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Dirac states of relativistic electrons channeled in a crystal

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Abstract

Dirac wave functions for high energy electrons channeled in crystals are obtained for crystal string potentials. Specifically, we study partial cylindrical wave expansions for cylindrical constant and $1/\rho$ potentials. The periodicity along the crystal axis is taken into account as a perturbation to the cylindrical wave functions. We also find a Sommerfeld - Maue like solution for the $1/\rho$ potential.

1 INTRODUCTION

The phenomenon of the channeling states of charged particles in a crystal was introduced by J.Lindhard in his classical paper [1] in 1965. The existence of bound states of channeled electrons was pointed out [2] by Vorobiev's group as early as in 1973. In fact, energies and angular distributions were calculated and compared for bound states of channeling electrons of energies of a few MeV. In fact, they were the first to use a string potential $V(\rho) \sim 1/\rho$, showing that this potential is closely similar to the Lindhard potential [1]. More recent work involves crystal inhanced bremstrahlung and pair production , also for much higher energies , which is reviewed in recent books and articles [3].

In the present paper we derive Dirac channeling wave functions including relativistic effects and spin effects, for use in calculations of channeling problems in crystals for very high electron or positron energies. The solutions are given as cylindrical waves for a transverse potential $V(\rho)$, with (ρ, ϕ, z) cylindrical coordinates. To obtain specific solutions we consider the $1/\rho$ dependent potential where Dirac solution including the order

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$\sqrt{\varepsilon/E}$ is obtained , with ε the transerve energy and E the total energy of the relativistic electron or positron. Both continuous and bound states are considered. We also include the effect of the lattice periodicity , the dependence of the potential on z . Since the main effect of the crystal in this high energy region comes from the transverse degree of freedom , in particular for bound electron states , the effects of the longitudinal potential variation is included as a perturbation . We also give the Dirac wave functions for (step - wise) constant transverse potential which can be of use for channeling conditions where strong screening effect are important. Perhaps the most convenient wave functions for high energy applications are Sommerfeld - Maue like wave functions. These are obtained in Chaper 6 for a $1/\rho$ potential.

2 THE DIRAC EQUATION IN CYLINDRICAL COORDINATES

The Dirac equation

$$(i\vec{\gamma}\nabla + \gamma_0(E - V(\rho)) - m)\psi(\vec{r}) = 0 \ , \tag{2.1}$$

for a static, cylindrically symmetric potential $V(\rho)$ is in the standard representation

$$\vec{\gamma} = \begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix} \ , \ \gamma_0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \ , \ \psi(\vec{r}) = N \begin{pmatrix} \varphi(\rho,\phi) \\ \chi(\rho,\phi) \end{pmatrix} e^{ip_z z} \ , \tag{2.2}$$

given by

$$\begin{aligned} (i\vec{\sigma}_\perp \nabla_\perp - \sigma_z p_z)\chi + (E - V(\rho) - m)\varphi = 0 \ , \\ (i\vec{\sigma}_\perp \nabla_\perp - \sigma_z p_z)\varphi + (E - V(\rho) + m)\chi = 0 \ , \end{aligned} \tag{2.3}$$

where

$$\vec{\sigma}_\perp \nabla_\perp = \sigma_\rho \frac{\partial}{\partial \rho} + \sigma_\phi \frac{1}{\rho}\frac{\partial}{\partial \phi} \ , \tag{2.4}$$

with $\sigma_\rho = \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix}$ and $\sigma_\phi = \begin{pmatrix} 0 & -ie^{-i\phi} \\ ie^{i\phi} & 0 \end{pmatrix}$, satisfying the usual $SU(2)$ characteristic equation

$$[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k \ ,$$

with indices $(\rho, \phi, z) = (1, 2, 3)$.

