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LETTER TO THE EDITOR

Scalar symmetry of the massless Dirac equation

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Abstract. The existence of a symmetry of the Dirac equation for a massless particle in a scalar field is demonstrated, and its effect on the bandstructure of certain arrays of scalar δ-function potentials is investigated. The implications of the symmetry for more general scalar potentials are also discussed.

Recently [1, 2] we obtained conditions for the existence of the band gaps of a massive relativistic particle in a one-dimensional disordered array of Lorentz scalar δ-function potentials possessing short-range order. For this array the distances between the δ-function potentials of strength λ were assumed to be independent random variables distributed in the interval $[l, l+d]$. The energy gap conditions are a pair of inequalities for the relativistic momentum k (in units $\hbar = c = 1$), and given by

$$n\pi - \pi q_{+1} \leqslant kl \leqslant n\pi + \pi q_{-1} - kd \tag{1}$$

for $n = 1, 2, 3, \ldots$ and $\lambda > 0$. Similarly for $\lambda < 0$ we obtained

$$n\pi - \pi q_{-1} \leqslant kl \leqslant n\pi + \pi q_{+1} - kd \tag{2}$$

where

$$q_t = \frac{2}{\pi} \operatorname{Pr} \arctan\left(r^t \tanh \frac{|\lambda|}{2} \right) \qquad \text{and} \qquad r = \frac{k}{E+m} \tag{3}$$

for a particle of energy E and mass m.

An intriguing feature of the above conditions occurs in the massless limit, where $r = 1$ and consequently $q_{+1} = q_{-1}$. In this limit we observe that the conditions specifying the gap structure, (1) and (2), become identical; the resulting band structure depends only on the magnitude of the δ-function strength and is independent of its sign. Furthermore, for the case of an exactly periodic lattice ($d = 0$), these gaps form regions which are symmetrical about the values $kl = n\pi$.

These two features suggest the existence of an underlying symmetry of the Dirac equation for a massless particle in a scalar field. Indeed such a symmetry does exist, a fact which has significant implications for the bandstructure of a system of such particles in a periodic scalar potential. It is the purpose of this letter to determine the origin of this symmetry and from this basis to investigate in detail its consequences for the bandstructure of the particle for an array of scalar δ-function potentials. Its consequences for more general scalar periodic structures will also be discussed.

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The well known chiral symmetry of the Dirac equation occurs because the Dirac equation is invariant under the transformation

$$\Psi(\boldsymbol{x}) \rightarrow \mathrm{e}^{\mathrm{i}\phi\gamma_5}\Psi(\boldsymbol{x}) \tag{4}$$

in the massless limit and this implies the existence of a corresponding conserved current, the axial vector current. Since a particle in a scalar potential has, in a sense, a position dependent mass, this result is of use only for a massless particle in a vector (i.e. electrostatic type) potential. In one dimension this symmetry implies conservation of the direction of motion of a particle [3]. This occurs because a reversal of momentum of the massless particle due to its interaction with a vector field would require a change in its helicity and this is forbidden by the symmetry (remember spin is not well defined in one dimension).

For a massless particle in a scalar field a similar, although less obvious, symmetry exists. To see how this symmetry arises consider the three-dimensional Dirac equation for a massless particle in a scalar field $S(\boldsymbol{x})$

$$[\boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta S(\boldsymbol{x})]\Psi(\boldsymbol{x}) = E\Psi(\boldsymbol{x}) \tag{5}$$

which we note is invariant under the transformations

$$\Psi(\boldsymbol{x}) \rightarrow \gamma_5\Psi(\boldsymbol{x}) \qquad \text{and} \qquad S(\boldsymbol{x}) \rightarrow -S(\boldsymbol{x}). \tag{6}$$

This is just the symmetry we are seeking.

In passing we note there is still a symmetry in the massive particle case, in which case the symmetry transformation takes the form

$$\Psi(\boldsymbol{x}) \rightarrow \gamma_5\Psi(\boldsymbol{x}) \qquad \text{and} \qquad S(\boldsymbol{x}) \rightarrow -S(\boldsymbol{x}) - 2m. \tag{7}$$

(In one dimension these become $\Psi(x) \rightarrow \alpha_x\Psi(x)$ and $S(x) \rightarrow -S(x)$.)

