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Relativistic quarks in one-dimensional periodic structures

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We obtain the band condition for relativistic quarks moving in one-dimensional periodic potentials using the transfer matrix method. Using a strong electrostatic type of potential in the Dirac equation does not give confining properties, while Lorentz scalar potentials do. We give an analytic form for the wave function which results when the potential is taken to a delta function limit, and discuss the discrepancy between this result and that obtained by "solving" the Dirac equation for a delta function potential.

I. INTRODUCTION

With the widespread realization that quarks, as the constituents of nucleons, can be expected to play a role in the physics of the nucleus, a number of models have been developed which seek to define that role. Bag models either expand the bag from a nucleon bag to a nuclear bag and look for clustering effects to define nucleonic structures, or else allow 6,9,... quark bags when 2,3,... nucleon bags overlap. Potential models introduce potentials which tend to confine quarks to individual sites, but which are not completely confining and thus permit quarks to tunnel from one nucleon site to another. Soliton bag models describe hadrons as quarks moving freely in the interior of a small bag which are coupled in an essential way to pion fields in the bag exterior. Each of these classes of models is, of course, a simplified approach to a very complicated many quark problem in quantum chromodynamics whose solution is beyond our present technology. Focusing on some particular aspect of the nuclear problem can be expected to offer us some insight on that aspect, but not a great deal of insight into other features.

This paper adopts a particularly special model of the potential type—a one-dimensional periodic lattice of "nucleons." There are a number of papers which have introduced periodic one- and three-dimensional potential models, see for example, Goldman and Stephenson,[1] or crystalline structures of soliton bags, see Achtzehnter, Scheid and Wilets.[2] It is a straightforward application of the usual analysis, which depends only on the periodicity of the Hamiltonian, to show that the solutions of the Dirac equation in this case have the familiar Bloch wave form.

Our purpose in studying the simplest such one dimensional model available for relativistic quarks—the classic Kronig-Penney model adapted to the Dirac equation—is threefold.

(i) We wish to further investigate the merits of electrostatic and Lorentz scalar potential models as models of confinement, a point we recently studied in the context of a single nucleon.[3]

(ii) We wish to study and clarify the discrepancy between the results obtained by first solving for a square barrier potential and then taking the delta function limit, and those obtained by solving the Dirac equation with a delta function potential. This discrepancy has been noted, in the case of electrostatic potentials, in the solid state literature.[4]

(iii) We want to lay the basis for studying random lattices[5] and surface states[6] in one dimension before moving to three dimensional problems.

There are two basic ingredients in our calculation: the solution of the Dirac equation in the unit cell, and the connection of solutions from one cell to another which we accomplish by the transfer matrix method. Since our work builds on the classic nonrelativistic Kronig-Penney model, in Sec. II we review this model, which serves to introduce the transfer matrix method. Then in Sec. III we show how the general transfer matrix method may be adapted to the Dirac equation.

Section IV is devoted to the solution of the Dirac equation in the unit cell. We first discuss the rectangular barrier and the form the Klein paradox takes in these circumstances. Then we take the delta function limit of our result, and contrast this with the results obtained by solving the Dirac equation with a delta function potential. We also obtain the formal general solution to the Dirac equation for a general potential in which we can take the limit that the potential becomes a delta function and obtain a result which agrees with that obtained by taking the limit of the square barrier potential. Since we find that solving the Dirac equation and then taking the delta function limit gives a unique result we suggest that the direct solution of the Dirac equation with delta function potentials should be regarded as unphysical—a point to which we return in subsequent sections.

In Sec. V we combine the results of Sec. IV and the methods of Sec. III to obtain the band structure in our various models. We discuss the form exhibited by the Klein paradox in this case, and examine the paradoxical results obtained by using the δ function as a potential in

the Dirac equation.

Section VI is devoted to the computation of the energy of the one dimensional model system.

Our conclusions are collected in Sec. VII.

II. REVIEW OF THE TRANSFER MATRIX METHOD AND THE NONRELATIVISTIC KRONIG-PENNEY MODEL

Our analysis is based on the well known one dimensional model for crystals which was first formulated by Kronig and Penney.[7] This model is nonrelativistic and must be recovered when we take the nonrelativistic limit of our results. We propose to use the transfer matrix method[8] in our analysis of the relativistic case, and as this method and indeed the Kronig-Penney model itself may not be totally familiar to nuclear physicists, it is appropriate to briefly review the transfer matrix approach to the Kronig-Penney model. We follow the approach of James[9] which is suitable whatever the potential structure in the unit cell.

We begin with the Schrödinger equation for a single particle in a periodic potential

$$-\frac{1}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi(x)=E(x)\psi(x)\ , \tag{2.1}$$

where $V(x+l)=V(x)$ and we have set $\hbar=1$. It convenient to define $U(x)=2mV(x)$ and $k^2=2mE$, so that the Schrödinger equation becomes

$$\frac{d^2\psi}{dx^2}+[k^2-U(x)]\psi=0\ . \tag{2.2}$$

The nth unit cell is defined as the region $(n-1)l<x<nl$, and we take periodic boundary conditions with period $L=Nl$. N is the total number of unit cells, and the boundary conditions on ψ are

$$\psi(x)=\psi(x+L)\ . \tag{2.3}$$

In any unit cell, the solution may be written as the linear combination of independent elementary solutions ϕ_A,ϕ_B which are defined in the range $0<x<l$.

$$\psi(x)=A_n\phi_A[x-(n-1)l]+B_n\phi_B[x-(n-1)l] \quad \text{for } (n-1)l<x<nl\ . \tag{2.4}$$

The transfer matrix T relates the A_n,B_n,

$$\begin{bmatrix}A_{n+1}\\B_{n+1}\end{bmatrix}=T\begin{bmatrix}A_n\\B_n\end{bmatrix}\ , \tag{2.5}$$

and is simply computed by matching solutions and their first derivatives in the nth and $(n+1)$th cells at $x=nl$.

$$T=[W(0)]^{-1}W(l)\ , \tag{2.6}$$

where

$$W(x)=\begin{vmatrix}\phi_A(x) & \phi_B(x)\\ \phi'_A(x) & \phi'_B(x)\end{vmatrix} \tag{2.7}$$

is the Wronskian matrix of the solutions. (Although the Wronskian determinant $\det W$ is constant, the Wronskian matrix is not.)

