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Solution of the Klein-Gordon Equation for a Periodic Lattice

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A solution of the Klein–Gordon equation is obtained for a periodic lattice and from this a solution for a beam of electrons traversing a single set of crystal planes is derived. For the singly periodic case, the dispersion equation is found to have two branches but in addition to the energy gap at the Brillouin zone boundary there appears a gap in the momentum states at the centre of the zone. The relativistic extinction distances are also derived.

Introduction

The Klein–Gordon equation is the relativistic wave equation. It was derived independently by a number of workers, including Schrödinger, in 1926 by applying Schrödinger's rules to the relativistic Hamiltonian. (Gordon, 1926; Klein, 1926.) A more fundamental derivation is given in the Appendix. The equation may be written

$$\nabla^2\psi-\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2}=\frac{4\pi^2\nu'^2}{c^2}\psi \qquad (1)$$

where ψ represents any physical property or system whatsoever which is to be described in different reference frames. ν'^2 is a parameter defined for the frame in which $\nabla'^2\psi=0$. If ψ is a particle wave function then $h\nu'=\varepsilon'=$rest energy, h being Planck's constant. The significance of the Klein–Gordon equation is that it selects, from all possible continuous functions of the coordinates, those functions which are consistent with the postulates of the theory of relativity, that is, physically acceptable functions. ψ is not restricted to probability amplitudes but can represent any physical property whatsoever. It is well known, for instance, that all clcctromagnetic quantities must satisfy an equation of this kind.

If we assume solutions of the form

$$\psi=\psi(r)\exp(2\pi i\nu t)$$

then equation (1) can be written in the forms

$$\nabla^2\psi+\frac{4\pi^2}{c^2}(\nu^2-\nu'^2)\psi=0 \qquad (2)$$

or

$$\nabla^2\psi+\frac{4\pi^2}{h^2c^2}(\varepsilon^2-\varepsilon'^2)\psi=0 \qquad (3)$$

where ε is the total energy, and $\varepsilon^2-p^2c^2=\varepsilon'^2$, p being the momentum. Equation (3) reduces to Schrödinger's equation when the kinetic energy is small compared with the rest energy. For a particle of rest mass m_0, $\varepsilon'=m_0c^2$ and the total energy ε differs from this by only a relatively small amount so that we can put $\varepsilon+\varepsilon'\simeq 2m_0c^2$. In the notation of classical physics the difference between the total and the rest energy is written $\varepsilon-\varepsilon'=E-V$ where E is the classical total energy and V is the potential energy. Hence,

$$\varepsilon^2-\varepsilon'^2\simeq 2m_0c^2(E-V)$$

and this substituted into equation (3) yields Schrödinger's time independent equation.

1. Solution for a periodic lattice

A solution of the Schrödinger equation for a periodic lattice was first given by Bethe (1928). The same method can be used for the Klein–Gordon equation in the form equation (2). The parameter ν'^2 is periodic with the periodicity of the lattice and can be expanded in a Fourier series

$$\nu'^2(r)=\sum_m \nu^2_{mn}(g)\exp[2\pi i(\mathbf{g}_m-\mathbf{g}_n).\mathbf{r}] \qquad (4)$$

where $\mathbf{g}_m$ and $\mathbf{g}_n$ are vectors of the reciprocal lattice and $\mathbf{r}$ is a vector in the ordinary space. As a trial solution put

$$\psi(r)=\sum_m \psi_m(k)\exp[2\pi i(\mathbf{k}+\mathbf{g}_m).\mathbf{r}] \qquad (5)$$

where $\mathbf{k}$ is an arbitrary wave vector. The solution (5) is a Bloch wave function and may be written in the form

$$\psi(r)=u(r)\exp(2\pi i\mathbf{k}.\mathbf{r})$$

where $u(r)$ is periodic with the lattice periodicity. If equations (4) and (5) are substituted into equation (2) and coefficients of like exponential terms are equated we obtain

$$\{\nu^2-c^2(\mathbf{k}+\mathbf{g}_m)^2\}\psi_m=\sum_n \nu^2_{mn}\psi_n\,. \qquad (6)$$

This represents a set of simultaneous equations with one equation for each value of m. There will be a non-trivial solution only if

$$|\delta_{mn}\{\nu^2-c^2(\mathbf{k}+\mathbf{g}_m)^2\}-\nu^2_{mn}|=0\,. \qquad (7)$$

Equation (7) determines the permitted values for ν^2 and these, substituted into the equations (6), then determine the amplitudes ψ_m.

