

Casimir effect for impurity in periodic background in one dimension

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Received 2 April 2020, revised 7 May 2020

Accepted for publication 19 May 2020

Published 27 July 2020



CrossMark

Abstract

We consider a Bose gas in a one-dimensional periodic background formed by generalized delta function potentials with one and two impurities. We investigate the scattering off these impurities and their bound state levels. Besides expected features, we observe a kind of long-range correlation between the bound state levels of two impurities. Further, we define and calculate the vacuum energy of the impurity. It causes a force acting on the impurity relative to the background. We define the vacuum energy as a mode sum. In order to get a discrete spectrum we start from a finite lattice and use Chebychev polynomials to get a general expression. These allow also for quite easy investigation of impurities in finite lattices.

Keywords: quantum vacuum, Casimir effect (theory), periodic potential

(Some figures may appear in colour only in the online journal)

1. Introduction

One-dimensional systems provide a large number of examples to study quantum effects. These allow frequently for quite explicit and instructive formulas, but at the same time there are many one-dimensional and quasi-one-dimensional systems in physics which are frequently also of practical interest like nanowires and carbon nanotubes. A modern field of applications is also optical lattices. Among these systems, a special role plays periodic structures in which the potentials in each cell have point support. Such potentials are also known as ‘zero-range potentials’ and appear in various contexts. For a recent review see [1]. The most general case of such potentials can be found in [2], with applications to metamaterials in [3]. The easiest



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example for such potentials in the one-dimensional case is the ‘Dirac comb’, which is a special case of a Kronig–Penney potential [4]. In this case, the potential is a Dirac delta function in each cell. An interesting generalization is to include a derivative of a delta function (δ' -potential) (see equation (3) below). The most general case for selfadjoint operators was investigated also in [5].

It must be mentioned that the study of such one-dimensional systems is an actual topic. For example, recently in [6], the influence of impurity on the energy bands was considered, theoretically and with relation to an experiment [7], or effects an impurity may have on a transmission coefficient [8] and their relation to localization. Another example is the application of similar models to critical fluctuations in liquids [9]. It is also of interest to investigate Bose–Einstein condensation in one-dimensional systems, see [10–12].

In this paper, we consider a one-dimensional scalar field, i.e., a Bose gas, in a periodic background formed by generalized delta function potentials with point impurities. Our interest is focused on the bound states and on the vacuum energy of the impurities. It is a continuation of the investigations of the vacuum energy in [13, 14], and of free energy and entropy in [15]; both for generalized delta functions. We mention also the very recent paper [16] on fluctuation induced forces on an impurity, where, however, the case of a small coupling is considered.

The paper is organized as follows. After introducing in section 2 the necessary basic formulas for the periodic background, we introduce in section 3 an impurity in form of also a generalized delta function which may be located at any place in its cell. We demonstrate the transmission coefficient for the scattering on this impurity and the bound state level. The case of two impurities is treated in section 4. In the subsequent section, a ‘half infinite’ crystal is considered, including the corresponding surface (Tamm) state. Finally, in section 6 the vacuum energy of the system is investigated. First, we reproduce the results of [13] for the pure lattice, then we calculate the vacuum energy of the impurity.

Throughout the paper units with $\hbar = c = 1$ are used.

2. A scalar field in a one-dimensional periodic background

We start from the scalar field equation after Fourier transform in time,

$$(-\omega^2 - \partial_x^2 + V(x)) \phi(x) = 0, \quad (1)$$

where ω denotes the frequency. The potential $V(x)$ is assumed to be periodic,

$$V(x + a) = V(x). \quad (2)$$

In this paper we consider a lattice of generalized delta functions,

$$V_\delta(x) = \sum_n (\alpha \delta(x - an) + 2\beta \delta'(x - an)), \quad (3)$$

which we realize by matching conditions

$$\begin{pmatrix} \phi(an + 0) \\ \phi'(an + 0) \end{pmatrix} = \mathbf{M} \begin{pmatrix} \phi(an - 0) \\ \phi'(an - 0) \end{pmatrix} \quad (4)$$

with the matrix

$$M = \begin{pmatrix} \frac{1 + \beta}{1 - \beta}, & 0 \\ \alpha & \frac{1 - \beta}{1 + \beta} \end{pmatrix}. \quad (5)$$

For $\beta = 0$, this matrix delivers the well-known matching conditions for a simple δ -function. The generalization to include β can be found, for example, in [3], equation (9), and even more general, in [5] or as a most general self-adjoint extension in [2]. Because of the periodicity (2) of the potential we can find solutions obeying the Bloch condition,

$$\phi(x + a) = e^{iqa} \phi(x), \quad (6)$$

with a quasi momentum q , which we now consider in more detail.

2.1. The solutions

To describe the solutions we split the x -axis into intervals with characteristic functions,

$$\Theta_n = \begin{cases} 1 & \text{if } (n - 1)a \leq x \leq an, \\ 0 & \text{otherwise,} \end{cases} \quad (7)$$

and have within each interval plane wave solutions. Taking a linear combination in the form,

$$\phi(x) = \sum_{n=-\infty}^{\infty} \phi_n(x) \Theta_n, \quad (8)$$

with

$$\phi_n(x) = A_n e^{i\omega(x-an)} + B_n e^{-i\omega(x-an)}, \quad (9)$$

we have to find the coefficients A_n and B_n . From the matching conditions (4) we get

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = T \begin{pmatrix} A_n \\ B_n \end{pmatrix}, \quad (n = -\infty, \dots, \infty), \quad (10)$$

with

$$T = Q^{-1} K^{-1} M K, \quad Q = \begin{pmatrix} e^{-i\omega a}, & 0 \\ 0, & e^{i\omega a} \end{pmatrix}, \quad K = \begin{pmatrix} 1, & 1 \\ i\omega, & -i\omega \end{pmatrix}, \quad (11)$$

Explicit formulas are

$$T = \begin{pmatrix} w, & z \\ z^*, & w^* \end{pmatrix} \quad (12)$$

with

$$w = \frac{1 + \beta^2 - \frac{i\alpha}{2\omega}}{1 - \beta^2} e^{i\omega a}, \quad z = \frac{2\beta - \frac{i\alpha}{2\omega}}{1 - \beta^2} e^{i\omega a} \quad (13)$$

and

$$\det T = 1, \quad \text{or equivalently, } |w|^2 - |z|^2 = 1, \quad (14)$$

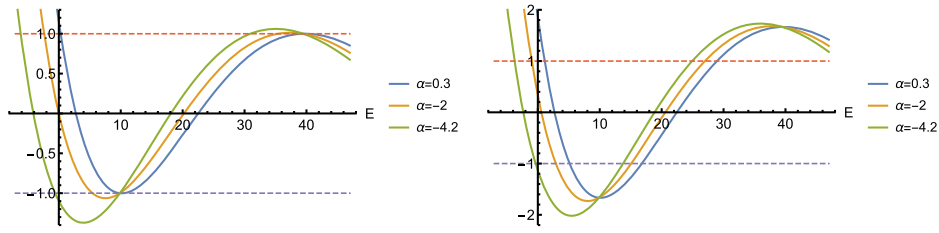


Figure 1. The right-hand side of equation (19) defining the spectrum as a function of the energy $E = \omega^2$, for several choices of α . The allowed values are in-between the dashed lines. The parameters are $\beta = 0$ (left panel) and $\beta = 0.5$ (right panel).

hold. From the periodicity (6) we find

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = e^{iqa} \begin{pmatrix} A_n \\ B_n \end{pmatrix}. \tag{15}$$

Now, taking (10) and (15) together, the equation

$$(T - e^{iqa}) \begin{pmatrix} A_n \\ B_n \end{pmatrix} = 0 \tag{16}$$

follows. This equation does not depend on n and calculating, say A_1 and B_1 , from (15) all other coefficients follow,

$$\begin{pmatrix} A_m \\ B_m \end{pmatrix} = e^{iq(m-1)} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}, \tag{17}$$

where m is any integer.

The existence of a non trivial solution to equation (16) demands

$$\det(T - e^{iqa}) = 0, \tag{18}$$

or, using (12) and (13),

$$\cos(qa) = \frac{w + w^*}{2} = \frac{(1 + \beta^2) \cos(\omega a) + \frac{\alpha}{2\omega} \sin(\omega a)}{1 - \beta^2}. \tag{19}$$

This is a secular equation determining the spectrum which shows the known band structure. Examples are shown in figure 1. For instance, it can be seen how the δ' -potential enhances the band gaps.

