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LETTER TO THE EDITOR

A simple numerical method for the determination of relativistic one-dimensional band structures

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Abstract. A discretized form of the one-dimensional Dirac equation is solved to study relativistic band structures. Properties of periodic continued fractions are used to find the dispersion relation inside allowed bands. The Mathieu potential is considered and it is found that relativistic effects cause a reduction of the width of allowed bands and gaps.

Properties of relativistic particles in one-dimensional periodic structures are of interest in solid state (Roy 1986) and nuclear physics (McKellar and Stephenson 1987, Clerk and McKellar 1990). Exact solutions of the Dirac equation for the Kronig-Penney potential—periodic array of square wells or barriers—have been found (Stéslicka and Davison 1970), even for the δ-function limit—wells or barriers with zero width and constant area—in monoatomic and polyatomic crystals (Dominguez-Adame 1987, 1989 and references therein). Nevertheless, better approximations to real systems may be reached by means of more structured potentials. In this way, the Mathieu potential is a good candidate for the crystal field for high energy electrons (Stéslicka *et al* 1970). Unfortunately, no exact solutions of the Dirac equation for potentials other than the Kronig-Penney potential are available. An alternative way to study relativistic effects on the energy spectrum could be the perturbative approach, by treating the mass-velocity correction as a perturbation term in the Schrödinger Hamiltonian (Stéslicka *et al* 1970). This approximation, however, remains valid whenever the momentum of the particle is negligible compared with its rest mass. Therefore, more accurate results may be found by solving numerically the Dirac equation.

There exist, at present, several numerical methods for one-dimensional band calculations based on the discretized Schrödinger equation (Vigneron and Lambin 1979, Killingbeck 1980), whereas the Dirac equation has received no attention. The present letter deals with a simple numerical method to solve the Dirac equation for one-dimensional periodic potentials. Our treatment adopts ideas of the previous work of Vigneron and Lambin (1979) for non-relativistic band structures. These authors have used a continued fraction approach to find the dispersion relation inside the allowed bands and the energy of band edges. We wish to show that this approach can be generalized to relativistic calculations with a little additional effort. Besides the periodicity, we require the potential to be symmetric around atomic positions. This limitation is not a several restriction to simulate real crystals.

We start with the one-dimensional Dirac equation for steady states ($\hbar = c = 1$)

$$[-i\alpha\partial + \beta m + V(x) - E]\psi(x) = 0 \tag{1}$$

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where $\psi(x)$ is the two-component wavefunction, α and β are 2×2 traceless, Hermitian matrices with square unity, and $\partial \equiv \mathrm{d}/\mathrm{d}x$. To solve the Dirac equation we set the standard representation $\alpha = \alpha_x$ and $\beta = \sigma_z$, σs being the Pauli matrices. Denoting by ϕ and χ the upper and lower components of the wavefunction, we obtain

$$-\mathrm{i}\partial\phi(x)+[V(x)-E-m]\chi(x)=0 \tag{2a}$$

$$-\mathrm{i}\partial\chi(x)+[V(x)-E+m]\phi(x)=0. \tag{2b}$$

For simplicity, we define $\varepsilon = E - m$ and take $m = \frac{1}{2}$. Hence we get

$$\chi(x)=\frac{\mathrm{i}\partial\phi(x)}{V(x)-\varepsilon-1} \tag{3a}$$

and

$$\partial^2\phi(x)-\frac{\partial V(x)}{V(x)-\varepsilon-1}\partial\phi(x)+[V^2(x)+\varepsilon(\varepsilon+1)-(2\varepsilon+1)V(x)]\phi(x)=0. \tag{3b}$$

We can deal only with the upper component since the lower component may be found using (3*a*).

Now we consider periodic potentials such that $V(x+L)=V(x)$, L being the period. Let us divide the unit cell $[0, L]$ into $N+1$ equal parts of length $h = L/(N+1)$, which defines the grid $x_n = nh$ $(n=0, 1, \ldots, N)$. The discretized form of (3*b*) at any point of the grid is

$$(1-a_n)\phi(x_{n+1})+(1+a_n)\phi(x_{n-1})-(2-b_n)\phi(x_n)=0 \tag{4}$$

where

$$a_n=(V(x_{n+1})-V(x_{n-1}))/4(V(x_n)-\varepsilon-1) \tag{5a}$$

$$b_n=h^2(V^2(x_n)+\varepsilon(\varepsilon+1)-(2\varepsilon+1)V(x_n)). \tag{5b}$$

