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# A relativistic equation for a slowly varying potential

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**Abstract.** A relativistic equation is derived for a slowly varying potential by suitably approximating the one-dimensional Dirac equation. This equation is shown to be akin to the Schrödinger equation with an effective potential and effective eigenvalues. An iterative procedure for solving this equation is indicated. As an application, the relativistic treatment of the Mathieu potential on the basis of this equation is considered and results are compared with those obtained by solving the exact one-dimensional Dirac equation. These results are likely to take adequate account of the relativistic impacts on electrons near Fermi levels in metals.

## 1. Introduction

The quantum mechanical behaviour of one-dimensional (1D) electrons with relativistic velocities has to be studied using the 1D Dirac equation. The 1D Dirac equation attracted the attention of many authors [1, 2] almost immediately after the formulation of the original Dirac equation. In particular, the 1D Dirac equation has found widespread applications in condensed matter physics [3–14].

In solving the Dirac equation, it is obviously necessary to handle coupled first-order differential equations involving the elements of the relevant spinors. Approximated solutions are frequently obtained by neglecting some elements of the spinor which are small only in the non-relativistic limit. In this paper, we report an approximate form of the 1D Dirac equation for slowly varying potential and indicate how this equation can be made akin to the Schrödinger equation by introducing the idea of an effective potential and effective eigenvalues. Furthermore, we (i) compare critically this equation with other approximate 1D Dirac equations relevant to high-energy electrons; (ii) elucidate an iterative procedure for solving this equation; (iii) point out the systems to which the equation can be applied; and (iv) indicate its degree of utility considering the case of the Mathieu potential.

The paper is organized as follows. Some general aspects of the 1D Dirac equation, which are required for obtaining our approximate equation, are first discussed in section 2. The derivation of the approximate equation and some related issues are presented in section 3. To check the accuracy of the approximate equation, the relativistic Mathieu potential, which is of interest in condensed matter physics, is considered in section 4. Finally, in section 5, the salient features of our equation, and its applicability, are discussed.

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## 2. Some aspects of the 1D Dirac equation

The (1D) time-independent Dirac equation for an electron of rest mass $m$, moving in an electrostatic-like potential $V(x)$ along the $x$-axis, appears as [3, 15]

$$-i\hbar c\sigma_x \frac{d\psi}{dx} + mc^2\sigma_z\psi = [E_R - V(x)]\psi \tag{1}$$

where $\psi$ is a two-component spinor given by

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \tag{2}$$

and where the $\sigma$'s denote the $2 \times 2$ Pauli matrices, $E_R$ is the relativistic energy eigenvalue and $c$ is the velocity of light. Equation (1) can be split into the following equations:

$$-i\hbar c\psi_2' = [\varepsilon - V(x)]\psi_1 \tag{3a}$$

$$-i\hbar c\psi_1' = [\varepsilon + 2mc^2 - V(x)]\psi_2. \tag{3b}$$

For convenience, we introduce the notation $\varepsilon \equiv E_R - mc^2$; $\varepsilon$ is nothing but the electron energy without the rest-mass energy and it can therefore be directly compared with the non-relativistic energy. The primes used in the above equations, and subsequently throughout this paper, denote differentiation with respect to $x$. We can decouple (3), in the standard fashion, to obtain the following two (second-order) equations:

$$\psi_1'' + f(x)\psi_1' + q^2(x)\psi_1 = 0 \tag{4a}$$

$$\psi_2'' + g(x)\psi_2' + q^2(x)\psi_2 = 0 \tag{4b}$$

with

$$f(x) = \frac{V'(x)}{\varepsilon + 2mc^2 - V(x)}$$

$$g(x) = \frac{V'(x)}{\varepsilon - V(x)}$$

$$q^2(x) = \left(\frac{1}{\hbar^2c^2}\right)[\varepsilon - V(x)][\varepsilon + 2mc^2 - V(x)].$$