Defining

$$q = \frac{1}{a} \arccos\left(\frac{w + w^*}{2}\right) \tag{20}$$

with $0 \leq q \leq \pi$, we have two solutions, with $\pm q$. We denote them by $\phi^+(x)$ and $\phi^-(x)$, accordingly. Accordingly, we have two solutions (9),

$$\phi^\pm(x) = \sum_{n=-\infty}^{\infty} \phi_n^\pm(x) \Theta_n, \quad \phi_n^\pm(x) = A_n^\pm e^{i\omega(x-an)} + B_n^\pm e^{-i\omega(x-an)}. \tag{21}$$

The condition (6) turns into

$$\phi_{n+1}^{\pm}(x) = e^{\pm iqa} \phi_n^{\pm}(x) \tag{22}$$

and allows for the continuation to all other intervals.

Solving equation (16) and inserting $\pm q$, we arrive at

$$\begin{pmatrix} A_1^+ \\ B_1^+ \end{pmatrix} = \begin{pmatrix} w^* - e^{iqa} \\ -z^* \end{pmatrix}, \quad \begin{pmatrix} A_1^- \\ B_1^- \end{pmatrix} = \begin{pmatrix} -z \\ w - e^{-iqa} \end{pmatrix}, \tag{23}$$

where now q is given by (19). It can be checked that in the case $\alpha = \beta = 0$ (no background potential) these turn into

$$\begin{pmatrix} A_1^+ \\ B_1^+ \end{pmatrix} = -2i \sin(\omega a) \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} A_1^- \\ B_1^- \end{pmatrix} = 2i \sin(\omega a) \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{24}$$

and correspond to right and left moving plane waves. Also we mention the Wronskian,

$$W = \phi^+(x)\phi'^-(x) - \phi^{+'}(x)\phi^-(x) = -2i\omega (2 - w e^{iqa} - w^* e^{-iqa}), \tag{25}$$

of these two solutions.

It should be mentioned that the above formulas are not new. Similar ones can be found in the literature. We take reference for instance to [17, 18]. However, the δ' -interaction was not included so far. To establish a relation to the literature we mention a slightly different derivation of the formulas (23) for the coefficients in the wave function.

We start from equation (4) with $n = 0$ and (9). The upper line in (4) reads

$$A_1 e^{-i\omega a} + B_1 e^{i\omega a} = \frac{1 + \beta}{1 - \beta} (A_0 + B_0) \tag{26}$$

Further, we use the Bloch condition (15). This allows writing the relation between the coefficients in the form

$$\left(\frac{1 + \beta}{1 - \beta} - e^{i(q-\omega)a} \right) A_0 + \left(\frac{1 + \beta}{1 - \beta} - e^{i(q+\omega)a} \right) B_0 = 0. \tag{27}$$

Introducing the notations

$$b_q = -\frac{e^{i(q+\omega)a} - \frac{1+\beta}{1-\beta}}{e^{i(q-\omega)a} - \frac{1+\beta}{1-\beta}}, \tag{28}$$

we rewrite equation (23), up to an overall factor, in the equivalent form

$$B_0^{\pm} = A_0^{\pm} b_{\pm q}. \tag{29}$$

This relation coincides with equation (14) in [18] up to some signs.

2.2. The current

We calculate the current from the formula

$$j^{\pm} = \frac{1}{2i\omega} \left(\phi^{\pm*}(x)\phi^{\pm}(x) - \phi^{\pm'*}(x)\phi^{\pm}(x) \right) = |A_n^{\pm}|^2 - |B_n^{\pm}|^2, \tag{30}$$

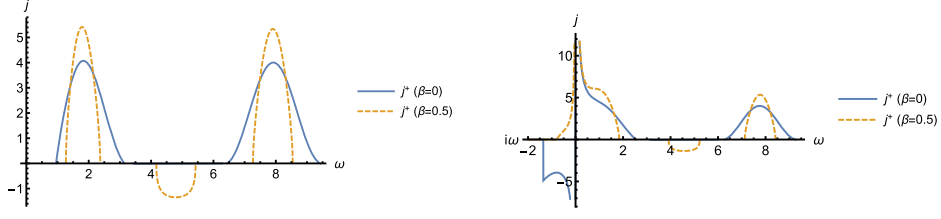


Figure 2. The current j^+1 , equation (31), as a function of ω . The parameters are $\alpha = 1$ (left panel) and $\alpha = -1.6$ (right panel). In the right panel, to the left of the ordinate axis, imaginary frequencies are taken.

It does not depend on x or on n . Inserting now (23) we arrive at

$$j^+ = 2 - w e^{iqa} - w^* e^{-iqa} = 2 (1 - |w| \cos(qa + \vartheta_w)), \quad j^- = -j^+, \quad (31)$$

with $w = |w| e^{i\vartheta_w}$ for these currents associated with the solutions $\phi_1(x)$ and $\phi_2(x)$, given by (21) with the coefficients (23). Up to a factor, these currents coincide with the Wronskian (25).

Some examples are shown in figure 2. As can be seen, the currents change their signs from zone to zone and may have very different sizes. The parameter β [strength of δ' -part in the potential (3)] changes the behavior significantly.

3. Single impurity

In this section, we assume a single impurity located at $x = x_0$. For the impurity potential, we take also a generalized delta function,

$$V_{\text{imp.}} = \tilde{\alpha}\delta(x - x_0) + 2\tilde{\beta}\delta'(x - x_0), \quad (32)$$

which we realize as matching conditions like before. For the wave function we make the ansatz

$$\phi_{\text{imp.}}(x) = (\mu_L \phi^+(x) + \nu_L \phi^-(x)) \Theta(-x + x_0) + (\mu_R \phi^+(x) + \nu_R \phi^-(x)) \Theta(x - x_0) \quad (33)$$

with the solutions $\phi_i(x)$, (21), and yet unknown coefficients $\mu_{L,R}$ and $\nu_{L,R}$.

Inserting (33) into a matching condition like (4),

$$\begin{pmatrix} \phi_{\text{imp.}}(x_0 + 0) \\ \phi'_{\text{imp.}}(x_0 + 0) \end{pmatrix} = \tilde{\mathbf{M}} \begin{pmatrix} \phi_{\text{imp.}}(x_0 - 0) \\ \phi'_{\text{imp.}}(x_0 - 0) \end{pmatrix}, \quad (34)$$

where

$$\tilde{\mathbf{M}} = \begin{pmatrix} \frac{1 + \tilde{\beta}}{1 - \tilde{\beta}}, & 0 \\ \tilde{\alpha}, & \frac{1 - \tilde{\beta}}{1 + \tilde{\beta}} \end{pmatrix} \quad (35)$$

involves the parameters from (32), we get

$$\begin{pmatrix} \mu_R \\ \nu_R \end{pmatrix} = \tilde{\mathbf{T}} \begin{pmatrix} \mu_L \\ \nu_L \end{pmatrix} \quad (36)$$

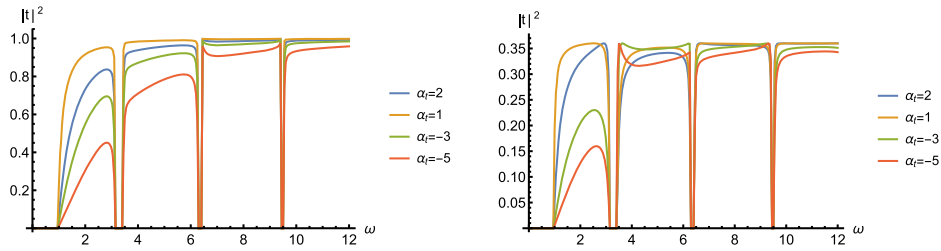


Figure 3. The scattering coefficient $|t|^2$, equation (39), for a single impurity given by the potential (32) as a function of the frequency ω . The parameters are $\beta = 0$, (left panel), $\beta = 0.5$ (right panel) and $\alpha = 1, \beta = 0, x_0 = 0.3$ in both panels.

with

$$\tilde{T} = \tilde{K}^{-1} \tilde{M} \tilde{K}, \quad \tilde{K} = \begin{pmatrix} \phi^+(x_0), \phi^-(x_0) \\ \phi'^+(x_0), \phi'^-(x_0) \end{pmatrix}. \tag{37}$$

The determinant of \tilde{K} is just the Wronskian, (25), of the two solutions, $\det(\tilde{K}) = W$.