From Eq.(2.3) follows

$$\chi = (E - V + m)^{-1}(\sigma_z p_z - i\vec{\sigma}_\perp \nabla_\perp)\varphi \ ,$$

and the Dirac wave function is given by

$$\psi(\vec{r}) = N \begin{pmatrix} 1 \\ (E - V + m)^{-1}(\sigma_z p_z - i\vec{\sigma}_\perp \nabla_\perp) \end{pmatrix} \varphi(\rho, \phi) e^{ip_z z} \ , \tag{2.5}$$

where the two component spinor $\varphi(\rho, \phi)$ satisfies the second order equation

$$\begin{aligned} &[\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial \phi^2} + (E - V)^2 - E_z^2 + \\ &i\sigma_\rho \frac{1}{(E - V + m)} \frac{dV}{d\rho}(\sigma_z p_z - i\vec{\sigma}_\perp \nabla_\perp)]\varphi(\rho, \phi) = 0 \ , \end{aligned} \tag{2.6}$$

where we have introduced the "longitudinal energy" E_z by

$$E_z^2 = p_z^2 + m^2. \tag{2.7}$$

The presence of $\sigma_\rho \vec{\sigma}_\perp \nabla_\perp$ in the last term of Eq.(2.6) shows that $\varphi(\rho, \phi)$ is not an eigenstate of the z - component of the angular monentum

$$L_z = -i\frac{\partial}{\partial \phi} \ .$$

The spinor $\varphi(\rho, \phi)$ is a superposition of states of $L_z = \mu$ and $L_z = \mu + 1$ as is easily seen since $\sigma_\rho \sigma_z = i\sigma_\phi$ essentially interchanges the ρ - dependent wave function $u(\rho)$ and $v(\rho)$ in $\varphi(\rho, \phi)$:

$$\varphi(\rho, \phi) = \begin{pmatrix} u(\rho) e^{i\mu\phi} \\ v(\rho) e^{i(\mu+1)\phi} \end{pmatrix} \ , \ i\sigma_\phi \varphi(\rho, \phi) = \begin{pmatrix} v(\rho) e^{i\mu\phi} \\ -u(\rho) e^{i(\mu+1)\phi} \end{pmatrix} \ . \tag{2.8}$$

In fact $\varphi(\rho, \phi)$ is an eigenstate of the z component of the total angular momentum

$$J_z = L_z + s_z = \mu + \frac{1}{2}.$$

The two differential equations of second order are from (2.6)

$$\begin{aligned} &(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho} - \frac{\mu^2}{\rho^2} + (E - V)^2 - E_z^2)u(\rho) + \\ &\frac{i}{(E - V + m)} \frac{dV}{d\rho}[i(\frac{\partial}{\partial \rho} - \frac{\mu}{\rho})u(\rho) - p_z v(\rho)] = 0 \ , \end{aligned}$$

$$(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{(\mu+1)^2}{\rho^2}+(E-V)^2-E_z^2)v(\rho)+$$
$$\frac{i}{(E-V+m)}\frac{dV}{d\rho}[i(\frac{\partial}{\partial\rho}+\frac{\mu+1}{\rho})v(\rho)+p_z u(\rho)]=0\ . \qquad (2.9)$$

Equations (2.5),(2.8) and (2.9) are the basis of our further discussion. These equations are exact. Related to channeling we shall discuss the case of very high longitudinal energies as compared to transverse and potential energies. We shall however first discuss the case of a free electron, $V=0$, described in cylindrical coordinates in order to relate our solution to the plane wave solution of a free electrton. At the same time we include the case of a constant potential

$$V(\rho)=V_0\ for\ \rho<\rho_0;\ V(\rho)=0\ for\ \rho>\rho_0\ , \qquad (2.10)$$

which we shall use as a strong screening potential for channeling process. It is to be noted that in this case the solution of the Dirac equation is exact, valid for all energies. This is a useful check on solutions to the channeling processes for which exact solution may not be obtained.

3 THE CASE OF A CONSTANT POTENTIAL, INCLUDING $V=0$, A FREE PARTICLE

Equation (2.9) for a constant potential, $V=V_0$ shows that $u(\rho)$ and $v(\rho)$ are Bessel functions

$$u(\rho)=u_0 J_\mu(\pi\rho)\ ,$$
$$v(\rho)=iv_0 J_{\mu+1}(\pi\rho)\ , \qquad (3.1)$$

with π , a quantity of dimension momentum

$$\pi=((E-V)^2-E_z^2)^{\frac{1}{2}}\ , \qquad (3.2)$$

with u_0 and v_0 constants.

For a free particle, $\pi=p_\perp$, is the transverse momentum. For a bound state, for $V\neq 0$, π is imaginary and the Bessel functions in Eq.(3.1) are replaced by McDonald Bessel functions [4] $K_\mu(\pi\rho)$ and $K_{\mu+1}(\pi\rho)$.

