The energy spectrum of a one-dimensional periodic system with a model random potential

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On the basis of an exactly soluble model of a random field, a formula is obtained for the density of states averaged over the random amplitudes. The possibility of the appearance of singularities in the density of states at the band-edges of an ideal one-dimensional periodic system is analyzed, and the reasons for their appearance are elucidated. A slightly modified model in which these singularities disappear is proposed. The question of the degree of localization of the states is also considered.

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The solution of the model problem of a one-dimensional chain of equally-spaced centers with δ-function potentials with random amplitudes gives an exact and also somewhat unusual result[1,2] (see also the three-dimensional generalization[3]). The possibility of an exact solution of the problem for arbitrary values of the random-scatter parameter is highly attractive, but the appearance of singularities in the density of states at the upper edges of the allowed bands[1] and the peculiar behavior of the degree of localization in the same parts of the spectrum[2], which differs sharply from the behavior in the disordered model of a liquid[4], require a detailed investigation with the purpose of elucidating the reasons for the appearance of these singularities. It is extremely important to clarify how sensitive these results are to variation of the model.

The latter should be emphasized once more, since a model problem can sometimes give not only quantitative but also qualitative results that are specific to just this model. Inasmuch as the one-dimensional formulation of the problem can acquire real physical meaning, e.g., in multi-layer structures (superlattices), it is natural to carry over the results of[1,2] to the case of such systems. In the effective-mass approximation these results can be used immediately, with the trivial replacement of the true electron mass by the effective mass. Then the theoretical possibility of observing effects associated with the singularities in the density of states would arise, if such singularities exist at all in a real random field. On the other hand, the use of the effective-mass approximation is not so necessary–in a model superlattice it is possible to take exact account of the arbitrary one-dimensional periodic field of the lattice[5]. Moreover, starting from[1,5,6], it turns out to be possible to obtain a general solution of the problem of the energy spectrum of an arbitrary one-dimensional periodic system with a model random field. At the same time, we shall elucidate the reasons for the appearance of the singularities and show that in a somewhat improved model the indicated singularities disappear.

1. PERIODIC SYSTEM WITH A RANDOM POTENTIAL

We shall consider a one-dimensional system possessing translational invariance (a one-dimensional perfect lattice), and impose on it an additional random field

$$U(x)=\sum_n U_n\delta(x-x_0-na). \tag{1}$$

Here the U_n are random quantities with the probability density used in[1,2], a is the lattice constant of the one-dimensional lattice, n = 0, ± 1, ± 2, ..., and, without limiting the generality, we can assume that $0\le x_0\le a/2$.

We shall take the arbitrary periodic field of the one-dimensional lattice into account exactly in terms of the Green function in this field[6], which possesses the well-known property:

$$G(x+na,\ x'+na)=G(x,\ x'). \tag{2}$$

The solution of the problem with the random field (1) is carried out in the same way as in[1]. We remark only that the averaging over the random amplitudes does not depend on the presence of the periodic field. The subsequent solution of the problem is analogous to that carried through in[5], except that the amplitude of the δ-function potentials becomes complex. The final dispersion equation takes the form (compare with[1,5])

$$\cos ka=\cos\beta a-\gamma_1 G(x_0,\ x_0)\sin\beta a. \tag{3}$$

Here β is the quasi-wavenumber of an electron in the perfect lattice, γ_1 is the parameter determining the random scatter, and k is the "quasi-wavenumber" in the presence of the random field and is complex here; the mean value of the random amplitude is included in the periodic field. The Green function $G(x_0, x_0)$ of the perfect lattice depends on β and α ($\alpha = (2mE)^{1/2}$, $\hbar = 1$), and the dependence of β on the energy E is given by the dispersion law of the perfect lattice.

The formula (3) is valid in the case when the energy runs over values in the allowed bands of the perfect lattice. Within the forbidden bands the spectrum is determined from an equation obtainable by analytic continuation ($\beta = i\gamma$, $\gamma > 0$) of Eq. (3):

$$\cos ka=\operatorname{ch}\gamma a-i\gamma_1 G(x_0,\ x_0)\operatorname{sh}\gamma a. \tag{4}$$

The averaged density of states in the case of (3) takes the form

$$\bar\rho(E)=\frac{1}{\pi a}\operatorname{Re}\left\{\frac{\partial}{\partial E}\sqrt{1-[\cos\beta a-\gamma_1 G(x_0,x_0)\sin\beta a]^2}\right.$$
$$\left.\times[\cos\beta a-\gamma_1 G(x_0,x_0)\sin\beta a]^{-1}\right\}, \tag{5}$$

and analytic continuation of this formula gives the form of the density of states in the forbidden bands.