3.1. Scattering setup

In this subsection we consider the scattering setup for the solutions (33) with impurity. In zones with $j_1 > 0$ and $j_2 < 0$ we consider first a right moving wave. With $\mu_L = 1$ and $\nu_R = 0$ we note

$$\phi_{\text{right}}(x) = (\phi^+(x) + r \phi^-(x)) \Theta(-x + x_0) + t \phi^+(x) \Theta(x - x_0), \tag{38}$$

where r and t have the meaning of reflection and transmission coefficients. Using (36) we get

$$r = -\frac{(\tilde{T})_{21}}{(\tilde{T})_{22}}, \quad t = \frac{1}{(\tilde{T})_{22}}, \tag{39}$$

where we used $\det(\tilde{T}) = 1$, which holds same way as (14). The left moving wave will be

$$\phi_{\text{left}}(x) = \bar{t} \phi^-(x) \Theta(-x + x_0) + (\bar{r} \phi^+(x) + \phi^-(x)) \Theta(x - x_0). \tag{40}$$

From unitarity $t = \bar{t}$ follows as usual, but $r = \bar{r}$ will hold for $\beta = \tilde{\beta} = 0$ (symmetric potential) only. Again from (35), we note

$$\bar{r} = \frac{(\tilde{T})_{12}}{(\tilde{T})_{22}}, \quad \bar{t} = \frac{1}{(\tilde{T})_{22}}. \tag{41}$$

Plots of the scattering coefficients are shown in figure 3. These are non zero within the bands only and show a rich diversity in their dependence on the parameters.

3.2. Bound states

Bound states require wave functions decreasing for $x \rightarrow \pm\infty$ for normalizability. From the repeated application of equation (6) it follows that the quasi momentum must be imaginary,

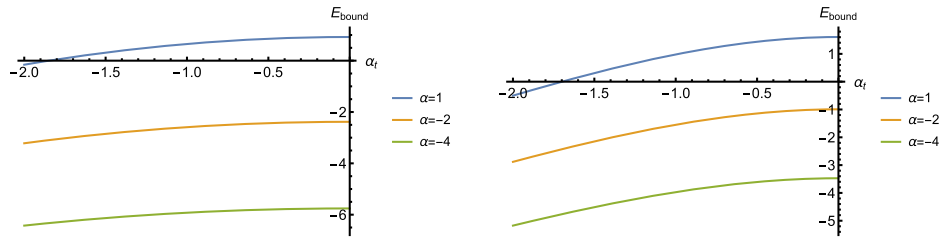


Figure 4. The bound state level for a single impurity given by the potential (32) as a function of the impurity strengths $\tilde{\alpha}$. The parameters are $\beta = 0$ (left panel), $\beta = 0.5$ (right panel) and $\beta = 0$, $x_0 = 0.3$ in both panels.

$q = i\eta$. Thus bound states may appear only outside the bands. The right side in equation (19) becomes larger than unity and we define

$$\eta = \operatorname{arccosh} \left(\frac{w + w^*}{2} \right) \quad (42)$$

with $\eta > 0$. Using the solutions $\phi_{1,2}(x)$, (21), and using

$$\phi^\pm(x + am) = e^{\mp\eta am} \phi^\pm(x), \quad (43)$$

which follows from (6), we get

$$\begin{aligned} \phi^+(x) &\xrightarrow{x \rightarrow \infty} 0, & \phi^+(x) &\xrightarrow{x \rightarrow -\infty} \infty, \\ \phi^-(x) &\xrightarrow{x \rightarrow \infty} \infty, & \phi^-(x) &\xrightarrow{x \rightarrow -\infty} 0, \end{aligned} \quad (44)$$

for the asymptotics. As a consequence we must have $\mu_R = \nu_L = 0$ in the ansatz (33),

$$\begin{pmatrix} \mu_R \\ 0 \end{pmatrix} = \tilde{T} \begin{pmatrix} 0 \\ \nu_L \end{pmatrix}. \quad (45)$$

This is possible only if

$$\tilde{T}_{22} = 0, \quad (46)$$

which is the frequency condition for a bound state.

In figures 4 and 5 several examples are shown. Bound states exist only for attractive impurity potential. The binding energies are below the lower boundary of the lowest band, reaching it at $\tilde{\alpha} = 0$. There are also bound states in-between the bands, which we, however, do not consider. In figure 5, where the binding energy is shown as a function of the location x_0 of the impurity inside a lattice cell, the lower curve is symmetric for $\beta = 0$ while $\beta \neq 0$ makes it non-symmetric. This function is periodic, i.e., it is the same in each lattice cell.

4. Double impurity

In this section we assume two impurities to be present, located at $x = x_0$ and $x = x_0 + L$, such that L is the separation between them and x_0 is the offset to the lattice. The discussion is to a large extent a simple generalization of the preceding section. However, the interaction between the two impurities will show some interesting features.

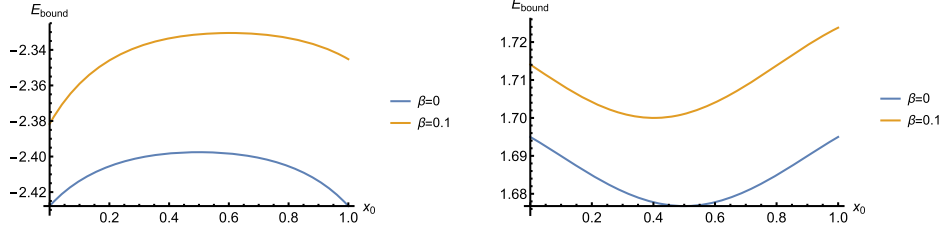


Figure 5. The bound state level for a single impurity given by the potential (32) as a function of the impurity location x_0 . The periodic potential is attractive ($\alpha = -2$) in the left panel and repulsive ($\alpha = 2$) in the right panel. The other parameters are $\beta = 0$, $\tilde{\alpha} = -0.3$ and $\tilde{\beta} = 0$.

The potential reads, symbolically,

$$V_{2\text{imp.}} = \tilde{\alpha}_1 \delta(x - x_0) + 2\tilde{\beta}_1 \delta'(x - x_0) + \tilde{\alpha}_2 \delta(x - (x_0 + L)) + 2\tilde{\beta}_2 \delta'(x - (x_0 + L)). \quad (47)$$

We realize it by matching conditions like before. For the solutions, we make the ansatz

$$\begin{aligned} \phi_{2\text{imp.}} = & (\mu_L \phi^+(x) + \nu_L \phi^-(x)) \Theta(-x + x_0) + (\mu \phi^+(x) + \nu \phi^-(x)) \Theta(x - x_0) \Theta(-x + (x_0 + L)) \\ & + (\mu_R \phi^+(x) + \nu_R \phi^-(x)) \Theta(x - (x_0 + L)), \end{aligned} \quad (48)$$

where the functions $\phi^\pm(x)$ are given by (21) and (23). The matching conditions, corresponding to (47), like (4) or (34), read

$$\begin{aligned} \begin{pmatrix} \phi_{2\text{imp.}}(x_0 + L + 0) \\ \phi'_{2\text{imp.}}(x_0 + L + 0) \end{pmatrix} &= \tilde{\mathbf{M}}_2 \begin{pmatrix} \phi_{2\text{imp.}}(x_0 + L - 0) \\ \phi'_{2\text{imp.}}(x_0 + L - 0) \end{pmatrix}, \\ \begin{pmatrix} \phi_{2\text{imp.}}(x_0 + 0) \\ \phi'_{2\text{imp.}}(x_0 + 0) \end{pmatrix} &= \tilde{\mathbf{M}}_1 \begin{pmatrix} \phi_{2\text{imp.}}(x_0 - 0) \\ \phi'_{2\text{imp.}}(x_0 - 0) \end{pmatrix}, \end{aligned} \quad (49)$$

where we defined

$$\tilde{\mathbf{M}}_i = \begin{pmatrix} \frac{1 + \tilde{\beta}_i}{1 - \tilde{\beta}_i} & 0 \\ \tilde{\alpha}_i & \frac{1 - \tilde{\beta}_i}{1 + \tilde{\beta}_i} \end{pmatrix}, \quad (i = 1, 2). \quad (50)$$

Similar to section 3 we rewrite these conditions in the form

$$\begin{pmatrix} \mu_R \\ \nu_R \end{pmatrix} = \tilde{\mathbf{T}}_2 \begin{pmatrix} \mu \\ \nu \end{pmatrix}, \quad \begin{pmatrix} \mu \\ \nu \end{pmatrix} = \tilde{\mathbf{T}}_1 \begin{pmatrix} \mu_L \\ \nu_L \end{pmatrix}, \quad (51)$$

with

$$\tilde{\mathbf{T}}_i = \tilde{\mathbf{K}}_i^{-1} \tilde{\mathbf{M}}_i \tilde{\mathbf{K}}_i, \quad (i = 1, 2), \quad (52)$$

and

$$\tilde{\mathbf{K}}_1 = \begin{pmatrix} \phi^+(x_0), \phi^-(x_0 + L) \\ \phi^{+'}(x_0 + L), \phi^{-'}(x_0) \end{pmatrix}, \quad \tilde{\mathbf{K}}_2 = \begin{pmatrix} \phi^+(x_0 + L), \phi^-(x_0 + L) \\ \phi^{+'}(x_0 + L), \phi^{-'}(x_0 + L) \end{pmatrix}. \quad (53)$$

Combining the two equations in (51), eliminating μ and ν , we arrive at

$$\begin{pmatrix} \mu_R \\ \nu_R \end{pmatrix} = \tilde{\mathbf{T}}_{2\text{imp.}} \begin{pmatrix} \mu_L \\ \nu_L \end{pmatrix}, \quad (54)$$

where

$$\tilde{\mathbf{T}}_{2\text{imp.}} = \tilde{\mathbf{T}}_2 \tilde{\mathbf{T}}_1. \quad (55)$$

Using these formulas, in parallel to sections 3.1 and 3.2, the transmission and reflection coefficients can be defined as well as the bound state condition. The latter reads

$$\left(\tilde{\mathbf{T}}_{2\text{imp.}} \right)_{22} = 0. \quad (56)$$

Again, for momenta in the forbidden regions, this is a real function and its zeros determine the bound state levels.