With $\varphi(\rho,\phi)$ given by

$$\varphi(\rho,\phi) = \begin{pmatrix} u_0 J_\mu(\pi\rho) e^{i\mu\phi} \\ i v_0 J_{\mu+1}(\pi\rho) e^{i(\mu+1)\phi} \end{pmatrix} , \tag{3.3}$$

and with the summation of Bessel functions [4]

$$\sum i^\mu J_\mu(\pi\rho) e^{i\mu\phi} = e^{i\pi\rho\cos\phi} ,$$

one obtaines the plane wave solution for $\rho > \rho_0$ i.e. for $\pi = p_\perp$

$$\sum \psi_\mu(\rho,\phi,z) = N \sum i^\mu \begin{pmatrix} 1 \\ \frac{-i\vec{\sigma}\nabla}{(E-V+m)} \end{pmatrix} \begin{pmatrix} u_0 J_\mu(\pi\rho) e^{i\mu\phi} \\ i v_0 J_{\mu+1}(\pi\rho) e^{i(\mu+1)\phi} \end{pmatrix} e^{ip_z z} =$$

$$\sqrt{\frac{E+m}{2m}} \begin{pmatrix} 1 \\ \frac{\sigma_x p_\perp + \sigma_z p_z}{(E-V+m)} \end{pmatrix} \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} e^{ip_\perp \rho\cos\phi + i p_z z} , \tag{3.4}$$

giving also the normalization constant. This is the partial cylindrical wave expansion for a free particle with the momentum $\vec{p}$ in the $x - z$ plane. By a rotation ϕ_p or by different choice of constants u_0 and v_0, $u_0 \exp(-i\mu\phi_p)$ and $v_0 \exp(-i(\mu+1)\phi_p)$ in Eq.(3.1)

$$\varphi(\rho,\phi) = \begin{pmatrix} u_0 J_\mu(\pi\rho) e^{i\mu(\phi-\phi_p)} \\ i v_0 J_{\mu+1}(\pi\rho) e^{i(\mu+1)(\phi-\phi_p)} \end{pmatrix} , \tag{3.5}$$

the asymptotic plane wave in an arbitrary direction with respect to the rotational symmetry z - axis is obtained , proportional to $\exp i[p_\perp \rho \cos(\phi - \phi_p) + p_z z]$.

4 CHANNELING STATES

From exact considerations so far, we now go over to discuss channeling approximations. For relativistic particles moving in directions close to a crystal axis the energy E_z defined in Eq.(2.7) is much larger than transverse and potential energies for the most important parts of space. In order to subtract out the longitudinal energy E_z we define ε by

$$\varepsilon = E - E_z , \tag{4.1}$$

which will be used for continuum as well as for transversely bound states. With the aproximations

$$\varepsilon \ll E_z \quad |V(\rho)| \ll E_z ,$$

Eq.(2.9) may be rewritten in the compact form

$$[\nabla^+\nabla^- + 2E_z(\varepsilon - V(\rho))]u(\rho) - i\frac{p_z}{E}\frac{dV}{d\rho}v(\rho) = 0 \ ,$$

$$[\nabla^-\nabla^+ + 2E_z(\varepsilon - V(\rho))]v(\rho) + i\frac{p_z}{E}\frac{dV}{d\rho}u(\rho) = 0 \ , \qquad (4.2)$$

where we have introduced

$$\nabla^+ = \frac{\partial}{\partial\rho} + \frac{\mu+1}{\rho} \ , \ \nabla^- = \frac{\partial}{\partial\rho} - \frac{\mu}{\rho} \ ,$$

$$\nabla^+\nabla^- = \frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho}) - \frac{\mu^2}{\rho^2} \ , \ \nabla^-\nabla^+ = \frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho}) - \frac{(\mu+1)^2}{\rho^2} \ . \qquad (4.3)$$

Equations (4.2) are dominated by the term $2E_z(\varepsilon - V)$. Assuming that $V(\rho)$ is of the order ε for the most importent values of ρ , we read from the equations that the terms $\nabla^+\nabla^-$ and $\nabla^-\nabla^+$ are of the order ρ^{-2} which must be of the order $E_z\varepsilon = (E_z/\varepsilon)\varepsilon^2$. Thus the terms which we have neglected $\varepsilon^2, \varepsilon V$ and V^2 are all of the order ε^2 and therefore negligible. Furthermore , the term $(p_z/E)(dV/d\rho)$ is of the order $\varepsilon/\rho = \sqrt{E_z/\varepsilon}\,\varepsilon^2$. This term may therefore be taken into account perturbatively. We shall show that the correction from this term to the wave function indeed is of relative order $\sqrt{\varepsilon/E_z}$.

