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Energy bands and forbidden gaps in the Kronig-Penney model

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The conventional form of the energy–crystal-momentum relations for the Kronig-Penney model is rewritten in a form amenable to qualitative analysis. The results of a complete analysis are summarized.

I. INTRODUCTION

The Kronig-Penney model[1] is an exactly soluble system which serves to illustrate many of the concepts basic to the quantum theory of periodic systems. It continues to be used by researchers, often as a starting point in studies of the effects of impurities, electric fields, or other complicating features on otherwise periodic systems[2] or to evaluate approximate calculation methods[3] with a system for which exact results are readily found.

Its mathematical tractability makes it an attractive instrument for learning about quantum particles in periodic systems and serves this purpose in numerous textbooks.[4] However, the energy–crystal-momentum relationship given in the textbooks may be characterized as qualitatively intractable. One may easily compute the dispersion curves, but only the most rudimentary features of the band structure may be discerned by qualitatively examining the energy–crystal-momentum relationship. This detracts from the effectiveness of the Kronig-Penney model as a teaching and research tool.

This paper shows that the energy–crystal-momentum relationship for the Kronig-Penney model can be expressed in a form which is amenable to a detailed qualitative analysis. The Kronig-Penney model is reviewed in Sec II. The resulting energy–crystal-momentum relationships are intimately tied to the symmetry of the wave function. The analysis is sketched in Sec. III and a summary of a complete analysis is provided in Sec. IV.

II. REVIEW OF THE KRONIG-PENNEY MODEL

The Kronig-Penney model is the nonrelativistic Schrödinger equation

$$H\psi=[p^2/2m+V(x)]\psi=E\psi \ , \tag{1}$$

where the potential consists of periodically repeated square wells,

$$V(x)=-\sum_n V_0\theta(a-|x-nL|), \quad \pm n=0,1,2,\ldots \ . \tag{2}$$

The depth of the well is measured by the positive, real number V_0. The θ functions [$\theta(x)=1$ if $x>0$ and $\theta(x)=0$ otherwise] assure that each potential well has a width $2a$ and that $V(x)=0$ outside the wells. The repeat distance or lattice constant is $L=2(a+b)$.

The Kronig-Penney Hamiltonian H is invariant to translations by a lattice vector, nL [$H(x-nL)=H(x)$] to inversion [$H(x)=H(-x)$], and to time-reversal K [$KH(x)=H(x)^*K=H(x)K$]. It is advantageous to utilize these symmetries in solving the problem.

Solutions in the "wells" are plane waves, $\exp(iKx)$ with

$$(\hbar K)^2/2m=E+V_0 \ . \tag{3}$$

In the complementary regions the plane-wave solutions, $\exp(ikx)$, have

$$(\hbar k)^2/2m=E \ . \tag{4}$$

Symmetric solutions in the symmetric zone, $-L/2\leq x\leq L/2$, are

$$\phi_+(x)=\cos(Kx)\theta(a-|x|)+G(x)\theta(x-a)\theta(\tfrac{1}{2}L-x)+G(-x)\theta(-a-x)\theta(\tfrac{1}{2}L+x) \tag{5a}$$

with

$$G(x)=\cos(Ka)\cos[k(x-a)]-K\sin(Ka)\sin[k(x-a)]/k \tag{5b}$$

and

$$\phi_-(x)=[\sin(Kx)/K]\theta(a-|x|)+U(x)\theta(x-a)\theta(\tfrac{1}{2}L-x)-U(-x)\theta(-a-x)\theta(\tfrac{1}{2}L+x) \tag{6a}$$

with

$$U(x)=\cos[k(x-a)]\sin(Ka)/K+\cos(Ka)\sin[k(x-a)]/k \ . \tag{6b}$$

The solutions have been written to make their inversion symmetry

$$\phi_+(-x)=\phi_+(x), \quad \phi_-(-x)=-\phi_-(x) \tag{7}$$

manifestly evident. These functions are real for negative energies when k is and K may be imaginary. Also, they are well-defined solutions in a limiting sense when k or K approaches zero.

A general solution in a symmetric zone is

$$\phi(x)=A_+\phi_+(x)+iA_-\phi_-(x) \ . \tag{8}$$

For real constants A_+, A_- $\phi(x)$ is invariant to time-reversal coupled with inversion, $\phi(-x)^*=\phi(x)$. A solution of the Kronig-Penney model is expressed as a Bloch function,

$$\psi_q(x)=\sum_n \exp(-inqL)\phi(x-nL) \tag{9}$$

with the translational symmetry, $\psi_q(x-L)=\exp(iqL)\times\psi_q(x)$. The parameter q is called the crystal momentum.