As example we investigated the bound state levels which are below the first zone. Examples are shown in figure 6. For small α , i.e., for nearly constant background, we have the known picture for two delta functions; at large separation two equal levels (in the shown case one is slightly oscillating), which split when the separation becomes smaller. The antisymmetric solution is expelled and moves into the continuum at a certain separation. With increasing α , i.e., with a more pronounced background, the picture stays in place to a large extend, however, oscillations of the levels increase. At large separation, the levels coincide only for special values of the separation and show a strong dependence on the lattice indicating some kind of long-range interaction between the two impurity potentials.

5. ‘Half’ infinite crystal

In this section, we consider a half infinite lattice (stretching from $x = x_0$ to infinity) to the right side and a potential step to the other side. This setup may serve as a model for a crystal in $x > x_0$ (‘inside’), terminated by a surface with a constant potential V_0 in $x < x_0$ (‘outside’). It is shown symbolically in figure 7.

In this setup, there is no periodicity of the potential and the usual arguments, following from translational invariance, are not applicable. We proceed in the following way. Let

$$\phi(c) = \phi_L(x)\Theta(x_0 - x) + \phi_R(x)\Theta(x - x_0) \quad (57)$$

be a solution of equation (1) composed from plane waves in the segment with constant potential,

$$\phi_L(x) = \mu_L e^{ip(x-x_0)} + \nu_L e^{-ip(x-x_0)}, \quad (58)$$

with the momentum

$$p = \sqrt{\omega^2 - V_0}, \quad (59)$$

and of plane waves in-between the delta-spikes,

$$\phi_R(x) = \sum_{n=0}^{\infty} \phi_n(x)\Theta_n, \quad (60)$$

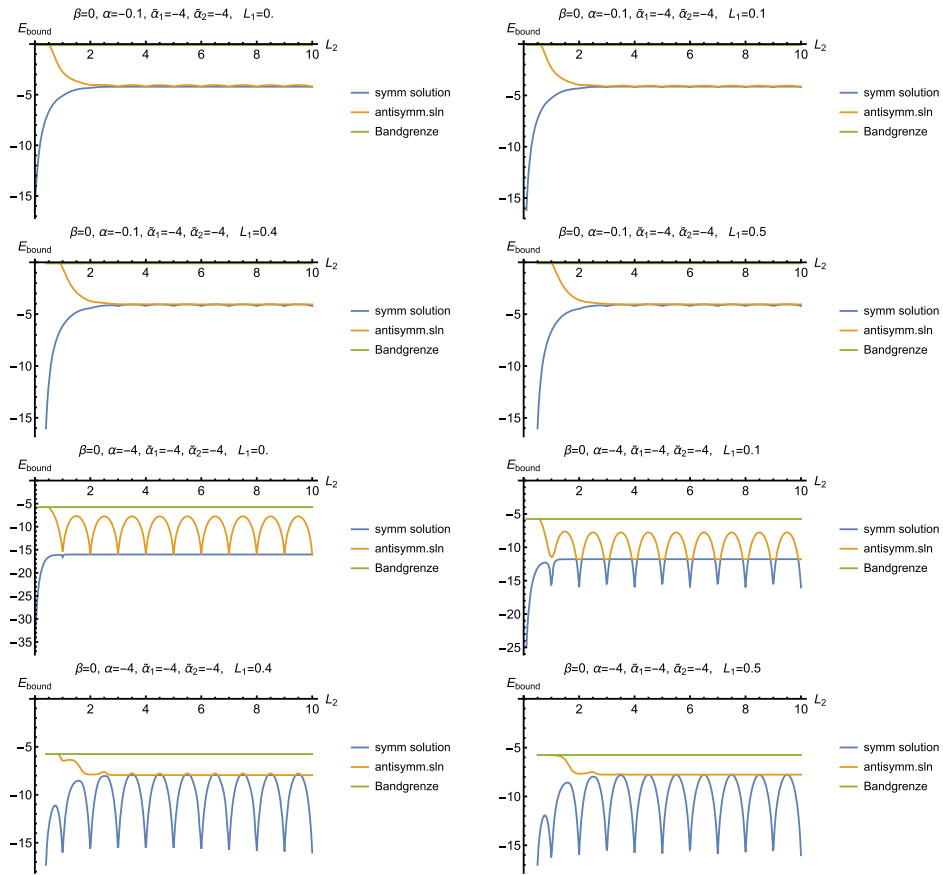


Figure 6. The bound state levels for a double impurity given by the potential (48) as a function of the separation $L = L_2 - L_1$ between the impurities; $L_{1,2}$ are their locations. L_1 changes from 0 to $\frac{1}{2}$ (in units of the lattice spacing a). The parameters are $\beta = \tilde{\beta} = 0$, $\tilde{\alpha}_1 = \tilde{\alpha}_2 = -4$ and $\alpha = -1$ (upper two rows) and $\alpha = -4$ (lower two rows).

where the $\phi_n(x)$ are given by equation (9). The matching conditions (10) are given by the same formula (10) as before, restricted however to $n \geq 0$.

We proceed by considering a finite comb. Using the matching condition (10) in the form

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = \mathbf{T}^n \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}, \quad (n = 0, 1, \dots), \quad (61)$$

with yet unknown coefficients. Following [19], we consider the eigenvalue (characteristic) equation of the matrix \mathbf{T} ,

$$\det(\mathbf{T} - \lambda) = \det(\mathbf{T}) - \lambda \operatorname{tr} \mathbf{T} + \lambda^2 = 0. \quad (62)$$

Further, we use the property $\det \mathbf{T} = 1$, (14), and introduce the notation

$$\xi \equiv \frac{1}{2} \operatorname{tr} \mathbf{T} = \frac{w + w^*}{2}, \quad (63)$$

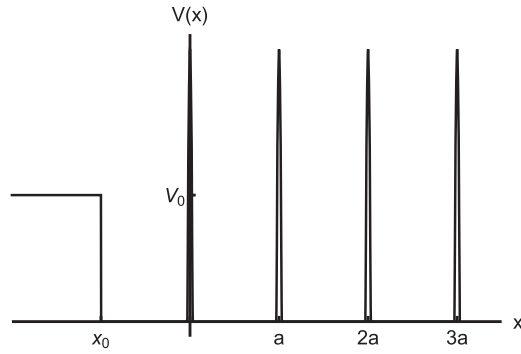


Figure 7. The potential for a ‘half’ infinite crystal.

where the last expression follows with (12). Using the Cayley–Hamilton theorem, stating that a matrix obeys its characteristic equation, we get the equation

$$T^2 = 2\xi T - 1. \tag{64}$$

Iterating this equation results in

$$T^n = T u_{n-1}(\xi) - u_{n-2}(\xi), \tag{65}$$

where

$$u_n(\xi) = \frac{\sin((n + 1)\gamma)}{\sin(\gamma)} \tag{66}$$

are the Chebychev polynomials and

$$\cos(\gamma) = \xi \tag{67}$$

holds. Comparing this equation with (63) and (19) we see that also for the finite lattice the same structure shows up which defines the bands in the infinite lattice. The difference is only that in a finite lattice there is no argument demanding that γ must be real. However, this argument appears in the half infinite lattice as can be seen from increasing n in (66) and demanding no growth.