Since the Bloch theorem must be satisfied, the upper component may be written as $\phi(x)=\exp(\mathrm{i}kx)U(x)$, with $U(x+L)=U(x)$ (equation (3) ensures that $\chi(x)$ is also a Bloch function). If we define

$$\alpha_n=(1-a_n)/(1+a_n) \tag{6a}$$

$$\beta_n=(2-b_n)/(1+a_n) \tag{6b}$$

$$R_n=\mathrm{e}^{-\mathrm{i}kh}U(x_n)/U(x_{n+1}) \tag{6c}$$

one can find the recurrence relation

$$R_{n-1}=\beta_n-\alpha_n/R_n \qquad n=1, 2, \ldots, N+1. \tag{7}$$

The definition of R_n and the periodicity of $U(x)$ give rise to the boundary condition $R_0 = R_{N+1}$. Hence (7) leads to the following periodic continued fraction

$$R_0=\beta_1+\cfrac{-\alpha_1}{\beta_2+\cfrac{-\alpha_2}{\beta_9+\ddots\cfrac{-\alpha_N}{\beta_{N+1}+(-\alpha_{N+1})/R_0}}} \tag{8}$$

which may be regarded as an equation for r_0. To solve (8) we define the nth numerator A_n denominator B_n through the relations (Wall 1967)

$$\begin{aligned} A_{n+1}&=\beta_{n+2}A_n-\alpha_{n+1}A_{n-1}\\ B_{n+1}&=\beta_{n+2}B_n-\alpha_{n+1}B_{n-1} \qquad n=0, 1, \ldots, N \end{aligned} \tag{9}$$

with the initial values $A_{-1}=B_0=1$, $A_0=\beta_1$ and $B_{-1}=0$. Note that $A_n=A_n(\varepsilon)$ and $B_n=B_n(\varepsilon)$ but they do not explicitly depend on any particular value of k. The determinant of the transformation is

$$A_{N-1}B_N-A_NB_{N-1}=\prod_{n=0}^{N}\alpha_n\equiv\delta_N. \tag{10}$$

The periodicity of the continued fraction allows us to write the equation for R_0 in terms of As and Bs

$$B_NR_0^2-(\alpha_{N+1}B_{N-1}+A_N)R_0+\alpha_{N+1}A_{N-1}=0. \tag{11}$$

Some particular results are required to complete our treatment. We quote these results as follows

$$\prod_{n=0}^{N}R_n=\mathrm{e}^{-\mathrm{i}kL} \tag{12a}$$

$$\prod_{n=0}^{N}R_n=A_{N-1}R_N-\alpha_NA_{N-2} \tag{12b}$$

$$\prod_{n=0}^{N}R_n=B_NR_0-\alpha_{N+1}B_{N-1}. \tag{12c}$$

The first equation is found by substituting the value of R_n (6c) in the left-hand side. Equation (12b) may be verified by induction, by analogy with the non-relativistic treatment of Vigneron and Lambin. Finally, (12c) is easily checked by using (11) and (12b).

If $V(x)$ is symmetric around atomic positions, one can show that (see appendix)

$$\delta_{N+1}=\prod_{n=0}^{N+1}\alpha_n=1. \tag{12d}$$

Note that this result is straightforward in the non-relativistic limit, since $\alpha_n\to 1$. Nevertheless, the result (12d) is only valid in the relativistic case provided $V(x)=V(-x)$.

In order to study the dispersion relation $\varepsilon=\varepsilon(k)$ of the Dirac particle in the periodic potential, we analyse the discriminant of the algebraic equation (11), defined as

$$\Delta\equiv(\alpha_{N+1}B_{N-1}+A_N)^2-4\alpha_{N+1}A_{N-1}B_N. \tag{13}$$

Using (10) and (12d), the discriminant may be written as

$$\Delta=(A_N-\alpha_{N+1}B_{N-1})^2-4. \tag{14}$$

There exist two possible cases, namely

(a) $\Delta\leqslant 0$. From (11) we obtain

$$R_0=\frac{1}{2B_N}(A_N+\alpha_{N+1}B_{N-1})\pm\frac{\mathrm{i}}{2B_N}\sqrt{-\Delta}. \tag{15}$$

Using the above results, (12), and defining the energy-dependent quantity

$$P_{N+1}=P_{N+1}(\varepsilon)\equiv(A_N-\alpha_{N+1}B_{N-1})/2 \tag{16}$$

which is calculated recursively from (9), one can get

$$\mathrm{e}^{-\mathrm{i}kL}=P_{N+1}(\varepsilon)\pm\mathrm{i}\sqrt{1-P_{N+1}^2(\varepsilon)} \tag{17}$$

so the dispersion relation is found to be

$$\cos kL = P_{N+1}(\varepsilon). \tag{18}$$

Therefore, the dispersion relation admits real values for the crystal momentum k and the corresponding energy belongs to an allowed band. From (17) we find that $\varepsilon(k) = \varepsilon(-k)$, as expected from time reversal invariance.

(b) $\Delta > 0$. In a similar way, it is an easy matter to show that in this case $|\exp(ikL)| > 1$ and then the crystal momentum k becomes complex. Hence forbidden gaps appear since the corresponding wavefunctions diverge at spatial infinity.

