.79; 6.97
-1.20	-1.40	14.60	1.72; 6.86; 14.14
-1.40	-1.80	16.20	1.64; 6.70; 14.61
-1.60	-2.20	17.80	1.54; 6.48; 14.79
-1.80	-2.60	19.40	1.43; 6.24; 14.81
-2.00	-3.00	21.00	1.31; 5.95; 14.72

The dependence of bound-state energy  $E$  on  $\beta$  will now be calculated again for two cases:  $k^2 = 0$  and  $k^2 = 0.35$ , while  $\beta$  will vary in the same interval  $[-2, 2]$  and  $\alpha$  will be fixed as  $\alpha = -1$ .

*Case  $k^2 = 0$ ,  $\alpha = -1$ ,  $\gamma = -\beta$ .* Here the upper limit  $V_0$  is linearly dependent on  $\beta$  and is given by

$$V_0 = 5 - 8\beta, \quad (5.12)$$

and the lower limit  $\tilde{V}_{\min}$  is same as given by (5.7). The results, shown in figure 4, are the following:

- No bound states for  $0.5 \leq \beta \leq 2$ ,
- One bound state for  $-0.1 \leq \beta \leq 0.4$ ,
- Two bound states for  $-1.0 \leq \beta \leq -0.2$ ,
- Three bound states for  $-2.0 \leq \beta \leq -1.1$ .

One can note that for  $\beta = 0.4$ ,  $V(x) \equiv 1.8$  is a constant potential (see table 3), but still there exists one bound state. However, we have already explained in section 3 that this apparently strange behaviour is perfectly consistent with constant-mass Schrödinger picture.

**Table 4.** The bound-state energies as a function of  $\beta \in [-2, 2]$  for  $\alpha = -1 \neq \gamma, k^2 = 0.35$  are given with  $V_{\min}$  and  $V_0$  ( $x_0 = 1.11$ ).

$\beta$	$V_{\min}$	$V_0$	$E$
0.40	1.96	1.98	1.98
0.20	1.35	3.01	2.20
0.00	0.74	4.05	2.24
-0.20	0.13	5.08	2.23
-0.40	-0.48	6.11	2.20; 5.67
-0.60	-1.09	7.14	2.16; 5.86
-0.80	-1.70	8.18	2.10; 5.89
-1.00	-2.31	9.21	2.04; 5.83
-1.20	-2.92	10.24	1.96; 5.71
-1.40	-3.53	11.27	1.87; 5.54; 11.04
-1.60	-4.14	12.31	1.77; 5.34; 11.35
-1.80	-4.75	13.34	1.66; 4.96; 11.43
-2.00	-5.36	14.37	1.53; 4.82; 11.40

In this context it may be mentioned that the existence of bound states for constant potential was also noted in [38] for  $m(x) = \text{sech}^2qx$ .

Case  $k^2 = 0.35, \alpha = -1, \gamma = -\beta$ . This case also corresponds to linear dependence of  $V_0$  on  $\beta$

$$V_0 = 4.05 - 5.16\beta, \tag{5.13}$$

and the lower limit is given by

$$\tilde{V}_{\min} = \begin{cases} 0.7, & \beta \geq -1/2, \\ -\infty, & \beta < -1/2. \end{cases} \tag{5.14}$$

The results shown in table 4 are the following:

- No bound states for  $0.5 \leq \beta \leq 2$ ,
- One bound state for  $-0.2 \leq \beta \leq 0.4$ ,
- Two bound states for  $-1.2 \leq \beta \leq -0.3$ ,
- Three bound states for  $-2 \leq \beta \leq -1.3$ .

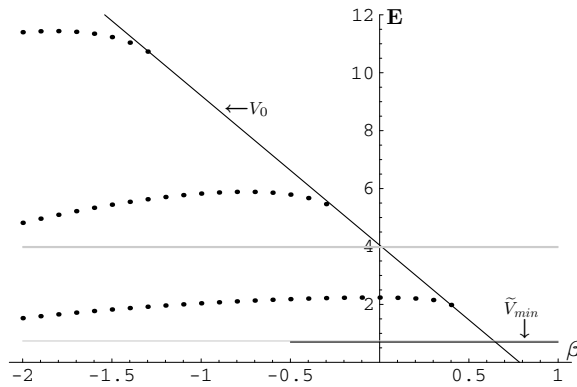
Once again we have observed that the ground state lies inside the allowed band and higher excited states are inside the continuum (see figure 5) for the constant-mass periodic associated Lamé potential characterized by  $\mu = \nu = 1; k^2 = 0.35$ .