Now we take λ as a solution of (62) and introduce the quasi momentum q by $\lambda = e^{\pm iqa}$. We get

$$\det(T - e^{\pm iqa}) = 0, \tag{68}$$

which is the same as (18), and can solve the equation

$$(T - e^{\pm iqa}) \begin{pmatrix} A_n \\ B_n \end{pmatrix} = 0. \tag{69}$$

This way we get the same solutions as in section 2.1 and, especially, the property (17). Inserting these into (60), and together with (57) and (58), we have complete solutions on both sides of the interface. It remains to match the solutions $\phi_L(x_0)$ and $\phi_R(x_0)$ by demanding continuity of the function and its derivative,

$$\begin{pmatrix} \phi_L(x_0) \\ \phi'_L(x_0) \end{pmatrix} = \begin{pmatrix} \phi_R(x_0) \\ \phi'_R(x_0) \end{pmatrix}. \tag{70}$$

From (58) we get

$$\begin{pmatrix} \phi_L(x_0) \\ \phi_L'(x_0) \end{pmatrix} = \mathbf{K}_p \begin{pmatrix} \mu_L \\ \nu_L \end{pmatrix} \quad \text{with } \mathbf{K}_p = \begin{pmatrix} 1 & 1 \\ ip & -ip \end{pmatrix}. \quad (71)$$

For $x > x_0$ we take a superposition of the solutions for $\pm q$,

$$\phi_R(x) = \mu_R \phi^+(x) + \nu_R \phi^-(x), \quad (72)$$

where the functions $\phi^\pm(x)$ entering (60) are given by (21). Rewriting,

$$\begin{pmatrix} \phi_R(x_0) \\ \phi_R'(x_0) \end{pmatrix} = \mathbf{K}_0 \begin{pmatrix} \mu_R \\ \nu_R \end{pmatrix}, \quad \text{with } \mathbf{K}_0 = \begin{pmatrix} \phi_0^+(x_0) & \phi_0^-(x_0) \\ \phi_0^{+'}(x_0) & \phi_0^{-'}(x_0) \end{pmatrix} \quad (73)$$

and inserting (71) and (73) into (70) we arrive at

$$\begin{pmatrix} \mu_R \\ \nu_R \end{pmatrix} = \mathbf{T}_0 \begin{pmatrix} \mu_L \\ \nu_L \end{pmatrix}, \quad \text{with } \mathbf{T}_0 = \mathbf{K}_0^{-1} \mathbf{K}_p. \quad (74)$$

This way, the complete solution of the problem is determined. There are two free parameters, μ_L , and ν_L for example.

From the asymptotic properties of the solutions, which follow either directly from (58) for ϕ_L or from (44) for ϕ_R , the possible solutions can be classified as follows.

(a) $E > V_0$, p and q real

These are plane wave solutions outside and Bloch wave solutions inside the crystal, energy must be in an allowed zone.

(b) $E > V_0$, p and η real ($q = i\eta$)

Energy is in a forbidden zone and in (72) one must take $\nu_R = 0$ following (44). This wave decreases exponentially inside. The incoming plane wave from outside is completely reflected. Together with (a), we have a completely continuous spectrum for $E > V_0$.

(c) $0 < E < V_0$, π and q real ($p = i\pi$)

Energy is in an allowed band and in (58) one must take $\mu_L = 0$ following (58). This wave decreases exponentially outside. We have a Bloch wave inside which is reflected at the surface.

(d) $0 < E < V_0$, $\alpha > 0$, π and η real ($p = i\pi$, $q = i\eta$)

Energy is in a forbidden zone. In (72) one must take $\nu_R = 0$ and in (58) one must take $\mu_L = 0$. The solution is decreasing to both sides of the interface and represents a so-called surface (Tamm) state. It existed only for repulsive delta potential in the lattice.

(e) $0 < E < V_0$, $\alpha < 0$, π and q real ($p = i\pi$)

Energy is in an allowed zone and one must take $\mu_L = 0$. We have a Bloch wave inside which is reflected at the surface. Since here $k = i\alpha$, in each cell the solutions are real exponentials. However, because of real q the solution does not decrease for $x \rightarrow \infty$.

5.1. Surface (Tamm) states

We consider case (d). The energy is below the potential step and outside any allowed band. In order to have a decrease of the wave function $\Phi_L(x)$, (58), for $x \rightarrow -\infty$, we must have imaginary momentum

$$p = i\pi, \quad \pi = \sqrt{U_0 - \omega^2}, \quad (75)$$

and we have to put $\mu_L = 0$. For decrease at $x \rightarrow \infty$, from $\Phi_R(x)$, (72), accounting for (44), we have to put $\nu_R = 0$. Using these settings in (74) we note

$$\begin{pmatrix} 0 \\ \nu_L \end{pmatrix} = T_0^{-1} \begin{pmatrix} \mu_R \\ 0 \end{pmatrix} \tag{76}$$

and the condition

$$(T_0^{-1})_{11} = 0 \tag{77}$$

follows. To get the explicit expression we rewrite (74),

$$T_0^{-1} = K_p^{-1} K_0, \tag{78}$$

and with (71) and (73) we arrive at

$$T_0^{-1} = \frac{1}{2\pi} \begin{pmatrix} (\pi - i\omega)e^{i\omega x_0} & (\pi + i\omega)e^{-i\omega x_0} \\ (\pi + i\omega)e^{i\omega x_0} & (\pi - i\omega)e^{-i\omega x_0} \end{pmatrix} \begin{pmatrix} A_0^+ \\ B_0^+ \end{pmatrix}, \tag{79}$$

where we used $\nu_R = 0$ and (79), (60). Using (79), the equation (77) turns into

$$(\pi - ik)e^{ikx_0} A_0^+ + (\pi + ik)e^{-ikx_0} B_0^+ = 0, \tag{80}$$

which is the frequency condition for surface states. The coefficients A_0^+ and B_0^+ can be substituted by A_1^+ and B_1^+ using (15) (the factor e^{-iqa} cancels out) and formulas (23) can be used. Equation (80) is a condition on the frequency ω . Its solution, ω_{Ta} , is the binding energy of a Tamm state.

As known, a bound state wave function, like $\phi(x)$, (57), with bound state momentum ω_{Ta} , can be chosen to be real. This circumstance allows to simplify equation (80), expressing it in terms of real entries. It must be mentioned that it is sufficiently inconvenient to transform equation (80), especially the coefficients A_0^+ and B_0^+ , which are given by equations (17) and (23). For this reason we will eliminate A_0^+ and B_0^+ .

To achieve this goal, we proceed as follows. First of all, we introduce the notation

$$\Psi(x) = \begin{pmatrix} \phi(x) \\ \phi'(x) \end{pmatrix} \tag{81}$$

for any of the solutions we consider below. These are, from (58),

$$\phi_L(x) = \nu_L e^{\pi(x-x_0)}, \quad (x < x_0), \tag{82}$$

where we accounted for $\mu_L = 0$ and (75). Further we have

$$\phi_R(x) = \mu_R \begin{cases} A_0^+ e^{i\omega x} + B_0^+ e^{-i\omega x}, & (x < 0), \\ A_1^+ e^{i\omega(x-a)} + B_1^+ e^{-i\omega(x-x_0)}, & (0 < x < a), \end{cases} \tag{83}$$

and we accounted for (60), (21) and for $\nu_R = 0$. Second, we use the matching conditions

$$\Psi_R(x_0) = \Psi_L(x_0), \quad (x = x_0), \tag{84}$$

$$\Psi_R(0) = M\Psi_R(0), \quad (x = 0). \tag{85}$$

The first one is equation (70) and the second one is (4) with M given by (5). Using (82) and (83) we get explicitly

$$\Psi_L(x_0) = \nu_L \begin{pmatrix} 1 \\ \pi \end{pmatrix}, \quad \psi_R(x_0) = \mathbf{K}\mathbf{Q}_0 \begin{pmatrix} A_0^+ \\ B_0^+ \end{pmatrix}, \quad (86)$$

with \mathbf{K} given by (11) and \mathbf{Q}_0 given by

$$\mathbf{Q}_0 = \begin{pmatrix} e^{i\omega x_0} & 0 \\ 0 & e^{-i\omega x_0} \end{pmatrix}. \quad (87)$$

Condition (84) can be used to express

$$\begin{pmatrix} A_0^+ \\ B_0^+ \end{pmatrix} = \nu_L \mathbf{Q}_0^{-1} \mathbf{K} \begin{pmatrix} 1 \\ \pi \end{pmatrix}. \quad (88)$$

Further, we note from (83)

$$\Psi_R(+0) = \mu_R \mathbf{K}\mathbf{Q} \begin{pmatrix} A_1^+ \\ B_1^+ \end{pmatrix}, \quad \Psi_R(-0) = \mu_R \mathbf{K} \begin{pmatrix} A_0^+ \\ B_0^+ \end{pmatrix}, \quad (89)$$

with \mathbf{K} and \mathbf{Q} given in (11). Further, using (17) and $q = i\eta$, the condition (85) can be written in the form

$$\mathbf{K}\mathbf{Q} e^{-\eta a} \begin{pmatrix} 1 \\ \pi \end{pmatrix} = \mathbf{M}\mathbf{K} \begin{pmatrix} A_0^+ \\ B_0^+ \end{pmatrix}, \quad (90)$$

where μ_R dropped out. Now we insert from (88) into this equation and arrive at

$$\Lambda e^{-\eta a} \begin{pmatrix} 1 \\ \pi \end{pmatrix} = \mathbf{M}\mathbf{K}\mathbf{Q}_0^{-1} \mathbf{k}^{-1} \begin{pmatrix} 1 \\ \pi \end{pmatrix}, \quad (91)$$

where we defined

$$\Lambda = \mathbf{K}\mathbf{Q}\mathbf{Q}_0^{-1} \mathbf{K}^{-1}. \quad (92)$$

We mention $\Lambda = \mathbb{1}$ for $x_0 = -a$, i.e., if the separation from the last delta function to the surface of the crystal is just equal to the lattice spacing.