Equation (9) is a solution everywhere except for the points, $(n+\frac{1}{2})L$, at the end points of the symmetric zones. Requiring continuity of function and derivative at the end points gives the Kronig-Penney energy–crystal-momentum relationship,

$$\tan^2(qL/2) = \frac{-G'(L/2)\,U(L/2)}{G(L/2)\,U'(L/2)} \quad . \tag{10}$$

Equation (10) may be shown to be identical to the conventional dispersion relations for the Kronig-Penney model.[4]

The factored form of Eq. (10) proves to be invaluable for qualitative analysis. One may easily verify the relation (the Wronskian),

$$GU' - G'U = 1 \quad . \tag{11}$$

Hence, alternatives to Eq. (10) are

$$\sin^2(qL/2) = -G'U, \quad \cos^2(qL/2) = GU' \quad . \tag{12}$$

Analysis shows that only when $\sin(qL/2)$ or $\cos(qL/2)$ is zero will the wave functions be of definite inversion symmetry. This symmetry can be discerned directly from the energy–crystal-momentum relationship by observing which factor is zero. When a factor G or G' is zero, the wave function is invariant with respect to inversion. If U or U' is zero the wave function is of odd parity. The nomenclature for the factors is intended to be a mnemonic aid in that factors G refer to the German word *gerade* (or even) and U refers to *ungerade* (or odd). It is also possible for $G' = U = 0$ or $G = U' = 0$. In such cases both even and odd parity wave functions exist simultaneously and an "accidental degeneracy" occurs.[5]

III. QUALITATIVE ANALYSIS OF THE KRONIG-PENNEY BAND STRUCTURE

Several observations follow immediately from Eq. (10). Distinct real-valued crystal momenta may be chosen in a Brillouin zone,

$$-\pi/L < q \leq \pi/L \quad .$$

With this choice of Brillouin zone (BZ) the allowed energies are symmetric about the BZ center, $q = 0$, since $\tan^2(qL/2)$ is an even function of q. Regions of unphysical energies or forbidden energy gaps can begin only at the BZ center $(q = 0)$ or at the BZ edge, $q = \pi/L$, because the right member of Eq. (10) is a continuous function of energy, E. Also, no physical solutions of Eq. (10) exist when the energy $E < -V_0$, since the right member of Eq. (10) is negative definite. It should be noted that the same observations can also be inferred from the conventional energy–crystal-momentum relationship.[4] However, much more qualtiative information is obtained from an analysis of Eq. (10) than from the conventional form.

For a more stringent analysis of Eq. (10) it is convenient to rewrite it as

$$\tan^2(qL/2) = (G_c'/G_c)\,U_c/U_c') \quad , \tag{13}$$

where the negative sign in Eq. (10) has been incorporated into G_c'

$$G_c = 1 - K\tan(Ka)\tan(kb)/k \quad , \tag{14}$$

$$G_c' = k\tan(kb) + K\tan(Ka) \quad , \tag{15}$$

$$U_c = \tan(Ka)/K + \tan(kb)/k \quad , \tag{16}$$

and

$$U_c' = 1 - k\tan(kb)\tan(Ka)/K \quad . \tag{17}$$

Each factor in Eq. (10) has simply been divided by $\cos(Ka)\cos(kb)$. The advantage of this form is that there are half as many functions to consider. The disadvantage is that tangent functions diverge. This is not a serious disadvantage because such divergences have little to do with the allowed energy-band structure. For example, when $\cos(kb) = 0$ (this can only occur for positive energies) Eq. (10) is evaluated to be

$$\tan^2(qL/2) = \cot^2(Ka) \quad . \tag{18}$$

Such a positive energy is allowed. Except for the unusual case of an accidental degeneracy it will not correspond to a BZ center or edge. Similarly, when $\cos(Ka) = 0$,

$$\tan^2(qL/2) = \cot^2(kb) \quad . \tag{19}$$

For negative energies the right member of Eq. (19) is nega-

TABLE I. Classification of Kronig-Penney energy bands for positive definite energies. The first column names the band type and the second column lists the conditions satisfied by an energy with this band type. The last two columns list the crystal momentum and parity of the lowest- and highest-band energies, respectively.

Band type	Conditions	$q_{\min}$ (parity)	$q_{\max}$ (parity)
$A+$	$\cos(kb)=0,\ \tan(Ka)>0$	$\pi/L(-)$	$0(+)$
$A-$	$\cos(kb)=0,\ \tan(Ka)<0$	$0(+)$	$\pi/L(-)$
$B+$	$\cos(Ka)=0,\ \tan(kb)>0$	$\pi/L(-)$	$0(-)$
$B-$	$\cos(Ka)=0,\ \tan(kb)<0$	$0(-)$	$\pi/L(-)$
$C+$	$\sin(kb)=0,\ \tan(Ka)>0$	$0(-)$	$\pi/L(+)$
$C-$	$\sin(kb)=0,\ \tan(Ka)<0$	$\pi/L(+)$	$0(-)$
$D+$	$\sin(Ka)=0,\ \tan(kb)>0$	$0(+)$	$\pi/L(+)$
$D-$	$\sin(Ka)=0,\ \tan(kb)<0$	$\pi/L(+)$	$0(+)$

tive and negative energies satisfying $\cos(Ka)=0$ are forbidden. Positive energies are allowed and will correspond to the BZ center or edge only in the case of an accidental degeneracy. Thus, the divergences of the tangent functions in Eq. (13) are benign and in general are not indicative of transitions between allowed and forbidden energy regions.