The periodicity requirement then demands that the solution in the first and $(N+1)$th cells be identical, i.e., that

$$\begin{bmatrix}A_{N+1}\\B_{N+1}\end{bmatrix}=\begin{bmatrix}A_1\\B_1\end{bmatrix}\ . \tag{2.8}$$

But we know that

$$\begin{bmatrix}A_{N+1}\\B_{N+1}\end{bmatrix}=T\begin{bmatrix}A_N\\B_N\end{bmatrix}=T^N\begin{bmatrix}A_1\\B_1\end{bmatrix}\ . \tag{2.9}$$

Thus $T^N=1$, so that the eigenvalues of T must be Nth roots of unity. Moreover, it is clear from (2.6) that $\det T=1$, so that we can write the eigenvalues of T as $e^{\pm i\theta}$ where $\theta=(2\pi p/N)$ for some integer p. It is customary to introduce a pseudo-wave-number $\kappa=p(2\pi/L)$, and write $\theta=\kappa l$. The eigenvalue condition that determines the band structure is then

$$2\cos\kappa l=\mathrm{Tr}T\ . \tag{2.10}$$

We can illustrate the method by considering the case where the potential has the form shown in Fig. 1—a potential step of height $U_0/2m$ and width a, with its left-hand edge at $x=0+\epsilon$, followed by a potential free region of length b, which extends a distance ϵ into the next cell. Clearly $a+b=l$. The elementary wave functions $\phi_A(x)$ and $\phi_B(x)$ may be chosen to be arbitrary linear combinations of those which start as $e^{\pm ikx}$ in the region $(0,\epsilon)$.

Writing

$$W_k(x)=\begin{bmatrix}e^{ikx} & e^{-ikx}\\ ike^{ikx} & -ike^{-ikx}\end{bmatrix}=\begin{bmatrix}1 & 1\\ ik & -ik\end{bmatrix}e^{ikx\sigma_z}\ , \tag{2.11}$$

where σ_z is the usual Pauli matrix, for the Wronskian matrix of the exponential solutions, and

$$F_0=\begin{bmatrix}A_A & A_B\\ B_A & B_B\end{bmatrix} \tag{2.12}$$

for the matrix of coefficients of the solutions

$$\phi_{A,B}=A_{A,B}e^{ikx}+B_{A,B}e^{-ikx}$$

in the region $(0,\epsilon)$, we see that

$$W(0)=W_k(0)F_0\ . \tag{2.13}$$

Similarly,

$$W(l)=W_k(l)F_l\ , \tag{2.14}$$

where F_l is the similar coefficient matrix in the region near $x=l$. Elementary quantum mechanics then shows that

$$F_l=\mathcal{M}F_0\ , \tag{2.15}$$

where

$$\mathcal{M} = W_k^{-1}(a)W_K(a)W_K^{-1}(0)W_k(0) \tag{2.16}$$

$$= e^{-ika\sigma_z}\cos Ka + \frac{i}{2}\left[\frac{K}{k}+\frac{k}{K}\right]\sin Ka\,\frac{i}{2}\left[\frac{K}{k}-\frac{k}{K}\right]\sin Ka - \frac{i}{2}\left[\frac{K}{k}-\frac{k}{K}\right]\sin Ka\,\cos Ka - \frac{i}{2}\left[\frac{K}{k}+\frac{k}{K}\right]\sin Ka \tag{2.16a}$$

is the matrix connecting the plane wave coefficients before and after the barrier. Here K is the wave number in the potential region,

$$K=(k^2-U_0)^{1/2}\ . \tag{2.17}$$

Thus

$$T=F_0^{-1}W_k^{-1}(0)W_k(l)\mathcal{M}F_0 \tag{2.18}$$

and the arbitrary coefficient matrix F_0 does not enter the band condition

$$2\cos\kappa l=\mathrm{Tr}[W_k^{-1}(0)W_k(l)\mathcal{M}]\ , \tag{2.19}$$

which may be written as

$$2\cos\kappa l=\mathrm{Tr}(e^{ikl\sigma_z}\mathcal{M}) \tag{2.20a}$$

or

$$2\cos\kappa l=\mathrm{Tr}[W_k(l)W_k^{-1}(a)W_K(a)W_K^{-1}(0)]\ . \tag{2.20b}$$

In this way we obtain the Kronig-Penney result for the allowed bands

$$2\cos\kappa l=2\cos kb\,\cos Ka-\frac{K^2+k^2}{Kk}\sin kb\,\sin Ka\ , \tag{2.21}$$

which in the δ function limit ($a\to 0$, $U_0\to\infty$ but $U_0a=2mS$, kept constant) becomes the perhaps more familiar band equation

$$\cos\kappa b=\cos kb+\frac{mS}{k}\sin kb\ , \tag{2.22}$$

which was also obtained by Kronig and Penney. In contrast to what happens with the Dirac equation, it should be emphasized that this same result is obtained if we solve the Schrödinger equation in the unit cell with a delta function potential.

Now we discuss the analogous solution of the Dirac equation for a barrier as the initial step in solving the Dirac equation in a periodic potential.

III. THE TRANSFER MATRIX METHOD FOR THE DIRAC EQUATION

The one dimensional Dirac equation has the form

$$(E-V_e)\psi+i\alpha_x\frac{\partial\psi}{\partial x}-\beta(m+V_s)\psi=0\ , \tag{3.1}$$

where we have introduced a Lorentz scalar potential $V_s(x)$ and an electrostatic type of potential $V_e(x)$ which is the time component of a four-vector potential. Both potentials are assumed to be periodic with period l. In one dimension it suffices to use two component spinors ψ. The 2×2 Dirac matrices α_x,β anticommute and are traceless Hermitian matrices with square unity. We may thus choose then two of the Pauli matrices. There are two standard choices:

(i) The Dirac representation

$$\alpha_x^D=\sigma_x,\quad \beta^D=\sigma_z\ , \tag{3.2}$$

which is convenient when considering the nonrelativistic limit, and

(ii) the Weyl representation

$$\alpha_x^W=\sigma_z,\quad \beta^W=\sigma_x\ , \tag{3.3}$$

which is particularly convenient for massless particles.

Note that the matrix

$$D=\frac{1}{\sqrt{2}}(\sigma_x+\sigma_z) \tag{3.4}$$

which satisfies $D^+=D$, $D^2=1$, effects the transformation between the Dirac and Weyl representations of the spinors.