2. Singly periodic lattice

For this case we consider wave vectors $\mathbf{g}_m$ and $\mathbf{g}_{-m}=-\mathbf{g}_m$ only and wave amplitudes ψ_m and ψ_{-m}. Equations (5) then reduce to

$$\{\nu^2 - \nu^2_{m,m} - c^2(\mathbf{k}+\mathbf{g}_m)^2\}\psi_m = \nu^2_{m,-m}\psi_{-m} \quad (8)$$
$$\{\nu^2 - \nu^2_{-m,-m} - c^2(\mathbf{k}-\mathbf{g}_m)^2\}\psi_{-m} = \nu^2_{-m,m}\psi_m$$

and the secular equation [equation (7)] becomes

$$\{\nu^2 - \nu^2_{m,m} - c^2(\mathbf{k}+\mathbf{g}_m)^2\}\ \{\nu^2 - \nu^2_{-m,-m} - c^2(\mathbf{k}-\mathbf{g}_m\} = (\nu^2_{m,-m})\ (\nu^2_{-m,m}). \quad (9)$$

The factor $\nu^2_{m,m}$ can be interpreted as the fraction of ψ_m which is scattered into itself and $\nu^2_{-m,-m}$ as the fraction of ψ_{-m} scattered into itself. As there is no means of distinguishing left from right in the lattice these two terms must be equal and both can be put equal to ν_0^2, say. The factor $\nu^2_{m,-m}$ is the fraction of ψ_{-m} scattered into ψ_m and conversely for $\nu^2_{-m,m}$. The product of these two factors reproduces the original direction and, for the case of elastic scattering processes, the twice scattered wave must be in phase with the original wave. The individual factors may include phase changes but the product must be real and can be replaced by the modulus $|\nu^2_{m,-m}|^2$. Equation (9) then becomes

$$\nu^2 = \nu_0^2 + c^2(k^2+g_m^2) \pm \{4c^4(\mathbf{k}\,.\,\mathbf{g}_m)^2 + |\nu^2_{m,-m}|^2\}^{1/2}. \quad (10)$$

3. The extinction distances

In equation (10) let $k=0$ and denote the solutions for the positive branch by ν_+^2 and for the negative branch by ν_-^2. Then

$$|\nu^2_{m,-m}| = \frac{\nu_+^2 - \nu_-^2}{2}.$$

In the general case when $k \neq 0$, let ν_2^2 and ν_1^2 refer to the positive and negative branches respectively. Then

$$\nu_2^2 - \nu_1^2 = 2\{4c^4(\mathbf{k}\,.\,\mathbf{g}_m)^2 + |\nu^2_{m,-m}|^2\}^{1/2}. \quad (11)$$

Divide both sides of equation (11) by $2kc^2$ and put

$$\frac{1}{\xi} = \frac{\nu_2^2 - \nu_1^2}{2kc}; \quad \frac{1}{\xi_g} = \frac{\nu_+^2 - \nu_-^2}{2kc^2}; \quad s = \frac{2\mathbf{k}\,.\,\mathbf{g}_m}{k}.$$

We then obtain

$$\frac{1}{\xi} = \left\{s^2 + \frac{1}{\xi_g^2}\right\}^{1/2}. \quad (12)$$

In electron-diffraction theory ξ is known as the extinction distance; ξ_g is the extinction distance when $\mathbf{k}\,.\,\mathbf{g}_m = 0$, that is to say, when Bragg's law is satisfied. The parameter s measures the departure from Bragg's law.