Before going over to the general case of an arbitrary ideal periodic potential, it is sensible to consider the particular model case when the potential is given in the form of the simple Kronig-Penney model, with the known expression for the Green function[6]:

$$G_r(x_0,x_0)=\frac{i}{2\alpha}\frac{|\sin\alpha a|}{\sin\beta a}\left[1+\frac{2P\sin\alpha x_0\sin\alpha(a-x_0)}{\alpha a\sin\alpha a}\right]$$
$$\cos\beta a=\cos\alpha a+(\alpha a)^{-1}P\sin\alpha a. \tag{6}$$

For $x_0 = 0$ the Green function (6) vanishes at the upper edges of the allowed bands ($\alpha a = \pi n$), and precisely this case was considered in[1]. If we put $x_0 = a/2$, it is not difficult to see that the expression (6) vanishes at the lower edges of the even-labeled allowed bands. The density of states (5) has exactly the same singularities at these points. In this case, the density of states no longer possesses singularities at the upper edges of the allowed bands. For intermediate values of $x_0 (0 < x_0 < a/2)$, the Green function (6) can vanish only within the forbidden bands, and thus the density of states (5) has no singularities anywhere. Proceeding from what has been said, it may be stated that the appearance of singularities in the density of states in the given model of a random field is caused by fortuitous circumstances: the vanishing of the Green function at the band-edges. If we go over to a more realistic model of the random field, or slightly smear out the δ-functions, these singularities disappear.

It is not difficult to understand the reason for the appearance of the singularities. In fact, the appearance of a finite density of states in the forbidden band is a consequence of the finite probability of the appearance of discrete levels. Inasmuch as the amplitudes of the δ-function potentials are random and independent in the model under consideration, the levels corresponding to them are random, but, nevertheless, interdependent. The interdependence of the levels here arises because of the overlap of the wavefunctions of the local states. In the case of one δ-function disturbing potential, the energy level in the forbidden band is determined by the well-known equation

$$1+U_n G(x_0, x_0)=0. \tag{7}$$

In the particular case $x_0 = 0$ the Green function $G(x_0, x_0)$ given by the expression (6) vanishes at the upper edges of the allowed bands and is positive in the forbidden bands. Then levels corresponding to positive values of U_n are not in a forbidden band (more precisely, these levels are pressed toward the lower edge of a forbidden band), and only levels that are split off from the upper allowed band correspond to negative U_n. Because of this, the density of states (5) has singularities at such points.

Going over to the general case of an arbitrary periodic field, we represent the Green function in this field in the form ($\epsilon \to +0$)

$$G_r(x_0, x_0)=-\sum_{l,\beta}\frac{|\psi_{l,\beta}(x_0)|^2}{E-E_l(\beta)+i\varepsilon}, \tag{8}$$

where $E_l(\beta)$ is the dispersion law, depending on the quasi-wavenumber β and the band index l; $\psi_{1,\beta}(x_0)$ are the Bloch wavefunctions.

In the region of the forbidden bands the Green function (8) is real and, as is not difficult to see, monotonically increasing in each of them. Inside each forbidden band, with the sole exception of the first low-lying one, it changes sign; consequently, at a certain energy value the function (8) vanishes. The positions of the zeros of the Green function in the forbidden bands undoubtedly depend on the specific periodic field. In particular, there may be fortuitous cases in which these zeros coincide with the edges of the forbidden bands. The Green function (6) has precisely such nontypical behavior.

In the region of the allowed bands the Green function (8) has the imaginary part

$$\operatorname{Im} G(x_0, x_0)=\pi a\rho_l(E)\,|\psi_{l,\beta}(x_0)|^2,$$

where $\rho_l(E)$ is the one-dimensional density of states of the ideal system.

Since the zone boundaries are determined by the condition $\sin \beta a = 0$, and the density of states $\rho_l(E)$ has singularities at these boundaries, the expression

$$\Delta=\gamma_1 \operatorname{Im} G(x_0, x_0)\sin \beta a\equiv-\gamma_1|\psi_{l,\beta}(x_0)|^2\frac{\partial}{\partial E}\cos \beta a, \tag{9}$$

remains finite, generally speaking, More precisely, at the actual band-edges we have the asymptotic form ($n' = 0, 1$)

$$\Delta=m^*\gamma_1 a^2|\psi_{l,\pi n'/a}(x_0)|^2, \tag{10}$$

where m^* is the effective electron mass near the edge of the corresponding band.