In this section we will establish the analog of James's general analysis for the Dirac equation, and we will preserve generality by not using any explicit representation of the Dirac matrices. Equation (3.1) may be rewritten in the standard form for linear first order equations

$$\frac{\partial\psi}{\partial x}=G\psi\ , \tag{3.5}$$

where

$$G=i\alpha_x[(E-V_e)-(m+V_s)\beta]\ . \tag{3.6}$$

According to the general theory of linear differential equations the first order equation (3.5) for the two dimensional vector $\psi=\binom{\psi_u}{\psi_l}$ has two linearly independent solutions. In the unit cell we select two independent solutions $\psi_A(x)$ and $\psi_B(x)$ and form the matrix

$$\Omega(x)=[\psi_A(x),\psi_B(x)]=\begin{bmatrix}\psi_{u,A} & \psi_{u,B}\\ \psi_{l,A} & \psi_{l,B}\end{bmatrix} \tag{3.7}$$

which plays the role the Wronskian matrix played in the discussion in the preceding section.

The general solution in the nth cell may be written as a linear combination of

$$\psi_A(x-[n-1]l),\ \psi_B(x-[n-1]l)\ ,$$

viz.,

$$\psi(x)=\Omega(x-[n-1]l)\mathcal{A}_n\ , \tag{3.8}$$

where $\mathcal{A}_n=\binom{A_n}{B_n}$ is the vector of coefficients.

Continuity of the upper and lower component solutions at $x=nl$ then requires that

$$\mathcal{A}_{n+1}=T_D\mathcal{A}_n\ , \tag{3.9}$$

where

$$T_D=\Omega^{-1}(0)\Omega(l) \tag{3.10}$$

is the Dirac transfer matrix.

It is a straightforward calculation to show that

$$\frac{\partial}{\partial x}\det\Omega=(\mathrm{Tr}G)\det\Omega \tag{3.11}$$

and because (3.6) implies that $\mathrm{Tr}G=0$, we see that

$$\det\Omega=\text{const} \tag{3.12}$$

and thus that

$$\det T_D=1\ , \tag{3.13}$$

just as for the Schrödinger equation.

The analysis of the preceding section leading to the general eigenvalue condition (2.10), and the specific form it takes when there are zero potential regions around $x=nl$, (2.19), may now be applied *mutatis mutandis* to the present case.

The general band condition for the Dirac equation is

$$2\cos\kappa l=\mathrm{Tr}T_D\ , \tag{3.14}$$

and for the special case that there are zero potential regions around $x=nl$,

$$2\cos\kappa l=\mathrm{Tr}[\Omega_k^{-1}(0)\Omega_k(l)\mathscr{M}_D]\ . \tag{3.15}$$

$\Omega_k(x)$ is the solution matrix of (3.5) for the plane wave solutions $e^{ikx}u_{k,+}$ and $e^{-ikx}u_{k,-}$, and $\mathscr{M}_D$ is the matching matrix relating the coefficients in the expressions

$$\psi(x\approx 0+)=A_0e^{ikx}u_{k,+}+B_0e^{-ikx}u_{k,-}\ , \tag{3.16}$$

$$\psi(x\approx l-)=A_le^{ikx}u_{k,+}+B_le^{-ikx}u_{k,-} \tag{3.17}$$

by

$$\begin{bmatrix}A_l\\B_l\end{bmatrix}=\mathscr{M}_D\begin{bmatrix}A_0\\B_0\end{bmatrix}\ . \tag{3.18}$$

It is also possible to write down a general analog of Eq. (2.20a), but this requires a little more analysis to show that it is independent of the particular choice of representation of the Dirac matrices and hence of the particular representation of the solution $u_{k,\pm}$. The clue is to realize that we may write

$$\Omega_k(x)=(u_{k+}e^{ikx},u_{k-}e^{-ikx})=(u_{k+},u_{k-})e^{ikx\sigma_z} \tag{3.19}$$

so that

$$\begin{aligned}\Omega_k^{-1}(0)\Omega_k(l)&=\Omega_k^{-1}(0)\Omega_k(0)e^{ikl\sigma_z}\\&=e^{ikl\sigma_z}\ .\end{aligned} \tag{3.20}$$

Thus we may rewrite (3.15) as

$$2\cos\kappa l=\mathrm{Tr}(e^{ikl\sigma_z}\mathscr{M}_D)\ , \tag{3.21}$$

in perfect analogy with (2.20a).

In the special case that the potentials V_e and V_s have an identical square barrier structure, the analog of (2.20b) is also a correct representation of the energy band condition, as we shall see in the next section.

IV. THE PENETRATION OF DIRAC PARTICLES THROUGH A BARRIER

A. The square barrier

We now develop the solution for the Dirac equation for a potential of the form shown in Fig. 1, where we may now set $\epsilon=0$ and allow the potential to extend from $-\infty$ to $+\infty$ without loss of generality. However, we now have to decide whether this potential is to be regarded as the time component of a Lorentz vector which we shall call an electrostatic potential, or whether it is to be regarded as a Lorentz scalar. We have argued elsewhere[3] that the appropriate representation of the confining potential for nuclear physics calculations involving quarks is to choose it as a Lorentz scalar. We will return to this point later but for the moment we will use the notation of the preceding section which allows both electrostatic and scalar potentials simultaneously.

Just as we did in Sec. II we can divide the line into three regions, where now

$$\begin{aligned}&R_{\mathrm{I}}=(-\infty,0),\quad x\in R_{\mathrm{I}},\quad V_e=V_s=0\\&R_{\mathrm{II}}=(0,a),\quad x\in R_{\mathrm{II}},\quad V_e=U_e,\quad V_s=U_s\\&R_{\mathrm{III}}=(a,\infty),\quad x\in R_{\mathrm{III}},\quad V_e=V_s=0\ .\end{aligned} \tag{4.1}$$

In regions I and III the solutions are linear combinations of $e^{\pm ikx}u_{k\pm}$, where $u_{k\pm}$ are eigenvectors of

$$G_0=i\alpha_x(E-m\beta)\ , \tag{4.2}$$

$$\Omega_k(x)=(e^{ikx}u_{k+},e^{-ikx}u_{k-})=\Omega_k(0)e^{ikx\sigma_z} \tag{4.3}$$

is the solution matrix, and, if $u_{k\pm}$ are normalized so that $u_{k\pm}^{+}u_{k\pm}=1$, it is also a unitary matrix which diagonalizes G_0.