In the Dirac–Pauli representation the γ_5 operator interchanges the upper and lower components of the wavefunction which, combined with the changing of the sign of the potential, suggests that the massless particle is unable to differentiate the sign of the potential. To examine this situation more closely we shall examine in detail a simple one-dimensional system.

In order to describe a relativistic particle in one dimension a two-component spinor wavefunction is required. In the Dirac–Pauli [4] representation in a field-free region the wavefunction may be written as

$$\Psi(x) = \begin{pmatrix} \Psi_1(x) \\ \Psi_2(x) \end{pmatrix}. \tag{8}$$

In many circumstances the lower component is much smaller than the upper, and many authors [5] have utilized this fact to neglect one of the components of the spinor, thus obtaining reasonable approximations to the relativistic system which differ marginally from those applicable to the single component non-relativistic systems. However, in the massless limit, both components are of the same order and a complete two-component description is necessary in any analysis.

The two components $\Psi_1(x)$ and $\Psi_2(x)$ satisfy

$$\mathrm{i}\Psi_1'(x) + (k+S(x))\Psi_2(x) = 0 \qquad \mathrm{i}\Psi_2'(x) + (k-S(x))\Psi_1(x) = 0 \tag{9}$$

which, upon the elimination of the appropriate components, can be rewritten as

$$\begin{aligned} &\Psi_1''(x) - \frac{S'(x)}{k+S(x)}\Psi_1'(x) + (k^2 - S^2(x))\Psi_1(x) = 0 \\ &\Psi_2''(x) + \frac{S'(x)}{k-S(x)}\Psi_2'(x) + (k^2 - S^2(x))\Psi_2(x) = 0. \end{aligned} \tag{10}$$

These equations appear to be uncoupled, but that is not the case as we must find solutions which are related through (9).

Examining these equations we verify that they remain invariant under the transformations

$$\Psi_1(x)\leftrightarrow\Psi_2(x) \qquad \text{and} \qquad S(x)\leftrightarrow -S(x). \tag{11}$$

This verifies the symmetry derived above, which may be interpreted as implying that, for a given scalar potential, the lower components of the wavefunction experience the opposite potential to that experienced by the upper components. Coupled with the necessity of a two-component description of the wavefunction this essentially implies that a massless particle is 'blind' to the sign of the scalar field. A direct result of this feature is that an infinite negative scalar field should confine a massless particle as effectively as an infinite positive scalar field, a property of the scalar potential which has been observed previously in the literature [6].

The above *symmetry of the Dirac equation for the scalar field* is obviously responsible for the results found for the band gap [1, 2], reviewed above. To show exactly how this symmetry manifests itself in the determination of the band gap structure we recall the origin of the band gaps themselves.

In the non-relativistic domain Bragg reflection in the lattice results in the formation of standing waves of either even or odd parity (when the origin is located at one of the δ-function sites and, as $kl = n\pi$, this implies that the odd wavefunction has its nodes occur exactly at the positions of the δ-function potentials comprising the array). A consequence of this property is that the odd wavefunction cannot interact with the lattice; its energy remains unaltered irrespective of the strength of the potential. (It is for this reason that the values $kl = n\pi$ always form one of the band edges [7] in the non-relativistic system.) Conversely the even wavefunction must have its antinodes coincide with the δ-function positions, thus implying that the energy of this state will be raised in energy due to its interaction with the lattice for $\lambda > 0$ (or lowered in energy for $\lambda < 0$). The difference between this value and $kl = n\pi$ then constitutes the energy gap.

In contrast, in the relativistic domain the two-component structure of the wavefunction ensures that if one component of the wavefunction has a node at one point then the other component must have an antinode at the same point (as is obvious from (9)). Therefore, in the relativistic system both the upper and lower band edges must be *functions of the δ-function* strength, a feature which is seen in our results. To see this explicitly we must consider the two-component structure of the wavefunctions.