As an example of this method, we have studied numerically the relativistic Mathieu problem. The Mathieu potential can explain the interaction of high-energy electrons with crystals, so the relativistic treatment is indeed required. This potential is written as

$$V(x) = V_0 \cos 2x$$

which satisfies the condition $V(x) = V(-x)$. The convergence of the numerical approach has been discussed by Vigneron and Lambin for the non-relativistic case. In the case of the Dirac equation, we have checked that accurate results are usually found taking about 50–100 points in the subdivision. However, the number of these points have to be greater to calculate the dispersion relation of higher bands. For small values of V_0, both non-relativistic and relativistic numerical dispersion relations are rather similar, as could be expected from the general features of the Dirac equation. For large values of V_0, however, both treatments show different features, as seen in figure 1 for $V_0 = 0.2 = 0.4m$. We observe that relativistic effects reduce the width of allowed bands and gaps. Figure 2 shows the width of the first allowed band $\Delta\varepsilon_1$ as a function of the potential depth V_0, illustrating the reduction just mentioned. The variation of the first gap against V_0 is depicted in figure 3. This gap is of the form $\varepsilon_g = V_0$ in the non-relativistic case. In contrast, ε_g presents a sublinear dependence on V_0 for relativistic particles (the broken line shows the linear extrapolation of values up to $V_0 = 0.2$). The potential becomes overcritical for values of V_0 larger than $2m = 1$, since the minimum of $V(x)$ dives into the negative-energy states. Hence a single-particle treatment losses validity.

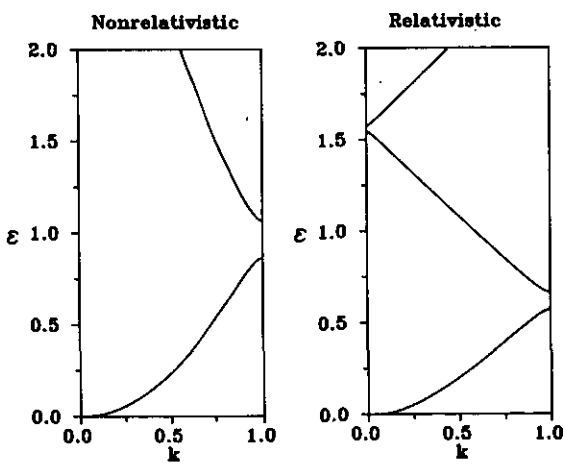

Figure 1. Non-relativistic and relativistic band structures for a particle of mass $m = 0.5$ in the potential $V(x) = V_0 \cos 2x$, with $V_0 = 0.2$.

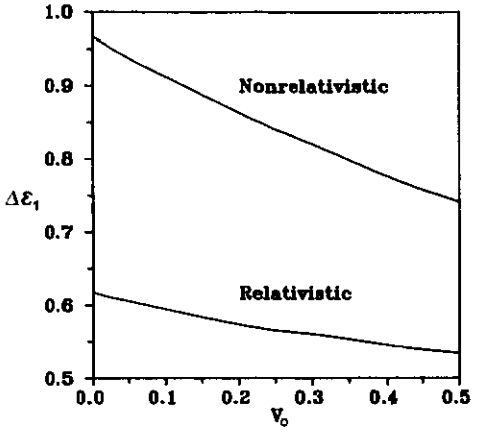

Figure 2. Variation of the width of the first allowed band as a function of the potential depth V_0, for both non-relativistic and relativistic treatments.

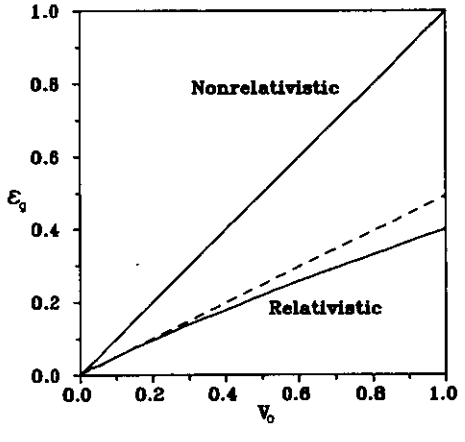

Figure 3. Variation of the width of the first gap as a function of the potential depth V_0, for both non-relativistic and relativistic treatments. The broken line shows the linear extrapolation for values up to $V_0 = 0.2$ for relativistic particles.

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Appendix

Equation (12*d*) can be written in the form

$$\delta_{N+1} = \frac{F(h)}{F(-h)} \tag{A1}$$

where

$$F(h) = \prod_{n=0}^{N+1} \{4[V(x_n) - \varepsilon - 1] - V(x_n + h) + V(x_n - h)\}. \tag{A2}$$

Reversing the order of the product with the substitution $n \to N+1-n$ and using that $x_{N+1-n} = L - x_n$ we obtain

$$F(h) = \prod_{n=0}^{N+1} \{4[V(L-x_n) - \varepsilon - 1] - V(L-x_n+h) + V(L-x_n-h)\}. \quad \text{(A3)}$$

The periodicity of the potential and the symmetry around the atomic positions lead to $V(L-x_n) = V(x_n)$, so we finally find that the function $F(h)$ satisfies

$$F(h) = F(-h). \quad \text{(A4)}$$

Therefore, equation (A1) ensures that $\delta_{N+1} = 1$.

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