Thus we may write the general solution in regions I and III as

$$\psi_\Gamma=\Omega_k(x)\mathscr{A}_\Gamma\ , \tag{4.4}$$

where $\Gamma=$I,III, and

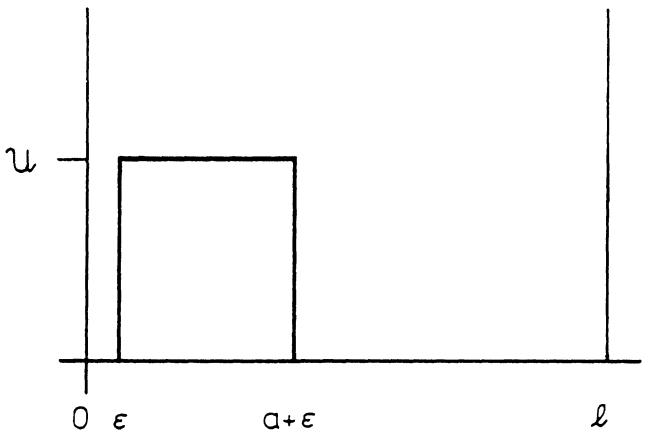

FIG. 1. A representation of one cell in the periodic lattice.

$$\mathscr{A}_\Gamma = \begin{bmatrix} A_\Gamma \\ B_\Gamma \end{bmatrix} \tag{4.5}$$

is the coefficient vector.

In a similar way we may write

$$\psi_{\rm II} = \Omega_K(x)\mathscr{A}_{\rm II} , \tag{4.6}$$

where

$$\Omega_K(x) = (e^{iKx}u_{K+}, e^{-iKx}u_{K-}) . \tag{4.7}$$

K is now the wave number in the barrier region and is given by

$$K^2 = (E-U_e)^2 - (m+U_s)^2 \tag{4.8}$$

and $u_{K\pm}$ are the eigenvectors of

$$G_1 = i\alpha_x[(E-U_e) - (m+U_s)\beta] , \tag{4.9}$$

with eigenvalues $\pm iK$.

Continuity of the solution at $x=0$ demands that

$$\mathscr{A}_{\rm II} = \Omega_K^{-1}(0)\Omega_k(0)\mathscr{A}_{\rm I} \tag{4.10}$$

and continuity at $x=a$ demands that

$$\mathscr{A}_{\rm III} = \Omega_k^{-1}(a)\Omega_K(a)\mathscr{A}_{\rm II} = \mathscr{M}_D\mathscr{A}_{\rm I} \tag{4.11}$$

with the matching matrix across the barrier identified as

$$\mathscr{M}_D = \Omega_k^{-1}(a)\Omega_K(a)\Omega_K^{-1}(0)\Omega_k(0) . \tag{4.12}$$

By the general result (3.12) on the constancy of $\det\Omega$, it is immediate that

$$\det\mathscr{M}_D = 1 . \tag{4.13}$$

A change in the representation of the Dirac matrices induces a change in the eigenstates

$$u'_{k\pm} = Du_{k\pm} \tag{4.14}$$

or

$$\Omega'_k(x) = D\Omega_k(x) \tag{4.15}$$

where D is a unitary matrix, such as that of Eq. (3.4).

It is then straightforward to demonstrate that

$$\mathscr{M}'_D = \mathscr{M}_D \tag{4.16}$$

so that the matching matrix is invariant under a change in representation for the spinors.

The current

$$j(x) = \psi^\dagger(x)\alpha_x\psi(x) \tag{4.17}$$

is continuous across the boundaries of the regions as a consequence of the matching conditions (4.10) and (4.11). Thus we can consistently define transmission and reflection coefficients for the barrier.

In the zero potential region, an explicit calculation in either the Dirac or Weyl representation shows that

$$j = \frac{k}{E}\mathscr{A}^\dagger\sigma_z\mathscr{A} = \frac{k}{E}(|A|^2 - |B|^2) \tag{4.18}$$

in accord with our intuition that $e^{ikx}u_{k+}$ represents a current to the right, and $e^{-ikx}u_{k-}$ represents a current to the left. The proportionality constant depends on the normalization of the state, and in Eq. (4.15) the normalization $u^+u=1$ is chosen in each representation.

In the finite potential region the analogous equation holds if the wave number K is real. However, if K is imaginary the expression for j in terms of A and B is more complicated and will not be reproduced here.

To obtain the transmission and reflection coefficients in a systematic way, we follow Saxon and Hunter[8] and introduce the $\mathscr{S}$ matrix by

$$\begin{bmatrix} A_{\rm III} \\ B_{\rm I} \end{bmatrix} = \mathscr{S}\begin{bmatrix} A_{\rm I} \\ B_{\rm III} \end{bmatrix} , \tag{4.19}$$

so that $\mathscr{T} = |\mathscr{S}_{11}|^2$ and $\mathscr{R} = |\mathscr{S}_{21}|^2$. $\mathscr{S}$ may be expressed in terms of the elements of $\mathscr{M}$ (remembering $\det\mathscr{M}=1$),

$$\mathscr{S} = \frac{1}{\mathscr{M}_{22}}\begin{bmatrix} 1 & \mathscr{M}_{12} \\ -\mathscr{M}_{21} & 1 \end{bmatrix} . \tag{4.20}$$

Conservation of the current can be shown to imply unitarity of $\mathscr{S}$, which in turn implies

$$\mathscr{R} + \mathscr{T} = 1 . \tag{4.21}$$

In terms of $\mathscr{M}$,

$$\mathscr{T} = \frac{1}{|\mathscr{M}_{22}|^2} , \tag{4.22}$$

$$\mathscr{R} = \left|\frac{\mathscr{M}_{21}}{\mathscr{M}_{22}}\right|^2 . \tag{4.23}$$

