Two- and three-dimensional Kronig-Penney model with δ-function-potential wells of zero binding energy

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An example of the Kronig-Penney model in the form of 1D (linear chain), 2D (square), and 3D (cubic) periodic lattices of 3D (three-dimensional) δ-function-potential wells is considered. For the states of negative energy the Bloch functions can be represented in an exact form and the dispersion law $E(\mathbf{k})$ can be obtained either analytically (for the 1D case) or from a numerical solution of the transcendental equation (for the 2D and 3D cases). A peculiar simplification is possible when the participating δ-function potentials have zero strength (i.e., when a single δ-function-potential well has just lost its only bound state). In this case the position of the lowest Bloch state depends only on the lattice constant d as $E_0 \sim d^{-2}$ while the effective mass does not depend on d at all and has the universal value of 1.161 69..., 1.184 75..., and 1.184 25... for the 1D, 2D, and 3D cases, respectively. For the 3D case, m^* is greater by 1.9% than m^*(1D), but at the same time m^*(3D) is *smaller* than m^*(2D) by only 0.04%.

I. INTRODUCTION

Since the one-dimensional (1D) Kronig-Penney model was first introduced in 1931,[1] a tremendous number of papers have been published on various 1D models for band structure, electron dynamics, localization phenomena, and other aspects. In many cases 1D models provide an exact solution—a fact which significantly increases their heuristic value (see, e.g., Refs. 2–4, and references therein).

In contrast, there are relatively few papers in which the exactly solvable models are extended to the three-dimensional (3D) case. An attempt to generalize the traditional 1D Kronig-Penney model to a 3D lattice has been made by Maleev[5] on the basis of the earlier paper by Goldberger and Seitz.[6] The model used in Ref. 5 is a cubic lattice of δ-function-potential wells which, in principle, provides a transcendental equation for the dispersion law. From this equation one can further calculate the exact value of the effective mass m^*. However, in Ref. 5 Maleev does not provide any explicit calculations of the position of the lowest band or of m^*. It is the purpose of this paper to perform such a calculation for the specially simplified version of the 3D cubic lattice when the δ-function potentials have zero strength. As we will see, the position of the lowest band level (E_0) depends only on the lattice constant d ($E_0 \sim -d^{-2}$), while the effective mass does not depend on d at all and has a "universal" value: $m^* = 1.184 m_0$. Comparisons with similar results for the 1D and 2D cases will also be given.

To avoid possible ambiguity, we have to note that our use of the term "δ potential" is equivalent to "zero-range potential" or "point interaction." This means that the interaction of an electron with a scatterer is locally pointwise in three-dimensional space in the sense defined by Eq. (4) below.

II. POLYCENTER PROBLEM FOR 3D δ-FUNCTION-POTENTIAL WELLS

The model of the δ-function well potential could be considered as a limiting version of the Hulthén potential model[7] when the actual radius of the force action tends to zero. To accomplish this transition one has to send both parameters a and b of the Hulthén potential

$$V(r) = -b/[\exp(ar) - 1]$$

to infinity in such a way that the ratio $b/a^2 \to \frac{1}{2}$. This procedure is fully explained in Ref. 7. The ground-state wave function of the particle in the field of a single δ potential has the form

$$\psi(\mathbf{r}) = \left[\frac{\gamma}{2\pi}\right]^{1/2} \frac{\exp(-\gamma r)}{r}, \tag{1}$$

where γ is usually called the "strength" or the "effective depth" of the δ-potential well. Therefore, for the case of a single δ-potential well the model has only one parameter γ and the ground state of the particle has an energy $E_0 = -\gamma^2/2$ (in atomic units). There are no excited bound states for the particle in the field of a *single* δ-potential well and, therefore, the next energy level (unbound) corresponds to the ionization limit $E \to 0$.

In the field of several origins (or reference points) of the δ potentials, the wave function has the form:[8–10]

$$\psi(\mathbf{r}) = \sum_{p=1}^{N} A_p \frac{\exp(-\alpha |\mathbf{r} - \mathbf{R}_p|)}{|\mathbf{r} - \mathbf{R}_p|}, \tag{2}$$

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where $\mathbf{R}_p$ $(p=1,2,\ldots,N)$ are the radius vectors of δ-potential wells.

We assume here that all δ potentials are attractive force centers, i.e., all $\gamma_p>0$. To determine the possible values of the parameter α and, correspondingly, the energy levels

$$E=-\alpha^2/2\ , \tag{3}$$

one has to apply the boundary condition to the wave function at each origin of the δ potentials[8,9]

$$\psi(\mathbf{r})\,|_{\mathbf{r}-\mathbf{R}_p}\sim A\left[\frac{1}{|\mathbf{r}-\mathbf{R}_p|}-\gamma_p\right]\ . \tag{4}$$

The set of Eqs. (4) written for each participating δ-potential well is equivalent to the Schrödinger equation (the particle is "free" everywhere, except for the points where it interacts with δ potentials).