To highest order in E_z/ε , the wave functions , which we denote U_μ and $U_{\mu+1}$, satisfy

$$[\nabla^+\nabla^- + 2E_z(\varepsilon - V(\rho))]U_\mu(\rho) = 0 \ ,$$

$$[\nabla^-\nabla^+ + 2E_z(\varepsilon - V(\rho))]U_{\mu+1}(\rho) = 0 \ , \qquad (4.4)$$

where we have used the fact that in Eq.(4.4) $v_\mu(\rho) = U_{\mu+1}(\rho)$

In Eq.(4.2) we introduce

$$u(\rho) = U_\mu(\rho) + \Delta_u(\rho) \ ,$$

$$v(\rho) = U_{\mu+1}(\rho) + \Delta_v(\rho) \ ,$$

where $\Delta_u(\rho)$ and $\Delta_v(\rho)$ are small corrections.

Keeping highest order terms in E_z/ε, we obtain from Eq.(4.2)

$$[\nabla^+\nabla^- + 2E_z(\varepsilon - V(\rho))]\Delta_u(\rho) = i\frac{dV}{d\rho}U_{\mu+1}(\rho) \ ,$$

$$[\nabla^-\nabla^+ + 2E_z(\varepsilon - V(\rho))]\Delta_v(\rho) = -i\frac{dV}{d\rho}U_\mu(\rho) \ , \qquad (4.5)$$

where we have put $p_z/E = 1$ which is in accordance with our approximation .

When we operate on the first of Eq.(4.4) by ∇^- and on the second by ∇^+ we find the nice result

$$[\nabla^-\nabla^+ + 2E_z(\varepsilon - V(\rho))]\nabla^- U_\mu(\rho) = 2E_z \frac{dV}{d\rho} U_\mu(\rho) \ ,$$
$$[\nabla^+\nabla^- + 2E_z(\varepsilon - V(\rho))]\nabla^+ U_{\mu+1}(\rho) = 2E_z \frac{dV}{d\rho} U_{\mu+1}(\rho). \tag{4.6}$$

Comparing with Eqs.(4.5) we see that $\Delta_u(\rho)$ and $\Delta_v(\rho)$ satisy the same equations as $(i/2E_z)\nabla^+ U_{\mu+1}(\rho)$ and $(-i/2E_z)\nabla^- U_\mu(\rho)$ respectively . Therefore

$$\Delta_u(\rho) = \frac{i}{2E_z}\nabla^+ U_{\mu+1}(\rho) + const\ U_\mu(\rho) \ ,$$
$$\Delta_v(\rho) = -\frac{i}{2E_z}\nabla^- U_\mu(\rho) + const\ U_{\mu+1}(\rho) \ , \tag{4.7}$$

where the last terms are contributions from the homogenous equations Eq.(4.4) The constants are determined by the requirements that $\Delta_u(\rho)$ and $\Delta_v(\rho)$ must vanish for $V(\rho) = 0$. This gives

$$\Delta_u(\rho) = \frac{i}{2E_z}(\nabla^+ U_{\mu+1}(\rho) - \sqrt{2E_z\varepsilon}\ U_\mu(\rho)) \ ,$$
$$\Delta_v(\rho) = -\frac{i}{2E_z}(\nabla^- U_\mu(\rho) + \sqrt{2E_z\varepsilon} U_{\mu+1}(\rho)) \ . \tag{4.8}$$

The spinor $\varphi(\rho,\phi)$ then becomes

$$\varphi(\rho,\phi) = (1 - i\sqrt{\frac{\varepsilon}{2E_z}} + i\frac{\sigma_z \vec{\sigma}_\perp \nabla_\perp}{2E_z})\varphi_\mu(\rho,\phi) \ , \tag{4.9}$$

with

$$\varphi_\mu(\rho,\phi) = \begin{pmatrix} U_\mu(\rho)e^{i\mu\phi} \\ U_{\mu+1}(\rho)e^{i(\mu+1)\phi} \end{pmatrix} \ , \tag{4.10}$$

and where we have used

$$\begin{pmatrix} \nabla^+ U_{\mu+1}(\rho)e^{i\mu\phi} \\ \nabla^- U_\mu(\rho)e^{i(\mu+1)\phi} \end{pmatrix} = \vec{\sigma}_\perp \nabla_\perp \varphi_\mu(\rho,\phi) \ ,$$