### 6. Some features of bound-state wavefunctions

In this section we will present some interesting properties of the wavefunctions  $\psi(x)$  that can be derived from the numerical results of the previous section with very good accuracy. A part of these properties, which seems to be difficult to prove analytically, does not concern the specific physical problem. We recall that  $\psi(x)$  is given by (up to the normalization factor)

$$\psi(x) = \begin{cases} m_0^{1/4} \chi^- e^{\kappa(x_0+x)}, & -\infty < x < -x_0, \\ f_m^{1/4}(x) \chi(z(x)), & -x_0 < x < x_0, \\ m_0^{1/4} \chi^+ e^{\kappa(x_0-x)}, & x_0 < x < \infty, \end{cases} \tag{6.1}$$





**Figure 5.** Bound-state energies (dots) as a function of  $\beta$  are plotted for  $\alpha \neq \gamma$ ,  $\alpha = -1$ ,  $k^2 = 0.35$ . The grey lines represent band-edge energies of corresponding associated Lamé potential.

where  $\chi(z(x)) = \chi_2(z(x)) + (d_1/d_2)\chi_1(z(x))$  and  $\chi^\pm \equiv \chi(\pm K/2)$ . Note that for  $k \neq 0$ ,  $\chi_i(z(x))$  are given by (2.23) for  $x(z) = \text{sn } z/\text{cn } z$ , and for  $k = 0$ ,  $\chi_{1,2}(z(x)) = \exp[\pm i\sqrt{E}z]$  for  $x(z) = \tan z$ . The quantity  $\kappa$  is to be computed from (2.19) for  $E = E_n$ ,  $E_n$  being the bound-state energies of our EM Hamiltonian. In the following we will use the notation

$$\kappa_n = \sqrt{m_0(V_0 - E_n)}, \quad n = 0, 1, 2. \tag{6.2}$$

6.1. Ground state

The two quantities  $a_1$  and  $a_2$  in (2.23) are complex and related by

$$a_1 = -a_2^*. \tag{6.3}$$

The real and imaginary parts of  $\chi_i(z)$  are respectively odd and even functions. Moreover  $\chi_i(z)$  satisfy following interesting relations with very high accuracy:

$$\chi_1(z) = \frac{d_2}{d_1}\chi_2(-z), \quad \chi_i(z) = -\chi_i^*(-z), \tag{6.4}$$

where the ratio  $d_2/d_1$  is a positive number. It will then follow that  $\chi(z)$  is an even function and

$$\chi(z) = \chi(-z) \propto \text{Im}[\chi_1(z)] \equiv v(z). \tag{6.5}$$

The ground state wavefunction is

$$\psi_0(x) = \begin{cases} C_0 m_0^{1/4} v\left(\frac{K}{2}\right) e^{\kappa_0(x_0+x)}, & x < -x_0, \\ C_0 f_m^{1/4}(x) v(z(x)), & |x| < x_0, \\ C_0 m_0^{1/4} v\left(\frac{K}{2}\right) e^{\kappa_0(x_0-x)}, & x > x_0. \end{cases} \tag{6.6}$$

It is straightforward to compute the normalization constant  $C_0$  from (2.17)

$$\frac{1}{C_0} = \left[ \frac{v^2(K/2)}{\sqrt{V_0 - E_0}} + \int_{-x_0}^{x_0} \sqrt{f_m(x)} v^2(z(x)) dx \right]^{1/2}. \tag{6.7}$$