Let $F_1(x)$ and $G_1(x)$ be two particular solutions of (4$a$). Then, its general solution can be simply written as follows

$$\psi_1 = aF_1(x) + bG_1(x) \tag{5}$$

where $a$ and $b$ are two arbitrary constants. Since the lower component $\psi_2$ is related to the upper component $\psi_1$ through (3$b$), we can obtain the spinor $\psi$ as

$$\psi = a\begin{pmatrix} F_1(x) \\ F_2(x) \end{pmatrix} + b\begin{pmatrix} G_1(x) \\ G_2(x) \end{pmatrix} \tag{6}$$

where we have defined

$$F_2(x) = \frac{-i\hbar c F_1'(x)}{\varepsilon + 2mc^2 - V(x)} \tag{7a}$$

$$G_2(x) = \frac{-i\hbar c G_1'(x)}{\varepsilon + 2mc^2 - V(x)}. \tag{7b}$$

The general spinor solution of the 1D Dirac equation (1) is given by (6). We insert here the form of (6) for the special case of a constant potential, as we shall require this form later. For a constant potential, say, $V_0$, the two functions $f(x)$ and $g(x)$ appearing in (4*a*) and (4*b*) vanish and $q(x)$ is constant. Solutions of (4*a*) and (4*b*) are plane waves of the form

$$F_1(x) = \exp(iKx) \tag{8a}$$

$$G_1(x) = \exp(-iKx) \tag{8b}$$

where $K^2 = (\varepsilon - V_0)(\varepsilon + 2mc^2 - V_0)/\hbar^2c^2$. Using (7), we obtain the following spinor for a constant potential

$$\psi = a\begin{pmatrix} 1 \\ \gamma \end{pmatrix}\exp(iKx) + b\begin{pmatrix} 1 \\ -\gamma \end{pmatrix}\exp(-iKx) \tag{9}$$

with $\gamma \equiv \sqrt{(\varepsilon - V_0)/(\varepsilon + 2mc^2 - V_0)}$.

## 3. The approximate relativistic equation (ARE) and related aspects

### *3.1. Derivation of the ARE*

The general spinor $\psi$, given by (6), can be written as

$$\psi = a\begin{pmatrix} 1 \\ A(x) \end{pmatrix}F_1(x) + b\begin{pmatrix} 1 \\ B(x) \end{pmatrix}G_1(x) \tag{10}$$

where

$$A(x) = \frac{F_2(x)}{F_1(x)} \qquad B(x) = \frac{G_2(x)}{G_1(x)}.$$

Hence, $A(x)$ and $B(x)$ may be used to obtain the relative phase of the upper and lower components of the particular spinors appearing in (10). Comparing (9) and (10), we find

$$A = \gamma \tag{11a}$$

$$B = -\gamma \tag{11b}$$

for the constant-potential case. For a slowly varying potential, we can reasonably assume that $A(x)$ and $B(x)$ correspond to (11*a*) and (11*b*), respectively, with replacement of $V_0$ by the slowly varying potential $V(x)$. The value of $\gamma$ is always less than unity and it increases with the velocity of the electron. However, even for velocities as high as $10^9$ cm s$^{-1}$, which

is of the order of velocities in crystalline solids of heavy atoms, $\gamma$ is around $10^{-4}$. We thus have the following condition on $\gamma$ for such velocities

$$\gamma \ll 1. \tag{12}$$

As $|A(x)|$ and $|B(x)|$ are formally close to $\gamma$ for a slowly varying potential, they would also conform to the following condition for electron velocities going up to about $10^9$ cm $s^{-1}$:

$$A(x) \ll 1 \tag{13a}$$

$$B(x) \ll 1. \tag{13b}$$

Using (10) and (13), we have

$$\psi = a\begin{pmatrix}1\\0\end{pmatrix} F_1(x) + b\begin{pmatrix}1\\0\end{pmatrix} G_1(x) \tag{14}$$

where $F_1(x)$ and $G_1(x)$ are particular solutions of (4*a*). Since we are considering high-velocity electrons in a slowly varying potential and $2mc^2$ is about 1 MeV, we can assume that