in Eq.(4.9) . The Dirac channeling wave function is then

$$\psi_{\mu,p_z}(\vec{r}) = N(1 - i\sqrt{\frac{\varepsilon}{2E_z}} + i\gamma_0\frac{\sigma_z \vec{\sigma}_\perp \nabla_\perp}{2E_z})\times$$

$$\begin{pmatrix} 1 \\ (E - V + m)^{-1}(\sigma_z p_z - i\vec{\sigma}_\perp \nabla_\perp) \end{pmatrix} \quad \varphi_\mu(\rho,\phi)e^{ip_z z} \ . \tag{4.11}$$

We have here used the fact that $\sigma_z\vec{\sigma}_\perp\nabla_\perp$ anticomutes with $(\sigma_z p_z - i\vec{\sigma}_\perp\nabla_\perp)$, and that $dV(\rho)/d\rho$ gives a negligible term in our aproximation. As seen from Eq.(4.11) the correction term are indeed of relative order $\sqrt{\varepsilon/E_z}$ as stated above.

5 THE $1/\rho$ POTENTIAL

The wave equations (4.4) can be written in the compact form

$$[\ \frac{d^2}{d\rho^2} + \frac{1}{\rho}\frac{d}{d\rho} - \frac{\kappa^2}{\rho^2} + 2E_z(\varepsilon - V(\rho)\ )\ ]U_\kappa(\rho) = 0 \ , \tag{5.1}$$

with $\kappa = \mu, \mu + 1$ for the upper and lower spinor components, respectively in Eq.(4.10) . We shall in this chapter discuss the solutions for the approximate crystal potential

$$V(\rho) = -\frac{Z\alpha}{\rho}\frac{a}{b}c = -V_0 a/\rho \ , \tag{5.2}$$

with b the interatomic distance in the crystal row, a the screening (e.g. Thomas - Fermi) lenght and c an empirical constant. The potential has been used in several calculations [5]. The potential may be considered reliable for ρ - distances larger than the interatomic distance along the crystal row. For applications the region of validity should be noted.

With the substitution

$$U_\kappa(\rho) = \sqrt{\rho} f_\kappa(\rho) \ , \tag{5.3}$$

the wave equation (5.1) becomes of the same form as the equation in a spherical symmetric potential, namely

$$[\ \frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} - \frac{\kappa^2 - \frac{1}{4}}{\rho^2} + 2E_z(\varepsilon - V(\rho)\ )\ ]f_\kappa(\rho) = 0 \ , \tag{5.4}$$

compared to the Schrödinger equation for a spherical symmetrical potential $V(r)$

$$[\ \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + 2m(\varepsilon - V(r)\ )\ ]R_l(r) = 0 \ . \tag{5.5}$$

At the same time the normalization for bound states are identical

$$\int U^2_{\kappa,n}(\rho)\rho d\rho = \int f^2_{\kappa,n}(\rho)\rho^2 d\rho = \int R^2_{l,n}(r)r^2 dr = 1. \tag{5.6}$$

This shows that the cylindrical wave functions and energy levels may be obtained directly from the corresponding sperical wave functions, if these are known. The substitutions are

$$l \to \kappa - \frac{1}{2} \ , \ m \to E_z \ , \ E \to \varepsilon \ , \ V(r) \to V(\rho) \ , \tag{5.7}$$

for potentials of identical functional dependencies.

For the potential (5.2) the substitution in the potential is

$$Z\alpha/r \to V_0 a/\rho \ , \ V_0 = cZ\alpha/b \ . \tag{5.8}$$

The continuum states are then obtained from the Hydrogenlike states [6] as

$$U_\kappa^\pm(\rho) = \exp(\mp i\sigma_{|\kappa|} + \frac{\pi}{2}\frac{V_0 a E_z}{p_\perp})\sqrt{\frac{2}{\pi}\rho}\ \frac{|\Gamma(-\eta+\kappa+\frac{1}{2})|}{\Gamma(2\kappa+1)}\exp(-ip_\perp\rho)(2p_\perp)\times$$
$$(2p_\perp\rho)^{\kappa-\frac{1}{2}}F(-\eta+\kappa+\frac{1}{2};\ 2\kappa+1;\ 2ip_\perp\rho) \ , \tag{5.9}$$