As last step we rewrite (92) in the form

$$\mathbf{T}_{\text{Ta}} \begin{pmatrix} 1 \\ \pi \end{pmatrix} = e^{-\eta a} \begin{pmatrix} 1 \\ \pi \end{pmatrix} \quad (93)$$

with

$$\mathbf{T}_{\text{Ta}} = \Lambda^{-1} \mathbf{M}\mathbf{K}\mathbf{Q}_0^{-1} \mathbf{K}^{-1}. \quad (94)$$

Multiplying by $(\pi, -1)$ from left, we arrive at

$$(\pi, -1) \mathbf{T}_{\text{Ta}} \begin{pmatrix} 1 \\ \pi \end{pmatrix} = 0, \quad (95)$$

which is the final form of the frequency condition for a Tamm state. It is equivalent to (80), but easier to use since in terms of real entries.

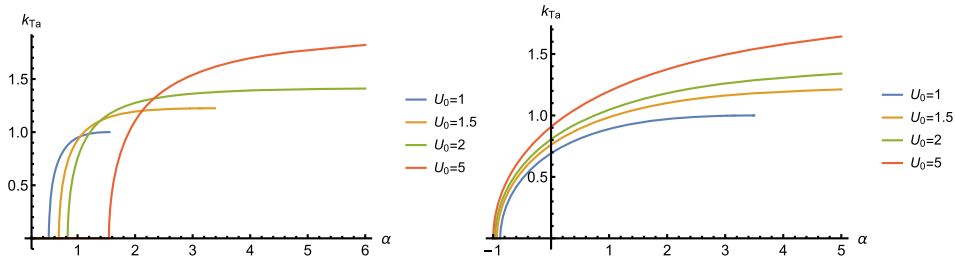


Figure 8. Tamm states below the lowest band as a function of the lattice coupling α for $x_0 = -a$ with $\beta = 0$ (left panel) and $\beta = 0.5$ (right panel).

The explicit form of (95) is, using $U_0 = \pi^2 + \omega^2$,

$$\alpha(\omega \cos(\omega a) + \beta \sin(\omega a))(\omega \cos(\omega(x_0 + a)) - \pi \sin(\omega(x_0 + a))) + \omega(4\beta\pi k \cos(\omega x_0) + 2\beta(\omega^2 - \pi^2) \sin(\omega x_0) - (1 + \beta^2)U_0 \sin(\omega(x_0 + 2a))) = 0. \tag{96}$$

It simplifies for $x_0 = -a$,

$$\omega(\alpha + 4\beta\pi) \cos(\omega a) + (\alpha\pi - 2\beta(\omega^2 - \pi^2) - (1 + \beta^2)U_0) \sin(\omega a) = 0. \tag{97}$$

Solutions are shown in figure 8. There is always some smallest coupling α for these solutions. For small U_0 there is also some largest α . Allowing for the δ' -function in the potential ($\beta \neq 0$), a solution exists also for $\alpha < 0$ (attractive delta potential).

6. The vacuum energy

In this section, we consider the vacuum energy of the scalar field $\phi(x)$ in the background of a comb with impurity. In general, the vacuum energy of a field in a one-dimensional background is a topic with a long history. However, in a periodic background interest grew up only quite recently. In [13] the vacuum energy for a comb of generalized delta functions was calculated (and in [15] generalized to finite temperature). Here we calculate the vacuum energy for a comb with single impurity. We start with a re-derivation, in a more simple way, of the vacuum energy for a pure comb, and, using similar methods, we consider the vacuum energy of the impurity.

6.1. The vacuum energy of a comb

In general, the vacuum energy is the half sum of energies over all excitations of a quantum field,

$$E_0 = \frac{1}{2} \sum_n \omega_n^{1-2s}. \tag{98}$$

Since this quantity has ultraviolet divergencies, one needs to introduce a regularization. We took in (98) the zeta functional one by introducing the parameter s in the power. For sufficiently large s the sum is convergent and to get E_0 for $s \rightarrow 0$ one has to make an analytic continuation. The regularization is removed for $s \rightarrow 0$. This regularization is called zetafunctional due

to its close relation to the zeta function $\zeta_P(s) = \sum_{(n)} \omega_{(n)}^{-2s}$ of the operator in (1), see, for example, the book [20]. For more details on this procedure, we refer also to chapter 4 in [21].

Equation (98) assumes a discrete spectrum. Now, the spectrum of a periodic potential is necessarily continuous due to the infinite extend of the lattice. For this reason, we first consider the vacuum energy of a finite comb, the length of which will then tend to infinity.

Let the finite comb have $2N$ peaks, located in $x = an$ with $n = -N + 1, \dots, N$. For the field, we modify the ansatz (8),

$$\phi(x) = \sum_{n=-N+1}^{N+1} (A_n e^{i\omega(x-an)} + B_n e^{-i\omega(x-an)}) \Theta_n, \tag{99}$$

with Θ_n given by (7). Now we impose Dirichlet boundary conditions in $x = L_1$ and $x = L_2$ with $L_1 = a(N + \frac{1}{2})$ and $L_2 = a(-N + \frac{1}{2})$, i.e., we terminate the function at a half interval outside the finite comb. This choice simplifies the calculations but does not pose any restrictions since we are interested in the limit $N \rightarrow \infty$. From (99) we get

$$\begin{aligned} \phi(L_1) &= A_{N+1} e^{-i\omega a/2} + B_{N+1} e^{i\omega a/2} = 0, \\ \phi(L_2) &= A_{-N+1} e^{-i\omega a/2} + B_{-N+1} e^{i\omega a/2} = 0. \end{aligned} \tag{100}$$

Further we use (10) repeatedly,

$$\begin{pmatrix} A_{N+1} \\ B_{N+1} \end{pmatrix} = T^{2N} \begin{pmatrix} A_{-N+1} \\ B_{-N+1} \end{pmatrix}, \tag{101}$$

and the system (100) turns into

$$\begin{aligned} & \left((T^{2N})_{11} e^{-i\omega a/2} + (T^{2N})_{21} e^{i\omega a/2} \right) A_{-N+1} + (T^{2N})_{12} e^{-i\omega a/2} \\ & + (T^{2N})_{22} e^{i\omega a/2} B_{-N+1} = 0, \\ & e^{-i\omega a/2} A_{-N+1} + e^{i\omega a/2} B_{-N+1} = 0. \end{aligned} \tag{102}$$

Its determinant is

$$(T^{2N})_{11} - (T^{2N})_{22} + (T^{2N})_{21} e^{i\omega a} - (T^{2N})_{12} e^{-i\omega a} = 0. \tag{103}$$

Next we use equations (65) and (12),

$$u_{2N-1}(\xi) (w - w^* + z^* e^{i\omega a} - z e^{-i\omega a}) = 0, \tag{104}$$

which with (66) implies

$$\sin(2N\gamma) = 0 \tag{105}$$

and

$$\gamma = \frac{\pi i}{2N} \tag{106}$$

takes discrete values. With (67) and (63) we arrive at the dispersion relation

$$\cos\left(\frac{\pi i}{2N}\right) = \frac{w + w^*}{2}. \tag{107}$$

At this place, it is convenient to introduce one more notation. Let

$$h(\omega) \equiv \frac{w + w^*}{2} = \frac{(1 + \beta^2) \cos(\omega a) + \frac{\alpha}{2\omega} \sin(\omega a)}{1 - \beta^2}, \quad (108)$$

where we used (19), denote the right side of the dispersion relation and let

$$q_i = \frac{\pi i}{2Na} \quad (109)$$

denote the discrete values of that quantity which in the infinite lattice will become the quasi momentum. With these notations, the dispersion relation can be recast in the form

$$\cos(qa) = h(\omega) \quad (110)$$

and inserting here q_i , (109), we have as solutions of $\cos(q_i a) = h(\omega_{i,n})$ frequencies $\omega_{i,n}$. Here, the index n numbers the groups of levels which in the limit will turn into the bands. The index i takes values $i = 0, \dots, N - 1$. All other values do not give new solutions in (107).