The set of Eqs. (4) leads to the transcendental secular equation for α:

$$\det||(\gamma_p-\alpha)\delta_{pq}+(1-\delta_{pq})\exp(-\alpha\,|\,\mathbf{R}_p-\mathbf{R}_q\,|\,)/|\,\mathbf{R}_p-\mathbf{R}_q\,|\,||=0\ , \tag{5}$$

which generally gives N different discrete energy levels.

III. PARTICLE IN A PERIODIC LATTICE OF DELTA POTENTIALS

Consider now an infinite linear chain of periodically arranged δ-potential wells with the same strength γ.[8-10] It should be stressed that this is *not* a one-dimensional model in the traditional sense, since we have here an array of 3D δ potentials in a 3D space, although these potentials are placed along a straight line. Similarly, we can consider a 2D or 3D lattice, and in the general case the coefficients A_p in Eq. (2) can be written in a Bloch form

$$A_p=A\exp(i\mathbf{k}\cdot\mathbf{R}_p)\ , \tag{6}$$

where $\mathbf{k}=(k_x,k_y,k_z)$ is the quasimomentum and $|\,k_{x,y,z}\,|\le d/\pi$ (d is the lattice spacing). The wave function of the particle now has the form

$$\psi_{\mathbf{k}}(\mathbf{r})=A\sum_p\exp(i\mathbf{k}\cdot\mathbf{R}_p)\frac{\exp(-\alpha\,|\,\mathbf{r}-\mathbf{R}_p\,|\,)}{|\,\mathbf{r}-\mathbf{R}_p\,|}\ . \tag{7}$$

Using the translational invariance of the lattice, one can easily verify that this function is representable in the form

$$\psi_{\mathbf{k}}(\mathbf{r})=U_{\mathbf{k}}(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r}),\quad U_{\mathbf{k}}(\mathbf{r}+\mathbf{a})=U_{\mathbf{k}}(\mathbf{r})\ , \tag{8}$$

which is the definition of the Bloch function ($\mathbf{a}$ is any integer translation).

Since all γ's are the same (all $\gamma_p=\gamma$), the application of the boundary condition (4) at any site $\mathbf{R}_0$ leads to the same transcendental equation, namely

$$\alpha-\gamma=\sum_p{}'\exp(i\mathbf{k}\cdot\mathbf{R}_p)\frac{\exp(-\alpha\,|\,\mathbf{R}_p-\mathbf{R}_0\,|\,)}{|\,\mathbf{R}_p-\mathbf{R}_0\,|}\ , \tag{9}$$

where the prime indicates the omission of the term $p=0$ from the summation.

For the 1D case the sum in Eq. (9) can be calculated analytically, and the above equation takes the form[8-10]

$$\cosh(\alpha d)=\cos(kd)+\tfrac{1}{2}\exp(\gamma d)\ . \tag{10}$$

By solving this equation one can obtain the dispersion law $E=E(\mathbf{k})$, i.e., the energy of the particle $E=-\alpha^2/2$ as a function of $\mathbf{k}$ (for a given value of γ). For the 2D and 3D cases Eq. (9) has to be solved numerically.

IV. BAND EDGE AND THE EFFECTIVE MASS OF AN ELECTRON IN THE MODEL OF ZERO-STRENGTH δ POTENTIALS

The approximation of zero strength δ potentials (ZSDP) assumes that all γ's have arbitrarily small (but still *positive*) values, i.e., $\gamma\to 0+$. For the case of just two potential wells the model of ZSDP leads to a nontrivial result[7,11] that the energy E_0 of the ground state of the particle at a fixed separation d between wells is finite, despite the apparent "disappearance" of the force centers in the limit $\gamma\to 0+$. Moreover, $E_0=-\text{const}/d^2$ which implies that $E_0\to-\infty$ if $d\to 0$. Again, as above, we note that our term "ZSDP" is equivalent to "zero-range potential of zero strength" or "point interaction of zero strength."

For $\gamma=0$, Eq. (9) takes the form (for the 3D case)

$$\beta=\sum_{n_x,n_y,n_z}{}'\exp[-i(k_xn_x+k_yn_y+k_zn_z)d]\times\frac{\exp[-\beta(n_x^2+n_y^2+n_z^2)^{1/2}]}{(n_x^2+n_y^2+n_z^2)^{1/2}}\ , \tag{11}$$

where we introduced the variable $\beta=\alpha d$. In Eq. (11) the summation over the integers n_x, n_y, and n_z extends from $-\infty$ to $+\infty$ and the point (0,0,0) is omitted. For the 2D and 1D cases Eq. (11) simplifies in a straightforward fashion.