Now it is necessary to become specific. If we introduce the parameters

$$\lambda = \frac{k}{E+m}, \quad \Lambda = \frac{K}{E-U_E+m+U_S} , \tag{4.24}$$

the wave function matrix in the Dirac representation is

$$\Omega_k(x) = N\begin{bmatrix} 1 & 1 \\ \lambda & -\lambda \end{bmatrix} e^{ikx\sigma_z} , \tag{4.25}$$

where N is a normalization constant. The matching matrix is independent of N, even if N is k dependent. The matching matrix is then

$$\mathcal{M}_D=\tfrac{1}{4}e^{-ika\sigma_z}\begin{bmatrix}1 & \frac{1}{\lambda}\\ 1 & -\frac{1}{\lambda}\end{bmatrix}\begin{bmatrix}1 & 1\\ \Lambda & -\Lambda\end{bmatrix}e^{iKa\sigma_z}\begin{bmatrix}1 & \frac{1}{\Lambda}\\ 1 & -\frac{1}{\Lambda}\end{bmatrix}\begin{bmatrix}1 & 1\\ \lambda & -\lambda\end{bmatrix}$$

$$=e^{-ika\sigma_z}\begin{bmatrix}\cos Ka+\frac{i}{2}\left[\frac{\Lambda}{\lambda}+\frac{\lambda}{\Lambda}\right]\sin Ka & \frac{i}{2}\left[\frac{\Lambda}{\lambda}-\frac{\lambda}{\Lambda}\right]\sin Ka\\ -\frac{i}{2}\left[\frac{\Lambda}{\lambda}-\frac{\lambda}{\Lambda}\right]\sin Ka & \cos Ka-\frac{i}{2}\left[\frac{\Lambda}{\lambda}+\frac{\lambda}{\Lambda}\right]\sin Ka\end{bmatrix}. \tag{4.26}$$

Note that the replacement $\Lambda/\lambda\rightarrow K/k$ transforms the Dirac matching matrix to the form of the Schrödinger matching matrix.

We can investigate the nonrelativistic limit of our result by setting

$$E=m+\epsilon \tag{4.27}$$

and working to lowest order in ϵ/m, U_e/m, U_s/m.

We find that

$$k\rightarrow(2m\epsilon)^{1/2}, \tag{4.28a}$$

$$K\rightarrow[2m(\epsilon-U_e-U_s)]^{1/2}, \tag{4.28b}$$

and

$$\frac{\Lambda}{\lambda}\rightarrow\frac{K}{k}. \tag{4.28c}$$

Thus in the nonrelativistic limit we obtain the result that the equivalent nonrelativistic potential is the sum of the electrostatic and the scalar potentials as we would have expected.

K can become imaginary, but $(\Lambda/\lambda\pm\lambda/\Lambda)\sin Ka$ and $\cos Ka$ are always real, so the transmission and reflection coefficients become

$$\mathcal{T}=\frac{1}{\cos^2Ka+\frac{1}{4}\left|\frac{\Lambda}{\lambda}+\frac{\lambda}{\Lambda}\right|^2|\sin Ka|^2} \tag{4.29}$$

$$\mathcal{R}=\frac{\frac{1}{4}\left|\frac{\Lambda}{\lambda}-\frac{\lambda}{\Lambda}\right|^2|\sin Ka|^2}{\cos^2Ka+\frac{1}{4}\left|\frac{\Lambda}{\lambda}+\frac{\lambda}{\Lambda}\right|^2|\sin Ka|^2}. \tag{4.30}$$

Much more interesting is the limit when the potentials become very strong, which leads us to a discussion of the Klein paradox for this potential.

B. The Klein paradox for a square barrier

In the classic discussion of the Klein paradox[10] a potential step is considered and it is shown that if $U_s=0$ and $U_e>E-m$ the transmission coefficient is negative and the reflection coefficient exceeds unity. In hole theory this is interpreted by noticing that the potential step raises the negative energy states to be at the same energy as the positive energy states outside the barrier. The particle in a filled negative energy state can then tunnel through to appear as a positive energy particle outside the barrier which is repelled to $-\infty$, leading to a reflected current exceeding the incident current. The empty negative energy state is an antiparticle which contributes to the transmitted current.

Arguing in this way, we see that we should expect that the particle in a filled negative energy state in the region of the barrier could tunnel through and appear as a particle on either side of the barrier. Thus, even for very strong electrostatic-type potentials we should expect a current on the "wrong" side of the barrier, showing that the particles cannot be confined by an electrostatic type barrier, however strong.

This expectation is confirmed by this analysis. For the case of interest $U_s=0$ and K is real ($K\approx\pm U_e$ for very large U_e), and

$$\mathcal{T}=\frac{1}{\cos^2Ka+\frac{1}{2}\sin^2Ka+\frac{1}{4}\left[\frac{\Lambda^2}{\lambda^2}+\frac{\lambda^2}{\Lambda^2}\right]\sin^2Ka}=\frac{1}{1+\frac{1}{4}\left[\frac{\Lambda}{\lambda}-\frac{\lambda}{\Lambda}\right]^2\sin^2Ka}. \tag{4.31}$$

Now for very large U_e, the transmission coefficient is bounded above *and below* by

$$1\geq\mathcal{T}\geq\frac{1}{1+\frac{1}{4}\left[\frac{\Lambda}{\lambda}-\frac{\lambda}{\Lambda}\right]^2}\approx\frac{1}{1+\frac{1}{4}(\lambda^{-1}-\lambda)^2}. \tag{4.32}$$

This shows that as $U_e\rightarrow\infty$, $\mathcal{T}$ remains finite, in agreement with the physical argument presented above. We note that in the massless limit $\Lambda=\lambda=\pm1$, and

$$\mathcal{T}=1 \text{ (massless limit)}, \tag{4.33}$$

so that there is no expectation of modeling confinement of quarks using potentials of the electrostatic type in the Dirac equation.

No such difficulty occurs with Lorentz scalar potentials. In this case ($U_e=0$, $U_s>E-m$) the wave number in the barrier is imaginary. Write

$$K=iK_1, \tag{4.34a}$$

where

$$K_1=[(m+U_s)^2-E^2]^{1/2} \quad . \tag{4.34b}$$

is now real; correspondingly, $\Lambda=i\Lambda_1$ and

$$\mathscr{T}=\frac{1}{\cosh^2 K_1 a+\frac{1}{4}\left[\frac{\Lambda_1}{\lambda}-\frac{\lambda}{\Lambda_1}\right]^2\sinh^2 K_1 a}$$
$$=\frac{1}{1+\frac{1}{4}\left[\frac{\Lambda_1}{\lambda}+\frac{\lambda}{\Lambda_1}\right]^2\sinh^2 K_1 a} \quad . \tag{4.35}$$

Now as $U_s\to\infty$ with a fixed, $\Lambda_1\to 1$ and $K\to U_s$ so

$$\mathscr{T}\approx\frac{1}{1+\frac{1}{16}(\lambda+\lambda^{-1})^2 e^{2U_s a}} \tag{4.36a}$$
$$\approx\frac{16}{(\lambda+\lambda^{-1})^2}e^{-2U_s a} \quad , \tag{4.36b}$$

which does indeed approach zero as $U_s\to\infty$, showing that the Lorentz scalar potential does provide an acceptable model for confinement in the Dirac equation. For future reference we note that, in the massless case for strong Lorentz scalar potentials,

$$\mathscr{T}\approx\operatorname{sech}^{-2}U_s a \quad , \tag{4.37}$$

as $U_s\to\infty$.