where $\sigma_{|\kappa|} = \arg\Gamma(-\eta+|\kappa|+\frac{1}{2})$, $\eta = -iV_0 aE_z/p_\perp$, $p_\perp = \sqrt{E^2-E_z^2} \approx \sqrt{2E_z\varepsilon}$ and $F(a;c,z)$ is the confluent hypergeometric function, the Kummer function. $U_\kappa^+(\rho)$ and $U_\kappa^-(\rho)$ are solutions with asymptotic form plane wave plus outgoing , ingoing cylindrical waves, respectively, as seen from the asymptotic form

$$U_\kappa^\pm(\rho) = \exp(\mp i\sigma_{|\kappa|})\sqrt{\frac{2}{\pi\rho}}cos(p_\perp\rho + \frac{V_0 aE_z}{p_\perp}\ln(2p_\perp\rho) - \frac{\pi}{2}(\kappa+\frac{1}{2}) - \sigma_{|\kappa|}) \ . \tag{5.10}$$

As usual with a Coulomb potential, in order to obtain pure outgoing or ingoing solutions, one has to assume a formal screening at $\rho \to \infty$ which removes the logarithmic function at large distances.

For bound states one obtains from Hydrogenlike atoms [6]

$$U_{n,\kappa}(\rho) = \sqrt{\rho}\frac{1}{\Gamma(2\kappa+1)}\left(\frac{\Gamma(\eta+\kappa+\frac{1}{2})}{\Gamma(\eta-\kappa+\frac{1}{2})2\eta}\right)^{1/2}\left(2\sqrt{-2\varepsilon_n E_z}\right)^{3/2}\exp(-\sqrt{-2E_z\varepsilon_n}\ \rho)\times$$
$$\left(2\sqrt{-2\varepsilon_n E_z}\ \rho\right)^{\kappa-\frac{1}{2}}F(-\eta+\kappa+\frac{1}{2};\ 2\kappa+1;\ 2\sqrt{-2E_z\varepsilon_n}\ \rho) \ , \tag{5.11}$$

with the energy eigenvalues , for $-\eta+\kappa+\frac{1}{2} = -n$

$$\varepsilon_n = -\frac{(Z\alpha)^2E_z}{2(n+\kappa+\frac{1}{2})^2}(c\frac{a}{b})^2 \ , \tag{5.12}$$

which gives a $(2n+1)$ degeneracy : $-n < \kappa < n$.

As shown in Appendix 1 , continuum and bound states Eq.(5.9) and (5.11) are valid for positive and negative values of κ i.e. μ and $\mu+1$. There are no singularities for negative values of κ.

6 TWO DIMENSIONAL SOMMERFELD - MAUE LIKE WAVE FUNCTIONS

Operating with $\gamma_0(-i\vec{\gamma}\nabla+\gamma_0(E-V(\rho))+m)\gamma_0$ on Eq.(2.1) one obtains the second order Dirac equation

$$(\nabla^2+p^2-2EV(\rho))\psi(\vec{r})=(-i\gamma_0\vec{\gamma}\nabla V(\rho)-V^2(\rho))\psi(\vec{r}) \ , \tag{6.1}$$

with the usual Sommerfeld - Maue [7] type approximate solution

$$\psi(\vec{r})=e^{i\vec{p}\vec{r}}(1-\frac{i}{2E}\gamma_0\vec{\gamma}\nabla)e^{-i\vec{p}\vec{r}}\psi_0(\vec{r}) \ , \tag{6.2}$$

where $\psi_0(\vec{r})$ is the solution of the equation

$$(\nabla^2+p^2-2EV(\rho))\psi_0(\vec{r})=0 \ . \tag{6.3}$$

The usual Sommerfeld - Maue solution is for the Coulomb potential. For a string $1/\rho$ potential the situation is different, still a solution similar to the Coulomb case is obtained.