Next, starting from formula (5), we see that the averaged density of states can have singularities only at the band-edges, provided that the expression (10) vanishes. At other points of the spectrum there are no singularities at all, even in the case when the expression (9) vanishes for $\beta a \neq \pi n$. The above has a clear physical interpretation. The vanishing of the modulus squared of the wavefunction, or of the probability of finding a particle, at a certain point at which a δ-function potential is localized leads to the result that this potential cannot be observed. Because of this, the corresponding points in the spectrum do not undergo any changes, and, in particular, the singularities in the density of states at the band-edges can remain. In our somewhat generalized model these singularities are completely absent, if we disregard fortuitous cases. In fact, near the band-edges the effective-mass approximation is usually valid, so that the Bloch wavefunctions can be replaced by plane waves. Then we have, simply, $\Delta = \gamma_1 m^* a$, and the density of states (5) does not depend on the parameter x_0. The latter fact is also clear physically. Near the band edges the electron wavelength is considerably greater than the lattice constant, so that the precise point, within the limits of the lattice constant, at which the potential is localized plays practically no role.

Thus, the formula (5) obtained for the averaged density of states gives the general solution of the problem of an arbitrary one-dimensional periodic system with a model random field of the form considered. It is important to stress that no restrictions are imposed on the random-scatter parameter γ_1, and this gives us the possibility of treating systems with large deviations from ideality.

The general formula (5) can also be applied in the case of a superlattice with a random field. Here a knowledge of the corresponding Green function is required. In the case of a model superlattice this is known (cf.[5]), and the model problem of a superlattice with a random field can thereby be solved completely. Here the arguments put forward above, concerning the averaged density of states, remain valid, except that the term "band" must be replaced by the customary name "miniband".

2. LOCALIZED CHARACTER OF THE STATES

The idea exists that in one-dimensional disordered systems all states are localized (cf.[7]). This question has become the subject of frequent studies, including some on exactly soluble models. The localized character of the states has been proved for a number of models (cf.[2, 7, 8]), but the universality of this idea cannot be

regarded as finally settled for all states (cf.[2, 9]). In the model under consideration this question is discussed in[2], where, alongside localized states, there are also nonlocalized states. It is precisely to the latter states that the singularities in the density of states correspond. However, as we saw in Sec. 1, the appearance of the singularities is due to fortuitous causes, and, therefore, the peculiar behavior of the degree of localization near the upper edges of the allowed bands[2] needs reconsideration. In our case an expression for the degree of localization can be obtained in the pattern of[2], but with allowance for the changes necessary for our model (see Sec. 1). As a result it turns out that the imaginary part of the complex quasi-wavenumber of (3), or more precisely, k_2a, serves as the degree of localization. For it we can easily obtain the expression

$$k_2a=\ln[\sqrt{1+z}+\sqrt{z}], \tag{11}$$

where

$$2z=(A^2-1+\Delta^2)+[(A^2-1+\Delta^2)^2+4\Delta^2]^{1/2},$$
$$A=\cos\beta a-\gamma_1\operatorname{Re}G(x_0,x_0)\sin\beta a.$$

The singularities in the density of states (5) arose because of the vanishing of the expression (9) for Δ. In our model, for $\gamma_1>0$, the quantity Δ is nonzero, and therefore the degree of localization k_2a is always positive and depends on the energy in a complicated way through formula (11). At the very edges of the bands it is easy to obtain the asymptotic form ($\sin\beta a=0$):

$$k_2a=\sqrt{\Delta}\ \text{ for }\ \Delta\ll1,\quad k_2a=\ln(2\Delta)\ \text{ for }\ \Delta\gg1.$$

Thus, in the model under consideration all states are found to be localized (in the sense in which this is discussed in[7]), the degree of localization being determined by the imaginary part of the complex quasi-wavenumber. Its real part determines the density of states (5), viz.,

$$\rho(E)=\frac{1}{\pi}\frac{dk_1}{dE},\quad k_1a=\arcsin\sqrt{y},$$
$$2y=1-A^2-\Delta^2+[(1-A^2-\Delta^2)^2+4\Delta^2]^{1/2}.$$

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