With these preparations, we return to the vacuum energy (98). Now we have two sums, over i and n . We transform the sum over n into a contour integral, using

$$\Delta(q, \omega) \equiv \cos(qa) - h(\omega) \quad (111)$$

as function whose zeros are the discrete frequencies,

$$E_0 = \frac{1}{2} \sum_{i=0}^{2N-1} \int_{\gamma} \frac{d\omega}{2\pi i} \omega^{1-2s} \partial_{\omega} \ln \Delta(q_i, \omega). \quad (112)$$

The integration path γ encircles the positive real half axis.

At this place, it is convenient to take the limit $N \rightarrow \infty$, i.e. to remove the ‘large box’. In doing so, the sum over i turns into an integral according to $\frac{\pi}{2aN} \sum_{i=0}^{2N-1} \rightarrow \int_0^{\pi/a} dq$ and $\frac{\pi i}{2Na} \rightarrow q$. The vacuum energy (112) becomes

$$E_0 = \frac{L}{2} \int_0^{\frac{\pi}{a}} \frac{dq}{\pi} \int_{\gamma} \frac{d\omega}{2\pi i} \omega^{1-2s} \partial_{\omega} \ln \Delta(q, \omega), \quad (113)$$

It is proportional to $L = 2aN$ which is the (infinite) length of the lattice. Dividing by L and multiplying by a one obtains the energy per unit cell. Simply dividing by L we would get the energy density.

The vacuum energy (113) is equivalent to that which was derived and investigated in [13, 15]. The representation presented here is better suited for the calculation of the vacuum energy for finite combs, which may have also different boundary conditions. For instance, it is easy to take periodic boundary conditions in place of (100).

We conclude this subsection by a further transformation of the vacuum energy (113) into a form well suited for numerical investigation. For this, we make a Wick rotation in the frequency integration, $\omega = i\xi$, in the upper half of the integration path γ and $\omega = -i\xi$ in the lower part. We arrive at

$$E_0 = -\frac{L}{2} \cos(\pi s) \int_0^{\frac{\pi}{a}} \frac{dq}{\pi} \int_0^{\infty} \frac{d\xi}{\pi} \xi^{1-2s} \partial_{\xi} \ln \Delta(q, i\xi), \quad (114)$$

where $\Delta(q, i\xi) = \Delta(q, i\xi)^*$ was used. Now we interchange the order of the integrations and using the explicit form (111). We can carry out the integration over q explicitly,

$$E_0 = -\frac{L}{2a} \cos(\pi s) \int_0^\infty \frac{d\xi}{\pi} \xi^{1-2s} \partial_\xi \ln \left(h(i\xi) + \sqrt{h(i\xi)^2 - 1} \right), \quad (115)$$

where the property $h(i\xi) > 1$, following from (108), was used. We note, that this formula does not contain the quasi momentum q . We use that to define a function $q(\omega)$ from the dispersion relation (110) and note

$$q(i\xi) \equiv \frac{1}{a} \operatorname{arccosh}(h(i\xi)) = \frac{1}{a} \ln \left(h(i\xi) + \sqrt{h(i\xi)^2 - 1} \right) - \frac{\ln 2}{a}, \quad (116)$$

such that (115) can be rewritten in the form

$$E_0 = -\frac{L}{2a} \cos(\pi s) \int_0^\infty \frac{d\xi}{\pi} \xi^{1-2s} \frac{\partial q(i\xi)}{\partial \xi}. \quad (117)$$

Defining $\eta(\xi) = q(i\xi)$, we get a monotonous function (in opposite to $q(\omega)$), and can change the integration variable from ξ to η . The inverse function $\xi(\eta)$ is well defined and we arrive at

$$E_0 = -\frac{L}{2a} \cos(\pi s) \int_0^\infty \frac{d\eta}{\pi} \xi(\eta)^{1-2s}, \quad (118)$$

which is probably the simplest form of representing the vacuum energy.

We conclude this section by a remark on the ultraviolet divergencies. We return to representation (117) and define the function $\eta(\xi) = q(i\xi)$. Also, we put $a = 1$ and restore the dependence on a later. For simplicity we restrict ourselves to $\beta = 0$, i.e., to the case with a simple delta function in the background potential (1). From (116) we get

$$\cosh(\eta(\xi)) = \cosh(\xi) + \frac{\alpha}{\xi} \sinh(\xi). \quad (119)$$

Now we represent

$$\begin{aligned} \eta &= \operatorname{arccosh}(\cosh(\eta)) = \ln \left(\frac{1}{2} \left(\cosh(\eta) + \sqrt{\cosh(\eta)^2 - 1} \right) \right), \\ &= \ln(\cosh(\eta)) + \ln \left(\frac{1}{2} \left(1 + \sqrt{1 - \cosh(\eta)^{-2}} \right) \right). \end{aligned} \quad (120)$$

The second term in the right side is decreasing for $\xi \rightarrow \infty$. The first one can be represented in the form

$$\ln(\cosh(\eta)) = \xi - \ln 2 + \ln \left(1 + \frac{\alpha}{\xi} \right) + \ln \left(1 + \frac{1 - \alpha/\xi}{1 + \alpha/\xi} e^{-2\xi} \right). \quad (121)$$

Here the first term is growing but does not depend on anything. This gives the contribution from the empty space which must be dropped. The constant term drops out under differentiation in (117). The third term is decreasing, but only like a power. It can be identified with the contribution from a single delta function taken alone (however in each cell). This contribution is sensitive only to a change in the strength α of the coupling. Finally, the fourth term is exponentially fast decreasing and, together with the second contribution in (120), gives rise to the renormalized vacuum energy of the comb,

$$E_0^{\text{ren.}} = -\frac{1}{2a} \int_0^\infty \frac{d\xi}{\pi} \xi \partial_\xi \left[\ln \left(1 + \frac{1 - \alpha a/\xi}{1 + \alpha a/\xi} e^{-2\xi} \right) \right]$$

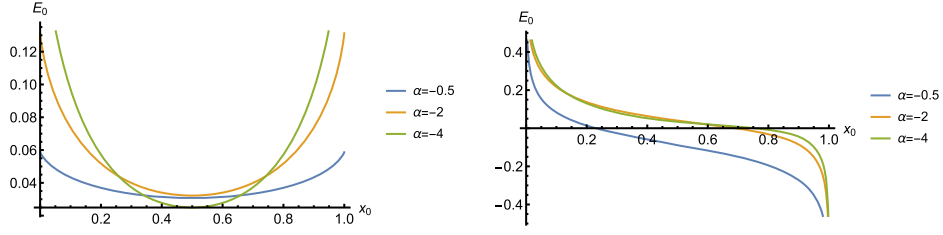


Figure 9. The vacuum energy for a single impurity as a function of its position x_0 inside a cell. Parameters are $\beta = 0$ (left panel), $\beta = 0.5$ (right panel) and $\tilde{\beta} = 0$, $\tilde{\alpha} = 2$ (both panels). The vacuum energy takes finite values for $x_0 = 0$ and $x_0 = 1$.

$$+ \ln \left(\frac{1}{2} \left(1 + \sqrt{1 - \left(\cosh \xi + \frac{\alpha a}{\xi} \sinh(\xi) \right)^{-2}} \right) \right), \quad (122)$$

taken now per unit cell. We have put $s = 0$ and restored the dependence on a . The last remark is that it is possible to integrate by parts in this formula, which simplifies the expression a bit further. Also, it can be seen that this vacuum energy takes only negative values, thus increasing the rigidity of the comb. A graphical representation of this vacuum energy is given in figure 1 in [13]. The case $\beta = 0$ corresponds to $\Omega = -1$ in [13] (the green curve). Also cases with $\beta \neq 0$, i.e., with a generalized delta function potential, are shown, where the vacuum energy may have both signs.