It should be emphasized that, while we found that an electrostatic potential in the Dirac equation was an inappropriate model for confinement, this does not imply that exchange of vector particles cannot create a confining potential—multiple vector exchanges can generate scalar potentials which in the Dirac equation can model confinement, as we saw above.

C. The delta function limit

One way to approach the delta function limit of the barrier is to solve the Dirac equation for a square barrier, and then allow U_e or U_s to become infinite at the same time as $a\to 0$, keeping

$$U_{e,s}a=S_{e,s}=\text{const} \quad .$$

We refer to $S_{e,s}$ as the strength of the delta function. Using (4.26) we can then immediately write down the matching matrices in the δ function limit. For example, for an electrostatic type of potential

$$\mathscr{M}_{D_e}=\begin{bmatrix}\cos S_e+\frac{i}{2}(\lambda+\lambda^{-1})\sin S_e & \frac{i}{2}(\lambda^{-1}-\lambda)\sin S_e \\ -\frac{i}{2}(\lambda^{-1}-\lambda)\sin S_e & \cos S_e-\frac{i}{2}(\lambda+\lambda^{-1})\sin S_e\end{bmatrix} \quad . \tag{4.38}$$

Using these relations we may compute the discontinuity in the wave function at the position of the δ function. The results have a very simple form. In the electrostatic case

$$\psi(0+)=e^{-iS_e\alpha_x}\psi(0-) \quad , \tag{4.39}$$

and in the scalar case

$$\psi(0+)=e^{-iS_s\alpha_x\beta}\psi(0-) \quad . \tag{4.40}$$

We see from these equations that, although the current $j_x=\psi^\dagger\alpha_x\psi$ is continuous at the position of the delta function, the density $\psi^\dagger\psi$ is discontinuous in the scalar case, but continuous in the electrostatic case. In contrast $\bar{\psi}\psi$ is continuous in the scalar case, but discontinuous in the vector case. That the scalar δ function potential gives a continuous $\bar{\psi}\psi$ but a discontinuous $\psi^\dagger\psi$ should not be surprising because the same situation pertains in the bag model,[11] which is equivalent to confinement in a scalar spherical well.[12]

In solid state literature, the solution of the Dirac equation for a one dimensional array of electrostatic delta function potentials has been discussed extensively.[4] It has been noted that if one attempts to solve the Dirac equation with a δ function potential directly, rather than taking the limit of the solution for a finite potential as we did above, one obtains results which differ from those of Eq. (4.39). The result given in the literature[4] is

$$\psi(0+)=e^{-i\Sigma_e\alpha_x}\psi(0-) \quad , \tag{4.41}$$

where

$$\frac{\Sigma_e}{2}=\tan^{-1}\frac{S_e}{2} \quad . \tag{4.42}$$

For the scalar potential we find the analogous result

$$\psi(0+)=e^{-i\Sigma_s\beta\alpha_x}\psi(0-) \quad , \tag{4.43}$$

where

$$\frac{\Sigma_s}{2}=\tanh^{-1}\frac{S_s}{2} \quad . \tag{4.44}$$

Note that both of these results reduce to the preceding case in the limit that the δ function is weak ($S_{e,s}\to 0$). The results (4.41) and (4.42) essentially depend on the definition of the product $\delta(x)\theta(x)$ by the relation

$$\delta(x)\theta(x)=\tfrac{1}{2}\delta(x) \quad . \tag{4.45}$$

A simple "derivation" of Eq. (4.45) is

$$\theta(x)\delta(x)=\theta(x)\frac{d}{dx}\theta(x)=\frac{1}{2}\frac{d}{dx}[\theta^2(x)]$$
$$=\frac{1}{2}\frac{d}{dx}\theta(x)=\tfrac{1}{2}\delta(x) \quad ,$$

but note that the product $\delta\theta$ is not well defined as a distribution.

Equations (4.43) and (4.44) imply that there is an infinite jump in the wave function when $S_s=2$, while for larger values of S_s (when Σ_s becomes complex) there is a discontinuity in both magnitude and phase of the wave function. These results do not occur when the δ function limit is taken after the solution of the wave function. Moreover, we can find no physical reason for a singularity at $S_s=2$. Thus we argue that the solution of the Dirac equation for a delta function potential produces spurious results, and should be discarded in favor of taking the δ function limit in solutions of the equation.

If we look at the Dirac equation as specifying an initial condition problem by which specifying $\psi(x)$ at $x=X_0$ determines $\psi(x)$ at other values of x, we can see a difficulty when a δ function potential is included at say $x=0$. This potential specifies that the wave function $\psi(x)$ should have a discontinuity at $x=0$ which is proportional to $\psi(0)$. However, $\psi(0)$ is not well defined. The prescription (4.45) is equivalent to the definition

$$\psi(0)=\tfrac{1}{2}[\psi(0-)+\psi(0+)] . \tag{4.46}$$

Although this definition is apparently reasonable, it is incompatible with the initial value problem approach to the differential equation, as it makes the value $\psi(0+)$ dependent on $\psi(0+)$ itself, which has not yet been defined. We thus discard the solution (4.41)—(4.44) as unphysical.

Because of these ambiguities it is desirable to verify that Eqs. (4.39) and (4.40) are independent of how the δ function limit is taken in the potential after the Dirac equation has been solved. This can be done by returning to the one dimensional Dirac equation (3.5), and noting (by analogy with the time dependent Schrödinger equation) that it has the formal solution

$$\begin{aligned}\psi(x)&=\left[1+\int_{x_0}^{x}G(x')dx'\right.\\&\quad\left.+\int_{x_0}^{x}dx'\int_{x_0}^{x'}dx''G(x')G(x'')+\cdots\right]\psi(x_0)\\&=P_x\exp\left[\int_{x_0}^{x}G(x')dx'\right]\psi(x_0) ,\end{aligned} \tag{4.47}$$

where P_x is the spatial ordering operator defined by

$$P_x[A(x)B(y)]=A(x)B(y)\theta(x-y)+B(y)A(x)\theta(y-x) . \tag{4.48}$$

Now suppose that either $V_E(x)$ or $V_S(x)$ (but not both) is very sharply peaked in the region $(-\epsilon,\epsilon)$ around $x=0$, and apply (4.47) to $x=+\epsilon$, $x_0=-\epsilon$ to obtain

$$\psi(\epsilon)=P_x\exp\left[\int_{-\epsilon}^{\epsilon}G(x')dx'\right]\psi(-\epsilon) . \tag{4.49}$$