6.2. First excited state

The quantity  $a_1$  is purely imaginary while the other quantity  $a_2$  is complex and they are related by

$$\text{Im}[a_1] = \text{Im}[a_2]. \tag{6.8}$$

The relation between  $\chi_1(z)$  and  $\chi_2(z)$  are

$$\chi_1(z) = -\frac{d_2}{d_1}\chi_2(-z), \tag{6.9}$$

where  $d_2/d_1$  is a positive number. Clearly this implies that

$$\chi(-z) = -\chi(z) = \text{complex} . \tag{6.10}$$

We have checked numerically with the same high accuracy that

$$\text{Re}[\chi(z)] \propto \text{Im}[\chi(z)], \tag{6.11}$$

and of course no degeneracy exists for  $E = E_1$ . The wavefunction is

$$\psi_1(x) = \begin{cases} -C_1 m_0^{1/4} \text{Re}[\chi^+] e^{\kappa_1(x_0+x)}, & x < -x_0, \\ C_1 f_m^{1/4}(x) \text{Re}[\chi(z(x))], & |x| < x_0, \\ C_1 m_0^{1/4} \text{Re}[\chi^+] e^{\kappa_1(x_0-x)}, & x > x_0. \end{cases} \tag{6.12}$$

6.3. Second excited state

The two quantities  $a_1$  and  $a_2$  have same properties as in the above case. The relation between  $\chi_1(z)$  and  $\chi_2(z)$  reads in this case

$$\chi_1(z) = \frac{d_2}{d_1}\chi_2(-z), \quad \left(\frac{d_2}{d_1} < 0\right). \tag{6.13}$$

Thus, here also  $\chi(z)$  is complex and

$$\chi(-z) = \chi(z), \tag{6.14}$$

but

$$\text{Re}[\chi(z)] \propto \text{Im}[\chi(z)]. \tag{6.15}$$

The wavefunction is

$$\psi_2(x) = \begin{cases} C_2 m_0^{1/4} \text{Re}[\chi^+] e^{\kappa_2(x_0+x)}, & x < -x_0, \\ C_2 f_m^{1/4}(x) \text{Re}[\chi(z(x))], & |x| < x_0, \\ C_2 m_0^{1/4} \text{Re}[\chi^+] e^{\kappa_2(x_0-x)}, & x > x_0. \end{cases} \tag{6.16}$$

The normalization constants  $C_n$ ,  $n = 1, 2$  may be expressed as

$$\frac{1}{C_n} = \left[ \frac{(\text{Re}[\chi^+])^2}{\sqrt{V_0 - E_n}} + \int_{-x_0}^{x_0} \sqrt{f_m(x)} (\text{Re}[\chi(z(x))])^2 dx \right]^{1/2}. \tag{6.17}$$

6.4. The limiting case for  $k \rightarrow 0$

In the limiting case for  $k \rightarrow 0$  the relation between  $x$  and  $z$  is very simple (see equation (4.4)), and it is convenient to express the corresponding properties in the variable  $x$ . Here we will

denote  $\chi_i(z(x))$  and  $\chi(z(x))$  by  $\chi_i(x)$  and  $\chi(x)$ . The relation between  $\chi_1(x)$  and  $\chi_2(x)$  is

$$\chi_1(-x) = \chi_2(x). \quad (6.18)$$

Let us introduce the parameters

$$\theta_n = \frac{\pi}{4} \sqrt{E_n}, \quad n = 0, 1, 2. \quad (6.19)$$

*Ground and second excited states* ( $k = 0$ ). In both cases the ratio  $d_2/d_1$  is unity. It then follows from the definition of  $\chi(x)$  that it is even function given by

$$\chi(-x) = \chi(x) = 2 \cos(\sqrt{E} \tan^{-1} x). \quad (6.20)$$

The wavefunctions are

$$\psi_n(x) = \begin{cases} C_n \sqrt{2} \cos \theta_n e^{\kappa_n(1+x)}, & x < -1 \\ \frac{2C_n}{\sqrt{1+x^2}} \cos(\sqrt{E_n} \tan^{-1} x), & |x| < 1 \\ C_n \sqrt{2} \cos \theta_n e^{\kappa_n(1-x)}, & x < -1, \end{cases} \quad (6.21)$$

for  $n = 0, 2$ .

