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ABSTRACT

An analytic solution for a Dirac particle in a one dimensional periodic square potential is obtained. The solution goes over in the non-relativistic limit to the famous Kronig-Penney one, and exhibits similar band structure of the energy spectrum.

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The motion of non-relativistic electrons in a periodic one-dimensional square well potential was solved long ago by Kronig and Penney, as a model of electrons in a crystal [1]. Their solution explicitly exhibits a band structure in the spectrum. There are also several physical systems where relativistic particles feel a periodic potential. The electrons in neutron stars are relativistic and if the neutrons of the dense core form a solid lattice, as has been conjectured, they would experience a periodic potential.

The particular interest that we have in this problem arises from recent interest in soliton models of the nucleon as representing a non-perturbative solution to Q.C.D. . We have studied a model of dense nuclear matter in which the nucleons are represented by quarks that are tightly bound to a topological configuration of meson fields (soliton). The solitons are arranged in a crystaline lattice. In this case the relativistic quarks experience the periodic field of the topological meson configurations. We have posed the question whether matter, described in this way might exhibit a phase transition in which, as in metals, the quarks become liberated from the solitons in which they are normally bound [2].

It is therefor of some interest to solve the relativistic analogue of the Kronig-Penney model.

The Dirac equation, in one space dimension can be written,

$$(\vec{\alpha} \cdot \vec{p} + \beta(m + U) - E)\,\psi(x) = 0 \;,\; \psi = \binom{u}{v} \tag{1}$$

where

$$\alpha = \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\; \beta = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{2}$$

The resulting linear coupled equations for u and v can be rewritten in terms of one of these, say u, which satisfies (units are $\hbar = c = 1$),

$$u'' + uU' = \left[(m + U)^2 - E^2 \right] u \tag{3}$$

For a periodic square potential, U, a discontinuity is produced in the derivative of the solution. For

$$U(x) = \begin{cases} 0 \;, & |x| \leqslant a \\ V \;, & a < |x| \leqslant a + b \end{cases} \tag{4}$$

we have

$$U' = -V\Big[\,\delta(x + a) - \delta(x - a)\Big] \tag{5}$$

and hence

$$u'' - uV\Big[\,\delta(x + a) - \delta(x - a)\Big]$$
$$= \Big[\,(m + U)^2 - E^2\,\Big]u \tag{6}$$

Integrate this about a small neighbourhood of each discontinuity to find the discontinuity in derivative of the solution,

$$u'(-a + \eta) - u'(-a - \eta) = Vu(-a)$$
$$u'(a + \eta) - u'(a - \eta) = -Vu(a) \tag{7}$$

Now define

$$Q^2 = (m + V)^2 - E^2 \;\;,\;\; K^2 = E^2 - m^2 > 0 \tag{8}$$

In each of the three regions the solution has the form,

$$u_1 = Ae^{Qx} + Be^{-Qx} \;\;,\;\; -(a + b) \leqslant x < -a$$
$$u_2 = \alpha e^{iKx} + \beta e^{-iKx} \;\;,\;\; -a \leqslant x < a \tag{9}$$
$$u_3 = Ce^{Qx} + De^{-Qx} \;\;,\;\; a < x \leqslant a + b$$

The Block theorem [3] can be used to relate the wave function at points separated by an integer number of cell lengths,

$$\psi(-a - b) = \psi(a + b)\exp(\,2i(a + b)k)$$
$$\psi'(-a - b) = \psi'(a + b)\exp(\,2i(a + b)k) \tag{10}$$

which solve to give

$$C/A = e^{-2(a+b)(Q+iK)}\,,\; D/B = e^{2(a+b)(Q-iK)} \tag{11}$$

The continuity of the function, and the specific discontinuity of the derivative derived above yield in particular

$$
\begin{aligned}
u_1(-a-\eta) &= u_2(-a+\eta) \\
u_1'(-a-\eta) + Vu_1(-a+\eta) &= u_2'(-a+\eta) \\
u_3(a+\eta) &= u_2(a-\eta) \qquad (12) \\
u_3'(a+\eta) + Vu_3(a+\eta) &= u_2'(a-\eta)
\end{aligned}
$$

in which the limit $\eta \rightarrow 0$ can now be taken. Taking into account (11), these four equations determine all the constants in the solution provided the determinant of the coefficients of the unknowns vanishes

$$
0 = \begin{vmatrix} 1 & 1 & 1 & -1 \\ Q+V & -(Q-V) & -iK & iK \\ e^{-2Qb}e^{-2ik(a+b)} & e^{2Qb}e^{-2ik(a+b)} & -e^{2iKa} & -e^{-2iKa} \\ (Q+V)e^{-2Qb}e^{-2ik(a+b)} & -(Q-V)e^{2Qb}e^{-2ik(a+b)} & -iKe^{2iKa} & iKe^{-2iKa} \end{vmatrix} \qquad (13)
$$

After some manipulation, this yields

$$
\frac{Q^2 - K^2 + V^2}{2QK} \sinh 2Qb \sin 2Ka + \cosh 2Qb \cos 2Ka = \cos 2k(a+b) \qquad (14)
$$

This provides the eigenvalues, E, in terms of the crystal momentum, k. The band structure arises because the left side cannot equal the right except over continuous ranges of energies that are separated by gaps. This is similar to the Kronig - Penney result but differs explicitly in the appearance of V on the left side, and implicitly in the relativistic relations (8). This result embraces the entire range of energies and reduces in the non-relativistic limit to the result of Kronig-Penney.