For small ϵ, only the strongly peaked potential contributes significantly to the integral in (4.49), and this gives a term proportional to either α_x or $\alpha_x\beta$ according to the type of potential which is large. This dominant term commutes at spatially separated points, so we may set $P_x=1$ for this term and obtain, after taking the limits that ϵ goes to zero and the potential magnitude becomes infinite

$$\psi(0+)=\exp(-i\alpha_x S_e)\psi(0-) \tag{4.50}$$

in the electrostatic case, and

$$\psi(0+)=\exp(-i\alpha_x\beta S_s)\psi(0-) \tag{4.51}$$

in the scalar case, where $S_{e,s}=\lim\int_{-\epsilon}^{\epsilon}V_{e,s}(x)dx$ is the strength of the δ function potential.

Equations (4.50) and (4.51) are identical to (4.39) and (4.40), demonstrating that the discontinuity in the wave function is independent of the particular representation of the δ function used to obtain the result, as long as the solution to the Dirac equation is obtained before the δ function limit is taken.

The uniqueness of this result, and the fact that it can be obtained in general, give us confidence in using it, or the equivalent matching matrices (4.38a) and (4.38b) as the basis for the discussion of the Dirac-Kronig-Penney model in the next section.

V. THE DIRAC-KRONIG-PENNEY MODEL

Now we simply have to insert the results for $\mathscr{M}_D$ obtained in the preceding section into Eqs. (3.15) or (3.21) to determine the band structure of the Dirac-Kronig-Penney model. We note that Kronig and Penney[7] considered both the finite square well potential and the delta function limit in their original paper, so it is appropriate to use the term Dirac-Kronig-Penney to refer to both the square barrier case and its delta function limit.

The result (2.20b) can be immediately transcribed to give an alternative form of eigenvalue condition (3.15) or (3.21) valid for the square barrier potential:

$$2\cos\kappa l=\mathrm{Tr}[\Omega_k(l)\Omega_k^{-1}(a)\Omega_K(a)\Omega_K^{-1}(0)] . \tag{5.1}$$

From this equation, or (3.21) and the form of $\mathscr{M}_D$ in Eq. (4.26), we obtain the general eigenvalue condition for the Dirac-Kronig-Penney model,

$$2\cos\kappa l=2\cos kb\cos Ka-\left[\frac{\Lambda}{\lambda}+\frac{\lambda}{\Lambda}\right]\sin kb\sin Ka , \tag{5.2}$$

where $\kappa=2\pi p/L$ for some integer p.

In the nonrelativistic limit described by Eqs. (4.28), the Dirac-Kronig-Penney eigenvalue condition (5.2) reduces to the Kronig-Penney eigenvalue condition (2.21). However, since we are considering a model for the binding of light quarks in a nucleus, we are much more interested in the form taken by (5.2) in the relativistic region. In fact, the limit of interest is

$$m\ll E\ll U_{e,s} . \tag{5.3}$$

In these circumstances it is desirable to consider the cases $U_e\gg E$, $U_s=0$ and $U_s\gg E$, $U_e=0$ separately.

In the first, electrostatic potential, case, $K\approx -U_e$ is real, $\Lambda\approx 1$, $\lambda\approx 1$, and (5.2) becomes

$$\cos\kappa l=\cos kb\cos Ka-\sin kb\sin Ka=\cos(kb+Ka) . \tag{5.4}$$

In this case there are no forbidden bands, as we may have anticipated, since we saw in Eq. (4.33) that the transmission coefficient for a single barrier becomes unity in these circumstances. The barriers are transparent to the quarks, and there are no band gaps.

The absence of band gaps is the manifestation of the

Klein paradox in this case, and again shows that an electrostatic type of potential cannot model confinement.

If we take the large U_e limit, but not the limit $E \gg m$, the eigenvalue condition becomes

$$\cos\kappa l = \cos kb \cos U_e a + \frac{E}{k} \sin kb \sin U_e a \ , \tag{5.5}$$

showing that forbidden bands can occur for heavy quarks in this limit.

Now we turn to the scalar potential, for $U_s \gg E,m$, $K \approx \pm i U_s$, $\Lambda \approx \pm i$ and so the eigenvalue condition becomes

$$\cos\kappa l = \cos kb \cosh U_s a + \frac{m}{k} \sin kb \sinh U_s a \ , \tag{5.6}$$

which can exhibit allowed and forbidden bands. If we take the limit in which the potential strength becomes infinite, the allowed bands become degenerate on the values of k determined by the transcendental equation

$$\tan kb + \frac{k}{m} = 0 \ . \tag{5.7}$$

This is, however, just the condition for the energies of quarks confined to a region of width b by an infinite scalar potential—or a one dimensional bag. Thus we see that a strong scalar potential effectively confines quarks to their individual cells.

The massless limit of (5.6) is

$$\cos\kappa l = \cos kb \cosh U_s a \ , \tag{5.8}$$

in which case the allowed bands are determined by the condition

$$|\cos kb| \leq \operatorname{sech} U_s a \tag{5.9}$$

explicitly showing how the bands narrow as U_s becomes large, and that they are centered on the points $k = (2n+1)(\pi/2b)$.

For the delta function potential we can obtain the eigenvalue condition simply by the replacement $Ua \to S$ in (5.5) and (5.6). This gives

$$\cos\kappa b = \cos kb \cos S_e + \frac{E}{k} \sin kb \sin S_e \tag{5.10}$$

for electrostatic delta function potentials, and

$$\cos\kappa b = \cos kb \cosh S_s + \frac{m}{k} \sin kb \sinh S_s \tag{5.11}$$

for Lorentz scalar delta function potentials. Note that for weak delta function potentials, and in the nonrelativistic limit, both of these equations reduce to the original Kronig-Penney eigenvalue condition (2.22).