For the limit $\mathbf{k}\to 0$, Eq. (11) turns into a dimensionless equation for the only remaining parameter β:

$$\beta=\sum_{n_x,n_y,n_z}{}'\frac{\exp[-\beta(n_x^2+n_y^2+n_z^2)^{1/2}]}{(n_x^2+n_y^2+n_z^2)^{1/2}}\ . \tag{12}$$

As a strictly numerical equation, Eq. (12) has an "absolute" (dependent only on the geometry of the lattice) root, namely $\beta_0=0.9624$, 1.5120, and 1.9458 for 1D, 2D, and 3D cases, respectively. Note, that while for 2D and 3D cases β_0 was obtained numerically, for the 1D case we, in fact, have an exact expression, namely $\beta_0=\ln[(3+\sqrt{5})/2]=0.962\,423\,65\ldots$.

Therefore, the position of the bottom of the conduction band has (similarly to the above-mentioned E_0 for just two ZSDP's) the "universal" dependence on the lattice period d; $E_0=-\beta_0^2/2d^2$. In atomic units of energy

$$E_d^{1D}=\frac{-0.463\,13}{d^2}\ ,$$
$$E_0^{2D}=\frac{-1.143\,01}{d^2}\ , \tag{13}$$
$$E_0^{3D}=\frac{-1.893\,01}{d^2}\ .$$

Assuming that close to the bottom of the conduction band (1) the dispersion law is isotropic, and (2) it is possible to use the parabolic approximation, one can obtain

$$E(\mathbf{k})=-\frac{\hbar^2\alpha^2(k)}{2m_0}\simeq E_0+\frac{\hbar^2k^2}{2m^*}\ , \tag{14}$$

where $\alpha(\mathbf{k})$ can be obtained from the solution of Eq. (11). Note that the isotropy of the dispersion law to the terms of second order can be easily verified by the direct differentiation of Eq. (11)—because of the terms n_xn_y, etc. all cross derivatives $\partial^2\alpha/\partial k_i\partial k_j$ (we use Cartesian coordinates) are zeros at $\mathbf{k}\to 0$ and the second derivative matrix turns out to be a multiple of the identity matrix. The anisotropy appears in the fourth-order terms of the Taylor series, which, however, are immaterial for the purpose of defining the effective mass.

The effective mass m^* in terms of the free-electron mass m_0 can now be expressed as

$$m^*/m_0=-\left[\alpha\left[\frac{\partial^2\alpha}{\partial k^2}\right]_{k\to 0}\right]^{-1}\ . \tag{15}$$

Using Eq. (11), one can turn Eq. (15) into the following form (for the 3D case):

$$\frac{m^*}{m_0}=\frac{3}{\beta_0}\frac{1+\sum'_{n_x,n_y,n_z}\exp[-\beta_0(n_x^2+n_y^2+n_z^2)^{1/2}]}{\sum'_{n_x,n_y,n_z}(n_x^2+n_y^2+n_z^2)^{1/2}\exp[-\beta_0(n_x^2+n_y^2+n_z^2)^{1/2}]}\ , \tag{16}$$

where β_0 is the root of Eq. (12). For the 2D and 1D cases the factor "3" in Eq. (16) should be replaced by "2" or "1," respectively.

In atomic units ($m_0=1$) the numerical values are

$$m^*(1D)=1.161\,69\ ,$$
$$m^*(2D)=1.184\,75\ ,$$
$$m^*(3D)=1.184\,25\ .$$

Again, for the 1D case the summation in Eq. (16) can be performed in closed form, which gives for m^*/m_0 the exact expression

$$m^*/m_0=\sqrt{5}/\ln[(7+3\sqrt{5})/2]=1.161\,685\,9\ldots\ .$$

V. CONCLUDING REMARKS

An attractive feature of the Kronig-Penney–ZSDP model is that it eliminates all characteristic parameters except for the lattice spacing d. This makes this model a kind of "absolute standard" for more elaborate multiparameter calculations.

The position of the bottom of the conduction band (E_0) in this model depends universally on the lattice constant d as $E_0=-C/d^2$. At the same time, the effective mass does not depend on d at all and, therefore, has universal values, which are close, but not equal, to unity. The peculiar fact is that while $m^*(3D)$ is *greater* than $m^*(1D)$ by 1.9%, $m^*(3D)$ is *smaller* than $m^*(2D)$ by just 0.04%.

A similar consideration can be performed for the ZSDP lattices with symmetries other than cubic, e.g., diamond lattice, etc.

The model of ZSDP described in the present paper can be applied, for example, for an estimate of the isotopic shift of the bottom of the conduction band. Isotopically pure crystals of the same element have slightly different lattice constants[12] which, according to the present model, can be straightforwardly related [through the Eqs. (13)] with the position of the lowest electronic state.

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