In Fig 1 we illustrate in a particular example chosen so that the particle is relativistic near and above the top of the potential, how the levels of the isolated potentials develop into bands, which merge for sufficiently close spacing of the wells. The band structure persists into the positive energy spectrum above the top of the potential, with the gaps tending toward zero with increasing energy.

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References

1. R. Kronig and W. Penney, Proc. Roy Soc A130 (1931) 451.
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3. C. Kittel, Introduction to Solid State Physics (John Wiley, New York, 1976)

Figure Captions

Fig. 1. Energy levels and band structure in a one dimensional periodic potential, for a Dirac particle, are shown as a function of separation between the attractive regions. At large separation the levels are degenerate and in the limit coincide with those of the isolated potential of width 2a. In units $\hbar = c = 1$, the mass and potential height are taken equal to 5 fm^{-1} so that the particle is relativistic and at above the potential.

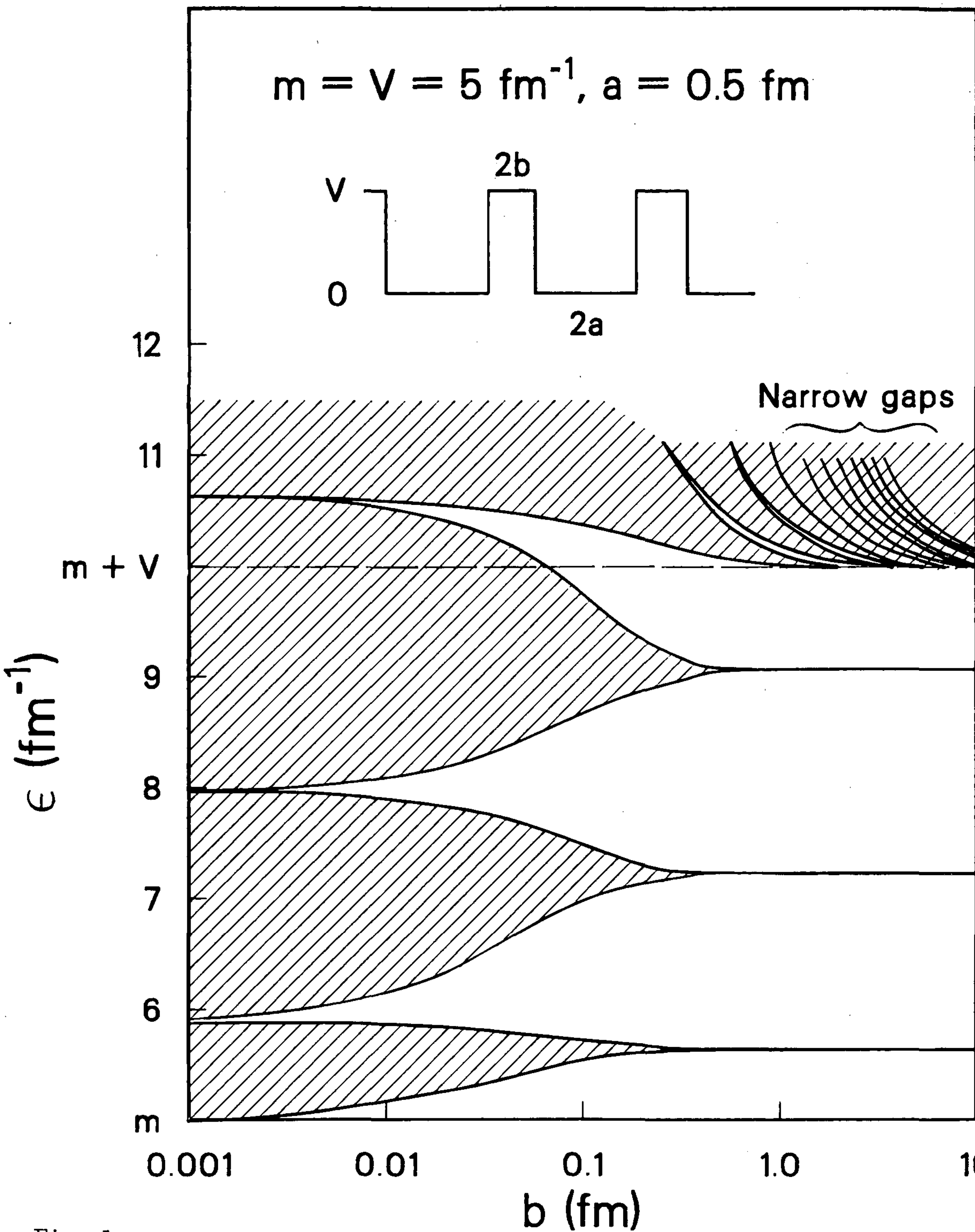

Fig. 1

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