The allowed energy bands in the region of negative energies exhibit a qualitatively different structure than those with positive energies. All the structure in the energy bands derives from the oscillations of $\tan(Ka)$.

It is possible for a band to begin in the negative-energy region and extend into the region of positive energies. If a half oscillation of $\tan(Ka)$, $-\infty<\tan(Ka)<0$ or $0<\tan(Ka)<+\infty$, includes some negative energies, then a nondegenerate band of a negative-energy character will begin in the negative-energy region.

The positive-energy region appears to be more complicated to analyze than the negative-energy region because both $\tan(Ka)$ and $\tan(kb)$ are oscillatory. However, the band structure in the positive region is remarkably simple.

Previously, it was noted that the positive energies for which $\cos(kb)=0$ or $\cos(Ka)=0$ are in allowed energy regions and have very simple energy–crystal-momentum relations, Eqs. (18) and (19). From Eq. (10) it is seen that when $\sin(kb)=0$ with $E>0$:

$$\tan^2(qL/2)=\tan^2(Ka) \tag{20}$$

and when $\sin(Ka)=0$,

$$\tan^2(qL/2)=\tan^2(kb)\ . \tag{21}$$

The somewhat surprising result is that each of the bands corresponding to Eqs. (18)–(21) are distinct bands and there are no other bands. Therefore, the positive-energy bands may be classified according to which condition is satisfied. The results of an analysis of the positive-energy bands are summarized in Table I. Accidental degeneracies may occur. In such a case the two-band types involved simply coalesce into one double band.

IV. SUMMARY

The Kronig-Penney band structure is remarkably simple. In the negative-energy region the bands are all nondegenerate and occur within the intervals,

$$n\pi/2<Ka<(n+1)\pi/2,\quad n=0,1,2,\ldots\ . \tag{22}$$

The highest band may extend into the positive-energy region. The wave functions corresponding to the BZ center and edge have the same parity. In this respect negative-energy bands may be said to have a definite parity. Even parity bands have their lowest energy at the BZ center and odd parity bands have their lowest energy at the BZ edge. The lowest-energy band has even parity. The negative-energy bands alternate parities.

Distinct bands in the positive-energy region include energies where

$$kb=m\pi/2,\quad E>0 \tag{23}$$

and

$$Ka=m\pi/2,\quad E>0\ , \tag{24}$$

where m is a positive integer. Accidental degeneracies occur only for energies where Eqs. (23) and (24) are simultaneously satisfied. No accidental degeneracy can occur between positive- and negative-energy bands.

No other allowed energies occur besides those in the bands described above. It is evident that the information included in this summary is a sufficient basis for writing an efficient computer program and obtaining a clear picture of the content of the Kronig-Penney model for use in simulating physical systems and classroom presentation.

[1]R. de L. Kronig and W. G. Penney, Proc. R. Soc. London, Sect. A 130, 499 (1931).

[2]Some examples include, S. Nagai and J. Kondo, J. Phys. Soc. Jpn. 49, 1255 (1980); H.-J. Unger, J. Phys. C 14, 3727 (1981); E. A. Babakharyan and Yu. V. Kononents, Phys. Status Solidi (b) 98, 59 (1980); C. Colvard, R. Merlin, and M. V. Klein, Phys. Rev. Lett. 45, (1980); M. Ya Azbel, *ibid.* 43, 1954 (1979); B. Seraphin, Z. Naturforsch. 94, 450 (1954).

[3]For example, see A. A. Bahurmuz and P. D. Lolt, Am. J. Phys. 49, 675 (1981); Grover C. Wetsel, Jr., *ibid.* 46, 714 (1978).

[4]R. B. Leighton, *Principles of Modern Physics,* 2nd ed. (Wiley, New York, 1970), p. 397; E. Merzbacher, *Quantum Mechanics,* 2nd ed. (Wiley, New York), p. 102.

[5]Shi-Tron Lin and Jan Smit [Am. J. Phys. 48, 193 (1980)] discuss conditions for obtaining zero gaps at the Brillouin-zone boundary [$\cos(qL/2)=0$] and give numerical examples in which zero gaps occur for the Kronig-Penney model and other simple-dimensional systems. Apparently, they have not considered the possibility of a zero gap at the Brillouin-zone center [$\sin(qL/2)=0$].