*First excited state* ( $k = 0$ ). The ratio  $d_2/d_1$  is equal to  $-1$  so that  $\chi(x)$  is an odd function given by

$$\chi(x) = -\chi(-x) = -2i \sin(\sqrt{E} \tan^{-1} x). \quad (6.22)$$

The wavefunction is

$$\psi_1(x) = \begin{cases} -C_1 \sqrt{2} \sin \theta_1 e^{\kappa_1(1+x)}, & x < -1 \\ \frac{2C_1}{\sqrt{1+x^2}} \sin(\sqrt{E_1} \tan^{-1} x), & |x| < 1 \\ C_1 \sqrt{2} \sin \theta_1 e^{\kappa_1(1-x)}, & x < -1. \end{cases} \quad (6.23)$$

In all the three cases the normalization constants  $C_n$  may be expressed as

$$\frac{1}{C_n} = \left[ \pi + 2 \left( \frac{1 + (-1)^n \cos 2\theta_n}{\sqrt{V_0 - E_n}} + (-1)^n \frac{\sin 2\theta_n}{\sqrt{E_n}} \right) \right]^{1/2}. \quad (6.24)$$

## 7. Conclusion

In this paper we have proposed a new solvable model wherein the potential and effective mass are rational functions of spatial coordinate. The novel feature of our model is that it may be mapped to well-known periodic associated Lamé potential in constant-mass scenario. This fact is clearly responsible for solvability of the model. It may be mentioned that the list of solvable models in effective mass framework is rather short. Our work has definitely enhanced this set by introducing a wide class of rational potential and mass functions. The important difference of our work compared to recent efforts is that we consider the variation of mass inside a finite region, and both potential and mass are constant outside. The advantage of considering variation of the mass inside a finite interval instead of a full line is that the mass remains finite and non-zero everywhere, as it should be.

We have examined the bound-state spectrum for different values of the ordering parameters  $\alpha, \beta, \gamma$  and elliptic modulus  $k^2$ , and have discussed the properties of the corresponding wavefunctions. It is observed for both  $\alpha = \gamma$  and  $\alpha \neq \gamma$  cases that the ordering parameter  $\beta$  has a critical value above which no bound state exists. But number of levels increases with decreasing values of  $\beta$ . Some peculiarities have been noted in the spectral properties (e.g. the existence of bound states for constant potential  $V(x)$ ) in contrast to the conventional situation where mass is constant. The qualitative observation is that the discrete energy levels

for bound states of our EM Hamiltonian for nonzero  $k$  lie only inside the allowed band and in the continuum for corresponding constant-mass periodic associated Lamé Hamiltonian. Moreover, as a by-product of our numerical procedure we have found some new curious relations for the solutions  $\chi_i(z)$  of associated Lamé equation, which seem to be universal. For example the form of the second relation of (6.4) for the solutions  $\chi_i(z)$  at  $E = E_0$  (inside the allowed band of corresponding associated Lamé potential) is not related with our physical problem.

Some direct generalizations of our model are possible. For instance, the application of SUSY transformations to enlarge the class of rational models and the inclusion of scattering states with  $E \geq V_0$  are under consideration. Further it will be interesting to investigate the validity of the above-mentioned relations between the solutions of associated Lamé equation for other values of  $E$ . The special exploration of  $k \rightarrow 1$  limit of our model also seems to be promising [59].

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### Appendix

In the following we will mention basic definitions and the relations involving elliptic functions, which we use in the text (for more details, see [59–61]). Consider two real numbers  $k^2$  and  $k'^2$  such that

$$k^2 \in (0, 1), \quad k'^2 = 1 - k^2. \quad (\text{A.1})$$

These two numbers are called respectively elliptic modulus and complementary modulus, and are basic parameters in the constructions of elliptic functions. The amplitude function is defined by

$$\varphi(z, k) = \text{am}(z, k), \quad z(\varphi, k) = \int_0^\varphi \frac{d\tau}{\sqrt{1 - k^2 \sin^2 \tau}}. \quad (\text{A.2})$$

From here the three Jacobian elliptic functions are defined by

$$\text{sn}(z, k) = \sin \varphi, \quad \text{cn}(z, k) = \cos \varphi, \quad \text{dn}(z, k) = d\varphi/dz. \quad (\text{A.3})$$