We begin by defining as even (odd) the wavefunction $\Psi(x)$ where $\Psi_1(x)$ is even (odd) and hence $\Psi_2(x)$ is necessarily odd (even). For an even wavefunction, the upper component $\Psi_1(x)$ peaks at the position of the δ-function potential and consequently we would expect the energy of this state to increase for $\lambda > 0$, in analogy with the non-relativistic result, while the lower component $\Psi_2(x)$ vanishes at the position of the δ-functions, and thus has no interaction with the lattice. Considering now the odd wavefunction we observe that it is the lower component $\Psi_2(x)$ that now interacts with the lattice whilst the upper component $\Psi_1(x)$ is oblivious to its presence. Since in the massless limit $\Psi_2(x)$ sees the negative of the potential experienced by $\Psi_1(x)$ the energy of this state should be lowered by an amount equivalent to that by which the even wavefunction was raised in energy. Thus the band gaps are symmetrical about $kl = n\pi$.

For $\lambda < 0$ we can show in an analogous fashion that the opposite situation to that described above would apply with the even component of $\Psi_1(x)$ ($\Psi_2(x)$ odd) forming the lower gap edge and the odd component of $\Psi_1(x)$ ($\Psi_2(x)$ even) forming the upper gap edge. This interchange of the upper and lower components of the wavefunction as the potential changes sign is thus the major effect arising from the symmetry mentioned above. Thus the band gaps must be independent of the sign of the δ-function potential.

These results lead us to ask the question: 'what happens to the gap structure for a periodic array of δ-function potentials of alternating strengths λ and $-\lambda$?'

To examine this case in detail we consider a potential of the form

$$S(x)=\lambda \sum_{n=1}^{\infty} [\delta(x-nl)-a\delta(x-[n-\tfrac{1}{2}]l)] \tag{12}$$

where $a \in [-1, 1]$. We note that $S(x+l)=S(x)$.

For this potential we can show that the energy gaps for a massless particle are the regions

$$\begin{gathered} 2n\pi-2 \operatorname{Pr} \arctan(p_1) \leqslant kl \leqslant 2n\pi+2 \operatorname{Pr} \arctan(p_1) \\ (2n+1)\pi-2 \operatorname{Pr} \arctan(p_2) \leqslant kl \leqslant (2n+1)\pi+2 \operatorname{Pr} \arctan(p_2) \end{gathered} \tag{13}$$

for $n=1, 2, 3, \ldots$ where

$$p_1=\sqrt{\frac{\cosh(a-1)\lambda-1}{\cosh(a+1)\lambda+1}} \qquad \text{and} \qquad p_2=\sqrt{\frac{\cosh(a+1)\lambda-1}{\cosh(a-1)\lambda+1}}. \tag{14}$$

The three cases of interest are treated below.

(i) $a=0$. Then $p_1=p_2=\tanh(\lambda/2)$ and we find

$$n\pi-2 \operatorname{Pr} \arctan\left(\tanh\frac{\lambda}{2}\right) \leqslant kl \leqslant n\pi+2 \operatorname{Pr} \arctan\left(\tanh\frac{\lambda}{2}\right) \tag{15}$$

in agreement with (1) for $m=d=0$.

(ii) $a=-1$. Then $p_1=\sinh\lambda$ and $p_2=0$ hence the gaps at $kl=(2n+1)\pi$ disappear. (Indeed it can be shown [3] that for these energies the transmission coefficient is unity and hence no reflection occurs and energy gaps cannot form.) This result is not surprising since the periodicity of the potential in (12) is now $S(x+l/2)=S(x)$ and as $\arctan(\sin\lambda)=2\arctan(\tanh[\lambda/2])$ we find the energy gaps to be now given by (15) with $l \to l/2$ in accordance with these observations.