With the substitution $\psi_0(\vec{r})=\exp(ip_z z)\varphi(\rho,\phi)$ and the coordinates

$$\xi=\rho(1+\cos\phi) \ , \ \eta=\rho(1-\cos\phi) \ ,$$

we find

$$\left(2\xi\frac{\partial^2}{\partial\xi^2}+\frac{\partial}{\partial\xi}+2\eta\frac{\partial^2}{\partial\eta^2}+\frac{\partial}{\partial\eta}+\frac{p_\perp}{2}(\xi+\eta)+2EV_0a\right)\varphi(\xi,\eta)=0 \ , \tag{6.4}$$

with the Sommerfeld - Maue like solution

$$\varphi(\xi,\eta)=Ne^{i\frac{p_\perp}{2}(\xi-\eta)}F(iV_0a\frac{E}{p_\perp} \ ; \ \frac{1}{2} \ ; \ ip_\perp\eta) \ , \tag{6.5}$$

where $F(\eta)$ is the Kummer function.

The wave function $\psi(\vec{r})$ is then

$$\psi(\vec{r}) = Ne^{i\vec{p}\vec{r}}(1 - \frac{i}{2E}\gamma_0\vec{\gamma}\nabla_\perp)F(iV_0a\frac{E}{p_\perp}\ ;\ \frac{1}{2}\ ;\ i(p_\perp\rho - \vec{p}_\perp\vec{\rho})\ )u\ . \tag{6.6}$$

The Dirac spinor effect has been taken into account by multiplication with the free particle Dirac spinor u . The asymptotic wave function is of the form

$$\psi_0(\vec{r}) = N\sqrt{\pi}\frac{e^{-\pi d/2}}{\Gamma(\frac{1}{2} - id)}\ e^{ip_z z}\ \times$$

$$\left[e^{i\vec{p}_\perp\vec{\rho} - id\ln(p_\perp\rho - \vec{p}_\perp\vec{\rho})} + \frac{\Gamma(\frac{1}{2} - id)}{\Gamma(id)}e^{-i\pi/4}\frac{e^{ip_\perp\rho + id\ln(p_\perp\rho - \vec{p}_\perp\vec{\rho})}}{\sqrt{p_\perp\rho - \vec{p}_\perp\vec{\rho}}}\right]u\ , \tag{6.7}$$

with $d = V_0aE/p_\perp$. This shows that $\psi(\vec{r})$ Eq.(6.6) describes a plane wave plus a cylindrical outgoing wave. The ingoing cylindrical wave solution is obtained by replacing $ip_\perp\rho$ in Eq.(6.6) by $-ip_\perp\rho$. Eq.(6.6) also shows that the normalizations constant N is given by

$$N = \frac{1}{\sqrt{\pi}}\Gamma(\frac{1}{2} - id)e^{\pi d/2} = \frac{1}{\sqrt{\pi}}\left|\Gamma(\frac{1}{2} - id)\right|e^{\pi d/2 + i\lambda} = (\cosh\pi d)^{-1/2}e^{\pi d/2 + i\lambda} \tag{6.8}$$

with

$$\lambda = \arg\Gamma(\frac{1}{2} - id)\ ,$$

which gives the plane wave part of $\psi(\vec{r})$ Eq.(6.7) $\exp(i\vec{p}\vec{r})u$ with the normalized free particle spinor u. It should also be noted that the asymptotic cylindrical wave Eq.(6.7) has the ρ dependence $1/\sqrt{\rho}$ as it should.

7 PERIODICITY ALONG THE CRYSTAL AXIS

We take into account the periodic variation of the potential along the crystal axis, $V(\rho, z)$, by an expansion in Fourier series

$$V(\rho, z) = V(\rho) + \sum_{k=1}^{\infty} V_k(\rho)\cos(g_k z)\ . \tag{7.1}$$

Here $V(\rho)$ is the potential used in the previous chapters , which can be written as

$$V(\rho) = \int_{z_0}^{z_0 + a_z} V(\rho, z)\frac{dz}{a_z}\ , \tag{7.2}$$

while the z dependence is taken into account by the coefficients $V_k(\rho)$

$$V_k(\rho) = \int_{z_0}^{z_0+a_z} V(\rho, z)\cos(g_k z)\frac{dz}{a_z} \;, \qquad (7.3)$$

where $g_k = 2\pi k/a_z$ - are reciprocal lattice vectors, with k an integer, and a_z is the atomic distance along the crystal axis and z_0 is arbitrary.

The Dirac equation Eq.(2.1) now becomes

$$(i\vec{\gamma}\nabla + \gamma_0[E - V(\rho) - Z(\rho, z)] - m)\psi_Z(\vec{r}) = 0 \;, \qquad (7.4)$$

where the index Z indicates the z - dependent potential

$$Z(\rho, z) = \sum_{k=-\infty}^{\infty} V_k(\rho)e^{ig_k z} \;, k \neq 0 \;,$$

and $\psi(\vec{r})$ is given by Eq.(2.5) for $Z(\rho, z) = 0$ with the z - dependence $exp(ip_z z)$.