These functions are called sine-amplitude, cosine-amplitude and delta-amplitude respectively. For simplicity, in equation (2.21) in the text, and also in the following, we have suppressed the explicit modular dependence and write simply  $\text{sn } z$ ,  $\text{cn } z$ ,  $\text{dn } z$ . These are doubly-periodic functions of periods  $(4K, 2iK')$ ,  $(4K, 4iK')$  and  $(2K, 4iK')$ , respectively, and are usually defined for a complex variable  $z$ . Nevertheless in our case  $z$  is always real. The quarter periods  $K$  and  $K'$  are the real numbers given by

$$K(k) \equiv K = z(\pi/2, k), \quad K'(k) \equiv K' = K(k'). \quad (\text{A.4})$$

$K$  is called complete elliptic integral of second kind. Noting the following relations

$$\operatorname{sn}(z + K) = \frac{\operatorname{cn} z}{\operatorname{dn} z}, \quad \operatorname{cn}(z + K) = -k' \frac{\operatorname{sn} z}{\operatorname{dn} z}, \quad \operatorname{dn}(z + K) = \frac{k'}{\operatorname{dn} z}, \quad (\text{A.5})$$

$$\operatorname{sn}(z + 2K) = -\operatorname{sn} z, \quad \operatorname{cn}(z + 2K) = -\operatorname{cn} z, \quad \operatorname{dn}(z + 2K) = \operatorname{dn} z, \quad (\text{A.6})$$

we see that the associated Lamé potential in equation (2.21) is  $2K$ -periodic or  $K$ -periodic, according as  $\mu \neq \nu$  or  $\mu = \nu$ . The function  $\operatorname{sn} z$  is odd with a simple zero at  $z = 0$ , while  $\operatorname{cn} z$ ,  $\operatorname{dn} z$  are even functions;  $\operatorname{cn} z$  has a simple zero at  $z = K$ , but  $\operatorname{dn} z$  has no zeros for real  $z$ . The precise value of the point  $x_0$  is obtained as  $x_0 = 1/\sqrt{k'}$  from the values

$$\operatorname{sn}\left(\frac{K}{2}\right) = \frac{1}{\sqrt{1+k'}}, \quad \operatorname{cn}\left(\frac{K}{2}\right) = \frac{\sqrt{k'}}{\sqrt{1+k'}}. \quad (\text{A.7})$$

Some other relevant relations are

$$\operatorname{sn}^2 z + \operatorname{cn}^2 z = 1, \quad \operatorname{dn}^2 z + k^2 \operatorname{sn}^2 z = 1, \quad (\text{A.8})$$

$$\operatorname{sn}' z = \operatorname{cn} z \operatorname{dn} z, \quad \operatorname{cn}' z = -\operatorname{sn} z \operatorname{dn} z, \quad \operatorname{dn}' z = -k^2 \operatorname{sn} z \operatorname{cn} z. \quad (\text{A.9})$$

In the two limits  $k \rightarrow 1$  and  $k \rightarrow 0$ , the elliptic functions degenerate into hyperbolic and trigonometric functions

$$\operatorname{sn} z \xrightarrow[k \rightarrow 0]{k \rightarrow 1} \begin{cases} \tanh z \\ \sin z \end{cases}, \quad \operatorname{cn} z \xrightarrow[k \rightarrow 0]{k \rightarrow 1} \begin{cases} \operatorname{sech} z \\ \cos z \end{cases}, \quad \operatorname{dn} z \xrightarrow[k \rightarrow 0]{k \rightarrow 1} \begin{cases} \operatorname{sech} z \\ 1 \end{cases}, \quad (\text{A.10})$$

where the quarter-periods go over

$$K \xrightarrow[k \rightarrow 0]{k \rightarrow 1} \begin{cases} \infty \\ \pi/2 \end{cases}, \quad K' \xrightarrow[k \rightarrow 0]{k \rightarrow 1} \begin{cases} \pi/2 \\ \infty \end{cases}. \quad (\text{A.11})$$