(iii) $a=1$. Then $p_1=0$ and $p_2=\sinh\lambda$ and hence the gaps at $kl=2n\pi$ disappear. (The transmission coefficient is unity for these energies as well [3].) This is a surprising result since the periodicity of the potential is still $S(x+l)=S(x)$. However, we do note that this potential also satisfies the condition

$$S\left(x+\frac{l}{2}\right)=-S(x). \tag{16}$$

The existence of this condition, combined with the inability of the massless particle to determine the sign of the potential, suggests that a pseudo-periodicity of length $l/2$ exists in the array and that this is responsible for the disappearance of the gaps at the values $kl=2n\pi$.

To elucidate this point we note that the phase of a relativistic solution of the Dirac equation may be defined by [2]

$$\tan\phi(k, x)=\frac{-\mathrm{i}\Psi_2(x)}{r\Psi_1(x)} \tag{17}$$

from which we can show that for a scalar δ-function of strength λ the change in phase over the δ-function is given by [1]

$$\mathscr{S}(\phi) = \mathrm{Pr}\arctan\left(\frac{-\tanh\lambda\cos 2\phi}{1-\tanh\lambda\sin 2\phi}\right) \tag{18}$$

for a phase ϕ immediately prior to the δ-function. From this result we can show that the following relationship exists between the phase change over a positive δ-function potential and that for a negative δ-function potential,

$$\mathscr{S}(\phi, -\lambda) = \mathscr{S}\left(\phi + \frac{\pi}{2}, \lambda\right). \tag{19}$$

The net effect on the phase of a δ-function potential of strength $-|\lambda|$ is thus equivalent to that of a δ-function potential of strength $|\lambda|$, combined with the addition of $\pi/2$ to the phase. The appropriate energies for Bragg reflection for the array for $a = 1$ must then be shifted by this amount and consequently are given by the energies $(kl/2) = n\pi + \pi/2$ or $kl = (2n+1)\pi$, as is found.

The origin of this phase shift of $\pi/2$ can also be simply understood. As stated previously when the potential changes sign the values of $\Psi_1(x)$ and $\Psi_2(x)$ are interchanged (i.e. $\Psi_{1/2}(x) \to \Psi_{2/1}(x)$ for $S(x) \to -S(x)$ due to the form of the equations coupling $\Psi_1(x)$ and $\Psi_2(x)$ in (9)). From the relationship for the phase in (17) for the massless case (i.e. $r = 1$), we observe that since $\tan(\phi + \pi/2) = -\cot\phi$, this interchange implies $\phi \to \phi + \pi/2$ as required.

Whilst it is well known that a symmetry associated with invariance under chiral transformations exists in systems comprising massless fermions interacting via external vector fields no such symmetry has been noted for the analogous scalar system, a subject of interest due to its application in some models of the nucleus [8, 9].

Our initial interest in the existence of this symmetry was first kindled during the analysis of some anomalous results from a simple one-dimensional nuclear model we had developed [3] which comprised an ordered array of scalar δ-function potentials with confining boundary conditions. In this model the scalar δ-function potentials were utilized to model the barrier to tunnelling of the massless quarks within the nucleus, a feature of the model which had been shown to produce significant binding energies in a previous treatment incorporating the Klein–Gordon equation [8]. In contrast in our model using the Dirac equation such an arrangement was shown to be exactly unbound; the binding produced was zero irrespective of the δ-function potential strengths.

Similarly, the occurrence of further anomalous results in our analysis of the bandstructure for arrays of scalar δ-function potentials indicated the existence of such a scalar symmetry, the origin of which we have detailed above.

The most visible consequence that we have thus far observed as originating from this symmetry is the complete disappearance of every second energy gap in the alternating array of scalar δ-function potentials. This effect, however, is not merely confined to such an analytically simple system as that involving the δ-function potentials. In fact any potential which satisfies (16) should exhibit this pseudo-periodicity and its consequent halving of the bandstructure.

To investigate this effect we have studied the bandstructure that occurs for a scalar cosine potential, one of the simpler potentials displaying this periodicity. For this potential we found [10] that the pseudo-periodicity of the potential causes the disappearance of the alternate band gaps exactly as expected.

The properties described above suggest that, while the consequences of this symmetry may be of less practical interest than those associated with the chiral symmetry, they are no less fascinating.

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