$$V'(x) \ll \varepsilon + 2mc^2 - V(x) \tag{15a}$$

$$f(x) \simeq 0. \tag{15b}$$

Therefore, taking $\phi$ for $F_1$ or $G_1$, we can reduce equation (4*b*) to

$$\phi''(x) + \frac{2m}{\hbar^2}[\eta - U(x)]\phi(x) = 0 \tag{16}$$

where

$$\eta = \frac{\varepsilon(\varepsilon + 2mc^2)}{2mc^2} \tag{17a}$$

$$U(x) = V(x) + V_1(x) \tag{17b}$$

$$V_1(x) = \frac{\varepsilon V(x)}{mc^2} - \frac{V^2(x)}{2mc^2}. \tag{17c}$$

The ARE we sought to derive is given by (16). The form of this equation is seen to be the same as the Schrödinger equation for a particle moving in a potential $U(x)$ with eigenvalue $\eta$. We may interpret $U(x)$ as an effective potential and $\eta$ as an effective eigenvalue. Instead of solving the 1D Dirac equation (1) involved with the two-component spinor $\psi$, we may now deal with (16) (with only a one-component wavefunction ($\phi$)) to obtain fairly reliable information about the quantum mechanical behaviour of high-energy electrons in a slowly varying potential.

*3.2. Comparison between ARE and other approximate relativistic equations*

Some authors [16] have used the following approximate equation to study relativistic impacts on the motion of electrons in a potential $V(x)$

$$\psi''(x) + \frac{2m}{\hbar^2}[E + W_1 - V(x)]\psi(x) = 0 \tag{18}$$

where $E$ is the energy eigenvalue and

$$W_1 = \frac{p^4}{8m^3c^2}. \tag{19}$$

$W_1$ decribes the mass–energy correction term, up to a first-order approximation, applied to the Hamiltonian given below

$$H = \sqrt{p^2c^2 + m^2c^4} - mc^2 + V(x). \tag{20}$$

Equation (18) is a Schrödinger equation with a Hamiltonian given by

$$H_s = H_0 - W_1 \tag{21}$$

where $H_0 = p^2/2m$ is the non-relativistic Hamiltonian. We note that (16) can be rewritten as

$$\psi''(x) + \frac{2m}{\hbar^2}[\varepsilon + W_1 - V(x) - V_1(x)]\psi(x) = 0. \tag{22}$$

In arriving at this equation, we have used the fact that $\varepsilon \simeq p^2/2m$; this assumption is not unjustified for high-energy electrons because the kinetic energy of such electrons is likely to be much higher than their potential energy. Now, equation (22) (or equivalently (16)) is seen to differ from (18) with respect to the presence of the term $V_1(x)$ in the former. Equation (18) is derived by adding the term $W_1$ to the non-relativistic Hamiltonian $H_0$. On the other hand, equation (22) (or (16)) is extracted from the 1D Dirac equation (1) (which is involved with a two-component spinor) and the occurrence of $V_1(x)$ is a consequence of this derivational procedure.

*3.3. Solution of the ARE*

Equation (16) may be solved by an iterative procedure. To arrive at the procedure, we first write this equation as

$$\phi''(x) + \frac{2m}{\hbar^2}[\eta - V_2(x) - V_3(x)]\phi(x) = 0 \tag{23}$$

where

$$V_2(x) = V(x) - \frac{V^2(x)}{2mc^2} \tag{24a}$$

$$V_3(x) = \frac{\varepsilon V(x)}{mc^2}. \tag{24b}$$

The entity $\varepsilon$ would generally conform to the condition $\varepsilon > -mc^2$, i.e. the quantum state does not dive into the negative energy continuum. Using this condition, along with the definition of the parameter $\eta$ (17*a*), one obtains