Although equation (12) is of the standard form the extinction distances as defined here differ somewhat from the usual form. In order to bring out the significance of the extinction distance let us consider the basic wave function which is formed by superimposing the four waves corresponding to frequencies ν_1 and ν_2, each frequency being associated with wave vectors $\mathbf{k}+\mathbf{g}_m$ and $\mathbf{k}-\mathbf{g}_m$. For our purpose we can assume the waves to have equal amplitudes; this simplifies the algebra without loss of generality as far as the extinction length is concerned. Summing the four waves we obtain a wave function of the form

$$4 \cos \pi(\nu_1 - \nu_2)t \cos (2\pi \mathbf{g}_m\,.\,\mathbf{r}) \times \exp [2\pi i\{(\nu_1+\nu_2)t - 2\mathbf{k}\,.\,\mathbf{r}\}].$$

The phase velocity is $u = (\nu_1+\nu_2)/2k$ and corresponds to a group velocity $v = c^2/u$. Hence we can write the first factor in the above expression

$$\cos \pi(\nu_1-\nu_2)t = \cos\left[\pi\left(\frac{\nu_1^2-\nu_2^2}{\nu_1+\nu_2}\right)t\right] = \cos\left[\pi\left(\frac{\nu_1^2-\nu_2^2}{2kc^2}\right)vt\right] = \cos\left[\pi\left(\frac{r}{\xi}\right)\right].$$

In electron diffraction, the electron beam in the crystal can be resolved into groups of four waves. Two of these with wave vector $\mathbf{k}-\mathbf{g}_m$, say, (frequencies ν_1 and ν_2) can be regarded as combining to form the incident wave whilst the remaining pair with wave vector $\mathbf{k}+\mathbf{g}_m$ make up the reflected wave. If unit amplitude is assigned to the incident wave at the entry surface (zero amplitude being assigned to the reflected wave at the same surface) then the amplitude of the total wave varies with the penetration, r, into the crystal as $\cos (\pi r/\xi)$.

From equation (8), the ratio of the wave amplitudes is given by

$$\frac{\psi_{-m}}{\psi_m} = \frac{\nu^2 - \nu_0^2 - c^2(\mathbf{k}+\mathbf{g}_m)^2}{\nu^2_{m,-m}}.$$

In electron-diffraction theory the parameter s is usually taken to be normal to $\mathbf{g}_m$. In practice, however, the angle of incidence of the beam on the crystal planes is very small and departures from Bragg's law are also small so the difference from the case here (where s is the projection of $\mathbf{g}_m$ onto $\mathbf{k}$) is relatively unimportant.

Finally, we can approximate for kinetic energies which are small compared with the rest energy in order to obtain a value for the extinction distance ξ_g.

The procedure is the same as that followed in the introduction in obtaining Schrödinger's equation. Again we can put $h(\nu+\nu') \simeq 2mc^2$, where m is the rest mass of the electron. However, now we must put the difference of the total and rest energies $h(\nu-\nu')$ equal to the classical value for the crystal potential energy, *i.e.* $2eV_g$, where e is the charge on the electron and V_g is the classical potential associated with the crystal Fourier component of wave vector $\mathbf{g}_m$. Thus

$$h^2(\nu_+^2 - \nu_-^2) \simeq 4mc^2eV_g$$

and

$$\xi_g \simeq \frac{h^2}{2me}\ \frac{K \cos \theta}{V_g}$$

where $K \cos \theta = k$ and θ is the Bragg angle.

4. The dispersion curve

Let k_g be the component of $\mathbf{k}$ in the direction of $\mathbf{g}_m$. The equation of the dispersion curve will then be taken to be

$$\nu^2 = \nu_0^2 + c^2(g_m^2 + k_g^2) \pm \{4c^4k_g^2g_m^2 + |\nu^2_{m,-m}|^2\}^{1/2} \quad (13)$$

with ν^2 plotted against k_g^2. (It is important to understand that in the relativistic Hamiltonian it is the square of the energy which is proportional to the square of the momentum and that the classical form, $E=p^2/2m$, is an approximation which is valid only for low kinetic energies.) When $k_g^2=0$, the wave system reduces to a standing wave combination so that this point corresponds to the usual Brillouin zone boundary. The separation of the upper and lower branches at this point is then $2|v^2_{m,-m}|$. The maximum of the upper branch and the minimum of the lower one occur when

$$\frac{\mathrm{d}(v^2)}{\mathrm{d}(k_g^2)}=c^2\pm\frac{2c^4g_m^2}{\{4c^4k_g^2g_m^2+|v^2_{m,-m}|^2\}^{1/2}}=0\,, \qquad (14)$$

that is when

$$k_g^2=g_m^2-\frac{|v^2_{m,-m}|^2}{4c^4g_m^2} \qquad (15)$$

and the separation of the branches is then $4c^2g_m^2$.