6.2. Vacuum energy with impurity

Also, in this case, the vacuum energy is given by the general formula (98), where now the frequencies ω_n are those in the presence of the impurity considered in section 3. To get these frequencies, we proceed differently from the preceding subsection and consider an infinite comb. We use the relation $q(\omega) = \arccos(h(\omega))$, following from (110). We start from the ansatz (33) and demand Dirichlet boundary conditions at $x = \pm \frac{L}{2}$, which result, using (33), in

$$\begin{aligned} \phi^+ \left(\frac{L}{2} \right) \mu_R + \phi^- \left(\frac{L}{2} \right) \nu_R &= 0, \\ \phi^+ \left(-\frac{L}{2} \right) \mu_L + \phi^- \left(-\frac{L}{2} \right) \nu_L &= 0. \end{aligned} \quad (123)$$

At once, the coefficients $\mu_{L,R}$ and $\nu_{L,R}$ have to obey (36). Inserting μ_R and ν_R from (36) into (123), we get a system,

$$\begin{pmatrix} \phi^+ \left(\frac{L}{2} \right) \tilde{T}_{11} + \phi^- \left(\frac{L}{2} \right) \tilde{T}_{21}, & \phi^+ \left(\frac{L}{2} \right) \tilde{T}_{12} + \phi^- \left(\frac{L}{2} \right) \tilde{T}_{22} \\ \phi^+ \left(-\frac{L}{2} \right) & \phi^- \left(-\frac{L}{2} \right) \end{pmatrix} \begin{pmatrix} \mu_L \\ \nu_L \end{pmatrix} = 0, \quad (124)$$

whose determinant must vanish,

$$\Delta(\omega) \equiv \phi^+ \left(\frac{L}{2} \right) \phi^- \left(-\frac{L}{2} \right) \tilde{T}_{11} + \phi^- \left(\frac{L}{2} \right) \phi^+ \left(-\frac{L}{2} \right) \tilde{T}_{21}$$

$$- \phi^+ \left(-\frac{L}{2} \right) \phi^- \left(\frac{L}{2} \right) \tilde{T}_{22} - \phi^+ \left(\frac{L}{2} \right) \phi^+ \left(-\frac{L}{2} \right) \tilde{T}_{12} = 0. \quad (125)$$

Assuming that not only L but also $\frac{L}{2}$ matches the lattice, using (22) we arrive at the relations

$$\begin{aligned} \phi^+ \left(\frac{L}{2} \right) &= e^{iqL/2} \phi^+ (0), & \phi^+ \left(-\frac{L}{2} \right) &= e^{-iqL/2} \phi^+ (0), \\ \phi^- \left(\frac{L}{2} \right) &= e^{-iqL/2} \phi^- (0), & \phi^- \left(-\frac{L}{2} \right) &= e^{iqL/2} \phi^- (0). \end{aligned} \quad (126)$$

Using these in (125), we arrive at

$$\Delta(\omega) = \left(e^{iqL} \tilde{T}_{11} - e^{-iqL} \tilde{T}_{22} \right) \phi^+(0)\phi^-(0) - \phi^+(0)^2 \tilde{T}_{12} + \phi^-(0)^2 \tilde{T}_{21} = 0, \quad (127)$$

where $q = q(\omega)$ is assumed to be inserted. The solutions ω_n of this equation are the (discrete) eigenfrequencies of the lattice with impurity within the box. In this case, the index n accompanies both, the number of the band and the quasi momentum inside each band.

We insert these frequencies ω_n into the vacuum energy (98) and transform the sum into a contour integral

$$E_0 = \frac{1}{2} \int_{\gamma} \frac{d\omega}{2\pi i} \omega^{1-2s} \partial_{\omega} \ln \Delta(\omega), \quad (128)$$

where the path γ encircles the solutions of (127) which are all assumed to be on the positive real axis. Now we perform the Wick rotation, $\omega \rightarrow i\xi$ on the upper half of the integration path γ and $\omega \rightarrow -i\xi$ on the lower part. We arrive at

$$E_0 = -\frac{\cos(\pi s)}{2\pi} \int_0^{\infty} d\xi \xi^{1-2s} \partial_{\xi} \ln \Delta(i\xi). \quad (129)$$

Now we perform the limit $L \rightarrow \infty$. We mention that $q(i\xi) \equiv i\eta(\xi)$ defines a function obeying $\eta(\xi) > 1$. It is a generalization of η used in the preceding subsection. With this property, for $L \rightarrow \infty$, we get

$$\Delta(i\xi) = \eta(\xi)L + \ln \tilde{T}_{22}(i\xi) + \ln (\phi^+(0)\phi^-(0)) + \dots \quad (130)$$

The dots denote terms vanishing for $L \rightarrow \infty$. Now, the first term gives the contribution from the comb without impurity; it coincides with (117). The second term is the contribution from the impurity,

$$E_0^{\text{imp.}} = -\frac{\cos(\pi s)}{2\pi} \int_0^{\infty} d\xi \xi^{1-2s} \partial_{\xi} \ln \left(\tilde{T}_{22}(i\xi) \right). \quad (131)$$

The third term gives a contribution that does not depend on the position of the impurity and we do not consider it.

Finally, we deal with the ultraviolet divergence. It is the same as for an impurity without background, i.e., for a simple delta function. In that case, the corresponding entry of the matrix \tilde{T} reads

$$\tilde{T}_{22}^{(0)} = \left(1 + \frac{\tilde{\alpha}}{2\xi} \right). \quad (132)$$

We perform the same subtraction as before and get

$$E_0^{\text{imp., ren.}} = -\frac{1}{2\pi} \int_0^\infty d\xi \xi \partial_\xi \ln \left(\frac{\tilde{T}_{22}(i\xi)}{\tilde{T}_{22}^{(0)}(i\xi)} \right) \quad (133)$$

for the renormalized vacuum energy. The integration in (133) converges and we have put $s = 0$.

This representation can be further simplified by partial integration and it allows for easy numerical evaluation. Examples are shown in figure 9. The interpretation of this vacuum energy is that it results in a force acting on the impurity relative to the lattice.

7. Conclusions

In the foregoing sections, we considered a scalar field in a periodic background without and with impurities. Although the corresponding formulas are, in general, not new, we think to have a more concise representation. Anyway, these formulas are needed for the subsequent section. Also, these formulas allow for easy generalization. For instance, for the transfer matrix T , (12), more general expressions can be taken in place of (12). Most generally, it can be composed of a general Sturm–Liouville problem inside a cell.

For the lattice and the impurities formulas were derived which are by no means surprising. However, the bound state levels for two impurities show unexpected behavior. For no background, i.e., for small coupling α of the background, one has a well-known picture. At small separation between the impurities, one has two distinct energy levels. For larger separation, with decreasing overlap of the corresponding wave functions, these levels become equal, matching the level of one impurity in the limit of infinite separation. However, with finite coupling α of the background, there remains a finite correlation between the levels. In figure 6 we kept the location of one impurity and moved the other away (with growing L). It is seen that both levels remain oscillating and do not become equal. This way, a kind of long-range correlation is seen. We investigated also the question whether these two levels may become equal in some points as the graphics suggest. In these points the difference between the two levels is of an order of $10^{-3} \dots 10^{-5}$ of its absolute value, but not zero. This statement is the result of a careful numerical investigation with appropriate numerical precision. At the moment we do not have an explanation for this effect.

Further, in this paper, we investigated the vacuum energy of a generalized comb without and with impurity. We demonstrated two possibilities to represent the vacuum energy starting from a mode sum over discrete frequencies. To get these, we used a ‘large box’, which subsequently was stretched to infinity. The first one is in terms of the discrete frequencies $\omega_{i,n}$, where n numbers the bands and q_i , (109), will become the quasi momentum. As a result, one arrives at a representation of the vacuum energy as a double sum. One of these, n , is transformed into a contour integral, the other becomes in the limit the integration over the quasi momentum. The latter can be carried out explicitly. One arrives finally at a very simple formula, equation (118). The other possibility is to transfer the sum over all discrete eigenfrequencies into a contour integral, equation (128). This representation allows for easy separation of the contribution from the impurity alone to the vacuum energy. This part of the vacuum energy depends on the position of the impurity and results in a force acting between impurity and lattice. An example is shown in figure 9. For the chosen parameters, the impurity is pushed into the middle between the neighboring delta function potentials, or towards the right end in case of generalized delta function potentials ($\beta \neq 0$).

There is a number of interesting possible generalization of the present work. First of all, the long-range correlation between the bound state levels of two impurities calls for a better understanding. Second, the above formulas allow for an easy generalization to finite temperature, for calculation of free energy and entropy, following the lines of [15]. Another extension could be the investigation of finite size effects using formulas like (65) and (66).

Acknowledgments

It is a pleasure to thank Sergey Leble for stimulating and interesting discussions. Open access funding provided by the University Library Leipzig as part of its license fee.

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