$$\varepsilon = mc^2\left[-1+\sqrt{1+\eta\hbar^2/m}\right]. \tag{25}$$

The term $V_3$ in (23) involves $\varepsilon$ and, hence, $\eta$. The presence of this term makes it difficult to solve (23). However, the value of $V_3$ is likely to be much smaller than $V_2$, due to the occurrence of the factor $mc^2$ in the denominator of the former. Hence, we can develop an iterative procedure for solving (24) as follows. We first take $V_3 = 0$ and solve the following equation for $\eta$

$$\phi_0''(x) + \frac{2m}{\hbar^2}[\eta - V_2(x)]\phi_0(x) = 0. \tag{26}$$

With $\eta$ thus obtained, we get $\varepsilon$ from (25) and then $V_3$ from (24*b*). With this $V_3$ we can solve (16) and the process is repeated until we attain self-consistency.

## 4. The relativistic Mathieu problem

In this section we study the relativistic Mathieu problem, that is, the dynamics of a relativistic particle under the action of a cosine potential. This allows us to investigate the accuracy of the ARE in dealing with a potential of interest in solid-state physics. In fact, the Mathieu potential can explain the interaction of high-energy electrons with crystals [16], so a relativistic treatment for this potential is indeed required. While the non-relativistic Mathieu problem has been well studied, and analytical solutions are available, very little work has been done in the relativistic regime. As regards the research done in this field, Steslicka *et al* [16] looked at the first-order relativistic corrections to the Schrödinger equation, whereas Méndez *et al* [17, 18] devised techniques for solving the 1D Dirac equation for general periodic potentials with application to the Mathieu potential. Scalar-like cosine potentials connected with 1D relativistic nuclear models were considered by Clerk [19].

The potential used in our numerical study is $V(x) = 0.2\cos 2x$. In what follows we use units such that $\hbar = 2m = c = 1$; the lattice period is $L = \pi$ in our case. Since the potential is periodic, the Bloch theorem holds so that the solution of the 1D Dirac equation (1) is of the form $\psi = \exp(ikx)\zeta$, where $\zeta$ is periodic with the same period as that of the potential, and $k$ is the crystal momentum. Since the effective potential $U(x)$, appearing in (16), is also periodic (with period $L = \pi$), the general solution of the ARE satisfies the Bloch theorem. We aim to compare the dispersion relation (energy against crystal momentum) obtained with ARE (16) with the dispersion relation obtained by directly solving the 1D Dirac equation (1). In addition, relativistic results are compared with non-relativistic ones. The wave equations (Schrödinger, Dirac, ARE) for the Mathieu potential have been solved numerically by following a technique outlined by Méndez *et al* [17] based on the properties of periodic-continued fractions. To this end, the corresponding wave equation is discretized on a grid of the unit cell $[0, \pi]$ (100 points are more than enough to obtain very accurate results); energy band edges and the dispersion law inside allowed bands are found by means of three-term recurrence relations (see [17] for details). Results are presented in figure 1.

Comparing the plots in figure 1 corresponding to relativistic calculations, we find that the dispersion relation given by the ARE agrees well with that corresponding to the 1D Dirac