The result (15) shows that there is a region of forbidden values of k_g^2 around the Brillouin zone centre ($k_g=g_m$). The explanation of this lies in the fact that the differential of v^2 with respect to k^2 in the Hamiltonian gives the square of the velocity of light and values of k_g^2 exceeding that given by equation (15) correspond to an imaginary component of the velocity of light in the direction g_m. The group velocity is given by

$$\frac{\mathrm{d}v}{\mathrm{d}k_g}=\frac{k_gc^2}{v}\pm\frac{g_mc^2}{v}\cdot\frac{1}{\{1+|v^2_{m,-m}|^2/4c^4k_g^2g_m^2\}^{1/2}}$$

and this also becomes zero when equation (15) is satisfied.

The equation for the dispersion curve is of the form of the pseudopotential developed by Harrison provided $v^2-v_0^2$ is replaced by $2mc^2E/h^2$, where E is the energy in the classical approximation (Harrison, 1966).

APPENDIX

Derivation of the Klein–Gordon equation

The d'Alembertian is invariant under a Lorentz transformation.

$$\nabla^2-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}=\nabla'^2-\frac{1}{c^2}\frac{\partial^2}{\partial t'^2}\,.$$

We can always construct a frame of reference so that $\nabla'^2=0$ and since in this frame the invariant is

$$-\frac{1}{c^2}\frac{\partial^2}{\partial t'^2}$$

this must be the value of the invariant in all frames.

If ψ represents one and the same physical property which is measured by two different observers, or, what is the same thing, is described in two different reference frames as $\psi(r,t)$ or $\psi(r',t')$, then

$$\nabla^2\psi-\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2}=-\frac{1}{c^2}\frac{\partial^2\psi}{\partial t'^2}\,;\quad \nabla'^2\psi=0\,.$$

The original Klein–Gordon equation was considered suspect for many years because it predicted negative energy states and the suspicion seems to have continued even after the problem was cleared up by Pauli & Weisskopf (1934). Basically, the equation is simpler than the Schrödinger equation if only because it is of the standard form for a wave equation. Part of the reluctance to use this equation seems to spring from a belief that Dirac's equations are necessary to describe the relativistic electron. This is mistaken. If ψ for instance, is replaced by the electric intensity E the above equation is the standard wave equation of the electromagnetic field and this can be resolved into the first-order Maxwell equations. In a similar way the Klein–Gordon equation can be resolved into Dirac's equations; each of the four components of ψ must then satisfy the general wave equation. The Klein–Gordon equation cannot provide information about spin (although it is incorrect to say that it can only describe particles of zero spin), for this it is necessary to go to the first-order equations.

To obtain equation (1) solutions of the form $\psi=\psi_0\exp(2\pi i v't')$ are assumed. Fundamentally, $1/v'$ is the defined unit of time in the primed reference frame but this unit can take different forms in different problems. In single particle theory, $hv'=mc^2$ is the rest or potential energy whilst in problems of the electromagnetic field $2\pi v'$ may be the plasma frequency.

$$2\pi v'=\left(\frac{e\varrho}{m\varepsilon_0}\right)^{1/2}$$

where ϱ is the charge density and ε_0 is the permittivity of free space.

In general v' is related to potential but although relativistic expressions can be approximated to classical ones in appropriate circumstances, the actual forms are quite different. For example the Coulomb energy of an electron at distance r from a proton is

$$E_r=\frac{mc^2}{\left(1+\dfrac{e^2}{2\pi\varepsilon_0mc^2r}\right)^{1/2}}\simeq mc^2-\frac{e^2}{4\pi\varepsilon_0r}$$

where the approximation is for $r\gg e^2/mc^2$. It will be noted that the relativistic energy goes to zero with r whereas the classical value goes to infinity. It is not justified in general to use classical coulomb energies in solutions of the wave equation.

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