VI. THE BINDING ENERGY OF THE MODEL SYSTEM

In the noninteracting quark approximation, the binding energy of the one dimensional model system may be calculated by the method originally used by Kronig and Penney.[7] The allowed states fill the lowest k band, and the equivalent band at the same energy corresponding to negative values of k. The states may be identified by the corresponding value of κ, which takes the values $\kappa = \pi p/Nl$, for integer $p \epsilon (0,N)$, and we can write

$$E_{\text{tot}} = \sum E(\kappa) = \frac{Nl}{\pi} \int_0^{\pi/l} d\kappa \, E(\kappa) \ . \tag{6.1}$$

Now change variables to k:

$$\langle E \rangle = \frac{E_{\text{tot}}}{N} = \frac{l}{\pi} \int_{k_{\min}}^{k_{\max}} dk \, E(k) \frac{d\kappa}{dk} \ , \tag{6.2}$$

where $(k_{\min}, k_{\max})$ is the first allowed band. The function $\kappa(k)$ is determined by the solution of the eigenvalue condition (2.10)

$$\kappa = l^{-1} \cos^{-1}(\tfrac{1}{2} \operatorname{Tr} T) \tag{6.3}$$

and $d\kappa/dk$ is proportional to the density of allowed states in k space. It is more useful to integrate (6.2) by parts:

$$\langle E \rangle = \frac{l}{\pi} E(k)\kappa(k) \int_{k_{\min}}^{k_{\max}} - \frac{l}{\pi} \int_{k_{\min}}^{k_{\max}} dk \frac{k}{E(k)} \kappa(k)$$
$$= E(k_{\max}) - \frac{l}{\pi} \int_{k_{\min}}^{k_{\max}} dk \frac{k}{E(k)} \kappa(k) \ . \tag{6.4}$$

To compute the binding energy we must subtract the binding energy of a quark in an isolated one dimensional bag. The quark energy levels in the bag are given by the solutions of (5.8).

As an example of illustrating the order of magnitude of the effects involved, we consider a system of bags of width $b = 1$ fm, represented as zero potential regions, separated by a potential barrier of width a and height U proportional to a. The proportionality between barrier height and width is adopted to simulate a rising potential as the quark leaves the attractive center.[1] The propor-

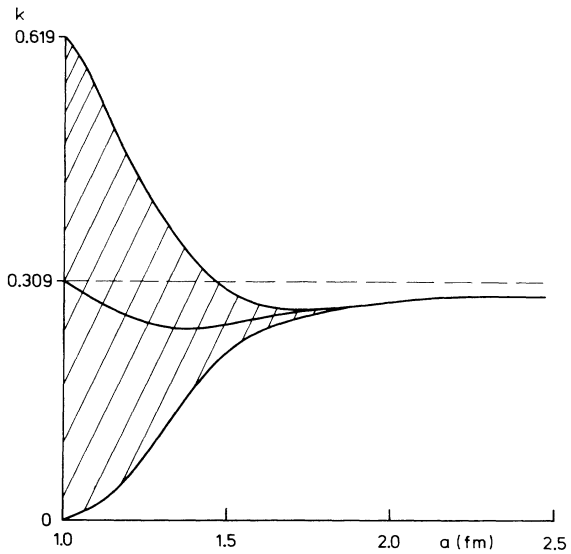

FIG. 2. Allowed values of k (in GeV/c) as a function of the unit cell size are shown as the cross-hatched area. The average energy per quark [Eq. (6.4)] is shown as the heavy line. For this example, $b = 1$ fm and $U = U_0 a$ with $U_0 = 1.65$ GeV/fm.

tionality constant was chosen to be 1.65 GeV/fm for our example. The quarks are taken to be massless, and the potential is assumed to be a Lorentz scalar. In Fig. 2 the allowed bands are shown cross-hatched as a function of the size of the unit cell, and the average energy is plotted as the solid line.

As the wells move apart from a configuration in which they touch, the bandwidth narrows dramatically, and the midpoint of the band drops from $\pi/2b$ when $a=0$, and then slowly moves back towards that value at infinite separation.

The behavior of the band is reflected in the energy. The system is not bound when the nucleons are very close together, and has an equilibrium binding energy of about 53 MeV/quark at a cell size of 1.4 fm. At this point the band gap is only 166 MeV/c, indicating a tight binding situation.

VII. CONCLUDING REMARKS

Our major results are:

(i) The one dimensional Dirac equation can be solved analytically for any very sharply peaked potential. The solution is quite different to that formally obtained for a delta function potential in the Dirac equation.

(ii) The first order nature of the Dirac equation makes it difficult to make physical sense of the delta function potential in the Dirac equation. For this reason we advocate the taking of the delta function limit after the solution of the equation.

(iii) The transfer matrix method is readily adapted to the solution of the Dirac equation for a one dimensional periodic potential.

(iv) A Lorentz scalar potential exhibits confinement in the Dirac-Kronig-Penney model, while an electrostatic type of potential does not.

(v) A model with a fixed bag size, and a barrier between wells whose height is proportional to its width exhibits saturation behavior.

These results are sufficiently encouraging to suggest that this model be further developed. Possible extensions are to random lattices and surface states in one dimension, and through the Green's function method to three dimensions.[13]

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[1]T. Goldman and G. J. Stephenson, Jr., Phys. Lett. **146B**, 143 (1984).

[2]J. Achtzehnter, W. Scheid, and L. Wilets, Phys. Rev. D **32**, 2414 (1985).

[3]B. H. J. McKellar and G. J. Stephenson, Jr., Los Alamos National Laboratory Report LA-UR-86-898, 1986.

[4]See, e.g., W. M. Fairbairn, M. L. Glasser, and M. Steslicka, Surf. Sci. **36**, 462 (1973); R. Subramanian and K. V. Bhagwat, J. Phys. C **5**, 798 (1972).

[5]See, e.g., P. Erdos and R. C. Herndon, Adv. Phys. **31**, 65 (1982).

[6]See, e.g., S. G. Davison and J. D. Levine, in *Solid State Physics,* edited by D. Turnbull, F. Seitz, and H. Ehrenreich (Academic, New York, 1970), Vol. 25, p. 1.

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

[8]D. Saxon and R. A. Hunter, Philips Res. Rep. **4**, 81 (1949).

[9]H. M. James, Phys. Rev. **76**, 1602 (1949).

[10]O. Klein, Z. Phys. **53**, 157 (1929).

[11]See, e.g., the review of A. W. Thomas, Adv. Nucl. Phys. **13**, 1 (1984).

[12]P. N. Bogolioubov, Ann. Inst. Henri Poincaré **8**, 163 (1967).

[13]S. Takada, Prog. Theor. Phys. **36**, 224 (1966); Y. Onodera and M. Okazaki, J. Phys. Soc. Jpn. **21**, 1273 (1966).