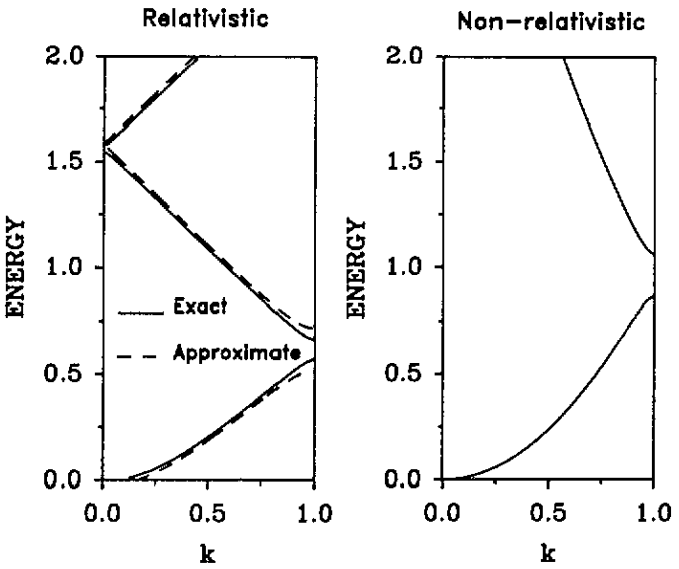


**Figure 1.** Relativistic (left) and non-relativistic (right) dispersion relations in the potential $V(x) = 0.2\cos 2x$ for a particle of rest mass $m = 0.5$. The ARE results (dashed curve) fit well with the exact results (solid curve) obtained by directly solving the 1D Dirac equation.

equation, except for $k$ values near the edge of the Brillouin zone ($k = 1$). The ARE predicts an energy gap somewhat larger than the (truly) relativistic value. It is worth mentioning that the ARE gap is almost the same as the non-relativistic one. This result agrees well with the perturbative calculations of Steslicka *et al* [16], who found that relativity (up to first order) causes a *shrinkage* of allowed bands, whereas the gaps remain unchanged. However, it is known that the 1D Dirac equation predicts a *shrinkage* of both allowed bands and gaps [17], as seen in figure 1. Hence, we may conclude that the decrease of the gap width comes mainly from the gradient of the potential which is neglected in ARE.

## 5. Discussion and conclusions

The course of derivation of our approximately relativistic equation (16) shows that it rests on two assumptions: (i) that $V(x)$ is slowly varying, and (ii) that the maximum velocity of the electrons goes to about $10^9$ cm $s^{-1}$. Both these assumptions are satisfied by electrons near the Fermi energy level in metals. Also, we have noted in the previous section that there exists a high degree of agreement between the results yielded by ARE (16) and the 1D Dirac equation. Hence, equation (16) is likely to provide an adequate account of the relativistic effects on the electronic properties of metals without requiring us to tackle the complications involved with two-component spinors in the corresponding Dirac equation. As an approximation, equation (16) is more accurate than (18). This is because the former incorporates a mass–energy correction as well as some influence from the (truly relativistic) Dirac equation, whereas the latter only includes the mass–energy correction.

## References


[1] Nikolosky K 1930 *Z. Phys.* **62** 677
[2] Sauter F 1931 *Z. Phys.* **69** 742
[3] Davison S G and Steslicka M 1969 *J. Phys. C: Solid State Phys.* **2** 1802
[4] Glasser M L and Davison S G 1970 *Int. J. Quantum Chem.* 4 867
[5] Subramanian R and Bhagwat K V 1971 *Phys. Status Solidi* b **48** 399
[6] Sen Gupta N D 1974 *Phys. Status Solidi* b **65** 351
[7] Sutherland B and Mattis D C 1981 *Phys. Rev.* A **24** 1194
[8] Roy C L 1982 *Physica* B **113** 94
[9] Roy C L and Pandey J S 1986 *Physica* A **137** 389
[10] Domínguez-Adame F 1989 *J. Phys.: Condens. Matter* **1** 109
[11] Domínguez-Adame F and Sánchez A 1991 *Phys. Lett.* **159A** 153
[12] Roy C L and Khan Arif 1992 *Indian J. Pure Appl. Phys.* **30** 432
[13] Roy C L and Khan Arif 1993 *J. Phys.: Condens. Matter* at press
[14] Domínguez-Adame F, Maciá E, Arif Khan and Roy C L 1994 (submitted for publication)
[15] Davydov A S 1965 *Quantum Mechanics* (Oxford: Pergamon) p 22
[16] Steslicka M, Davison S G and Fairbairn W M 1970 *J. Phys. C: Solid State Phys.* **3** 1207
[17] Méndez B and Domínguez-Adame F 1991 *J. Phys. A: Math. Gen.* **24** L331
[18] Méndez B, Domínguez-Adame F and Maciá E 1993 *J. Phys. A: Math. Gen.* **26** 171
[19] Clerk G 1991 *PhD Thesis* University of Melbourne, p 115