We shall solve the Dirac equation Eq.(7.4) assuming a solution

$$\psi_Z(\vec{r}) = (1 + \hat{Z}(\vec{r}))\psi(\vec{r}) \;, \qquad (7.5)$$

with $\hat{Z}(\vec{r})$ a small perturbation.

Introducing $\psi_Z(\vec{r})$ into Eq.(7.4) we find

$$(i\vec{\gamma}\nabla + \gamma_0[E - V(\rho) - Z(\rho, z)] - m)\hat{Z}(\vec{r})\psi(\vec{r}) = \gamma_0 Z(\vec{r})\psi(\vec{r}) \;. \qquad (7.6)$$

When we neglect the small terms $V\hat{Z}(\vec{r})$, $Z\hat{Z}(\vec{r})$ and $i\vec{\sigma}_\perp\nabla_\perp\hat{Z}(\vec{r})\psi(\vec{r})$ we find

$$(\; i\gamma_z\frac{\partial}{\partial z} + \gamma_0 E - m \;)\hat{Z}(\vec{r})\psi(\vec{r}) = \gamma_0 Z(\vec{r})\psi(\vec{r}).$$

Expanding $\hat{Z}(\vec{r})$

$$\hat{Z}(\vec{r}) = \sum_{k=-\infty}^{\infty} Z_k(\rho)e^{ig_k z} \;, \qquad (7.7)$$

we find

$$Z_k(\rho) = (\gamma_0 E - \gamma_z(p_z + g_k) - m)^{-1}\gamma_0 V_k(\rho) \;, \qquad (7.8)$$

and the wave function including the periodicity along the lattice string is given by Eq.(7.5), with

$$\hat{Z}(\vec{r}) = \sum_{k=-\infty}^{\infty} \frac{1}{2E_z(\epsilon - g_k)}(\gamma_0 E - \gamma_z(p_z + g_k) + m)\gamma_0 V_k(\rho)e^{ig_k z} \;, \; k \neq 0 \;, \qquad (7.9)$$

in our approximations $E_z \gg \varepsilon, E_z \gg g_k$.

The wave function for the potential $V(\rho, z)$ (Eq.(7.1)) is therefore given by Eq.(7.5)

$$\psi_Z(\vec{r}) = (1 + \hat{Z}(\vec{r}))\psi(\vec{r}) \ , \tag{7.10}$$

with $\hat{Z}(\vec{r})$ given by Eq.(7.9) and $\psi(\vec{r})$ by Eq.(4.10) and (4.11)

$$\psi(\vec{r}) = \psi_{\mu,p_z}(\vec{r}) \ , \tag{7.11}$$

where $U_\mu(\rho)$ and $U_{\mu+1}(\rho)$ are obtained from Eq.(5.9) and (5.11) for continuum and bound states , with $\kappa = \mu$ or $\kappa = \mu + 1$.

APPENDIX 1

The easily proved theorem [4]

$$\frac{1}{\Gamma(c)}F(a;c;z) = \frac{z^m\Gamma(a+m+1)}{\Gamma(a)}F(a+m+1;m+2;z)\ ,\ c=-m\ , \tag{A.1}$$

for the Kummer function

$$F(a;c;z) = \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(c)}{\Gamma(a)\Gamma(c+n)}\frac{z^n}{n!}\ ,$$

shows that the particular combination $[\Gamma(c)]^{(-1)}F(a;c;z)$ is finite for $c=-m$.

One then easily finds

$$z^{-\kappa-\frac{1}{2}}\frac{\Gamma(-\eta-\kappa+\frac{1}{2})}{\Gamma(-2\kappa+1)}F(-\eta-\kappa+\frac{1}{2}\ ;\ -2\kappa+1\ ;\ z) =$$

$$z^{\kappa-\frac{1}{2}}\frac{\Gamma(-\eta+\kappa+\frac{1}{2})}{\Gamma(2\kappa+1)}F(-\eta+\kappa+\frac{1}{2};\ 2\kappa+1;\ z)\ , \tag{A.2}$$

with no singularities , and positive and negative values of κ (μ or $\mu+1$) are equivalent and may be summed over. In fact, κ may be replaced by $|\kappa|$.

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