Weierstrass elliptic function  $\wp(z; g_2, g_3) \equiv \wp(z)$  is defined by

$$\wp(z) = \frac{1}{z^2} + \sum'_{m,n} \left[ \frac{1}{(z - 2m\omega_1 - 2n\omega_3)^2} - \frac{1}{(2m\omega_1 + 2n\omega_3)^2} \right], \quad (\text{A.12})$$

where the symbol  $\sum'$  means summation over all integral values of  $m, n$  except  $m = n = 0$ ,  $\omega_1$  and  $\omega_3$  being half-periods of  $\wp(z)$ . In our case, these are defined through

$$\omega_1 = K, \quad \omega_3 = iK', \quad (\text{A.13})$$

and the invariants  $g_2, g_3$  are given by

$$g_2 = \frac{4}{3}(k^4 - k^2 + 1), \quad g_3 = \frac{4}{27}(k^2 - 2)(2k^2 - 1)(k^2 + 1). \quad (\text{A.14})$$

The above choice corresponds to the case when the discriminant  $\Delta = g_2^3 - 27g_3^2 > 0$ , and so the three numbers  $\wp(\omega_i) \equiv e_i, i = 1, 2, 3$  are always real ( $e_1 > e_2 > e_3$ ), where  $\omega_2 = \omega_1 + \omega_3$ . It may be mentioned that  $e_i$  are the three roots of the equation

$$4t^3 - g_2 t - g_3 = 0, \quad (\text{A.15})$$

and, for simplicity, we have chosen the scale  $e_1 - e_3 = 1$ . Weierstrass elliptic function is an even function; its derivative  $\wp'(z)$  is an odd elliptic function with the same periods and satisfy following identity:

$$\wp'^2(z) = 4 \prod_{i=1}^3 [\wp(z) - e_i]. \quad (\text{A.16})$$

The relations between Weierstrass elliptic function and Jacobian elliptic functions, with our choice, are

$$\wp(z) = e_1 + \frac{\operatorname{cn}^2 z}{\operatorname{sn}^2 z} = e_2 + \frac{\operatorname{dn}^2 z}{\operatorname{sn}^2 z} = e_3 + \frac{1}{\operatorname{sn}^2 z}. \quad (\text{A.17})$$

Weierstrass zeta function  $\zeta(z; g_2, g_3) \equiv \zeta(z)$  and sigma function  $\sigma(z; g_2, g_3) \equiv \sigma(z)$  are quasi-periodic functions defined by

$$\dot{\zeta}(z) = -\wp(z), \quad \frac{\dot{\sigma}(z)}{\sigma(z)} = \zeta(z), \quad (\text{A.18})$$

and satisfy the following relations:

$$\begin{aligned} \zeta(-z) &= -\zeta(z), & \zeta(z + 2\omega_i) &= \zeta(z) + 2\zeta(\omega_i), \\ \sigma(-z) &= -\sigma(z), & \sigma(z + 2\omega_i) &= -\sigma(z) \exp[2\zeta(\omega_i)(z + \omega_i)]. \end{aligned} \quad (\text{A.19})$$

The addition formulae for these functions are

$$\wp(z_1 + z_2) = \frac{1}{4} \left[ \frac{\dot{\wp}(z_1) - \dot{\wp}(z_2)}{\wp(z_1) - \wp(z_2)} \right]^2 - \wp(z_1) - \wp(z_2), \quad (\text{A.20})$$

$$\zeta(z_1 + z_2) = \zeta(z_1) + \zeta(z_2) + \frac{1}{2} \frac{\dot{\wp}(z_1) - \dot{\wp}(z_2)}{\wp(z_1) - \wp(z_2)}. \quad (\text{A.21})$$

We will now derive the energy equation (2.34). Using relations (A.13)–(A.19) and the addition formula (A.21), and noting that

$$\begin{aligned} \wp(z + 2\omega_i) &= \wp(z), & \wp(-z) &= \wp(z), \\ \dot{\wp}(z + 2\omega_i) &= \dot{\wp}(z), & \dot{\wp}(-z) &= -\dot{\wp}(z), \end{aligned} \quad (\text{A.22})$$

it is not very difficult to derive the following relations:

$$\dot{\chi}_1^\pm = A_\pm \chi_1^\pm, \quad \dot{\chi}_2^\pm = -A_\mp \chi_2^\pm, \quad (\text{A.23})$$

where  $\chi_i(z)$  and  $A_\pm$  are given by (2.23) and (2.35). Inserting the expressions for  $\dot{\chi}_i^\pm$  from (A.23) into (2.33), the energy equation (2.34) will readily follow from (2.32).

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