On the momentum eigenfunctions for the periodic problem

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In a letter of this title (Pincherle and Lee 1962, to be referred to as I) it was shown how in energy band calculations by plane wave methods it is possible to derive the first derivatives, with respect to crystal momentum **k**, of the energy $E(\mathbf{k})$ and of the momentum eigenfunctions $v(\mathbf{k})$ along any direction in **k** space along which the symmetry is the same at all points.

We should like to add that in fact all the derivatives can be worked out with a procedure very suitable for a computer. Equation (3) of I can be differentiated any number of times, provided we are not at a point of degeneracy. The left-hand sides of the n-times differentiated equations are the same as in equation (3) of I, with the nth derivative replacing the first; the right-hand sides are (omitting the argument—$\mathbf{k}+\mathbf{K}_i$—of v)

$$\frac{\partial^n E}{\partial \alpha^n} v + \binom{n}{1} \frac{\partial^{n-1} E}{\partial \alpha^{n-1}} \frac{\partial v}{\partial \alpha} + \binom{n}{2} \frac{\partial^{n-2} E}{\partial \alpha^{n-2}} \frac{\partial^2 v}{\partial \alpha^2} + \ldots + \binom{n}{2} \left(\frac{\partial^2 E}{\partial \alpha^2} - 2 \right) \frac{\partial^{n-2} v}{\partial \alpha^{n-2}}$$

$$+ \binom{n}{1} \left[\frac{\partial E}{\partial \alpha} - 2(\mathbf{k}+\mathbf{K}_i) \, . \, \boldsymbol{\alpha} \right] \frac{\partial^{n-1} v}{\partial \alpha^{n-1}}.$$

If the calculation has already been carried out up to the $(n-1)$th derivative, all quantities on the right-hand side are known except $\partial^n E/\partial \alpha^n$ which then satisfies, as shown in I, an algebraic equation of the first degree. Having found its value, all the $\partial^n v(\mathbf{k}+\mathbf{K}_i)/d\alpha^n$ can be calculated from the system of equations, adding the further equation obtained by differentiating n times the condition of normalization

$$\sum_{\mathbf{K}_i} |v(\mathbf{k}+\mathbf{K}_i)|^2 = 1.$$

Thus, in principle, from a calculation at one point in the range, a Taylor series gives E and v at all points. The convergence of the series can be expected to be good for E, but not for v, since it is known that (E, k) curves are generally smooth, while the $v(\mathbf{k})$ functions are often rapidly varying.

The accuracy of the procedure depends on the number of equations considered in the original system. As an example, the method was applied at the centre and edge of the Brillouin zone for the lowest band for the one-dimensional potential

$$a^2 V = 2 \cos(2\pi x/a).$$

A system of five equations was used at $k = 0$ and of six equations at $k = \pi/a$, and derivatives up to the eighth were included; the energy a^2E was obtained correctly to three figures in the whole interval. The use of a system of five equations at the middle point gave inferior results.

While in practical cases such accuracy cannot be expected, the method allows, with little extra computer time, a fair picture to be obtained of the (E, k) curves along any direction, after carrying out the calculation at the end points. In many calculations of band structures that have been carried out in the past, these curves have been sketched using little more than the compatibility relations.

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Cylindrically symmetric radial electrostatic fields in general relativity

Abstract. This letter establishes the non-existence of any physically acceptable solution of the Einstein–Maxwell equations which can be identified as that of a charged infinite cylinder with a radial electrostatic field.

The purpose of the present letter is to point out the impossibility of constructing a solution of Einstein–Maxwell's equations satisfying the following conditions:

(i) The field is static and cylindrically symmetric and corresponds to a radial electrostatic field.

(ii) The source of the field is represented by a continuous distribution of matter and charge rather than as singularities of the field; the source distribution is assumed to be confined in a bounded region of the radial coordinate.

(iii) The energy density T_4^4 as well as $T_4^4 - \frac{1}{2}T$ shall be non-negative everywhere.

We start with the general line element of cylindrical symmetry

$$ds^2 = -A(dx_1^2 + dx_2^2) - C\,dx_3^2 + D\,dx_4^2 \tag{1}$$

where A, C and D are functions of x_1 only.

Now for regions in which there is only an electromagnetic field

$$R_\nu^\mu = -8\pi T_\nu^\mu \tag{2}$$

with

$$T_\nu^\mu = -F^{\mu\alpha}F_{\nu\alpha} + \tfrac{1}{4}g_\nu^\mu F^{\alpha\beta}F_{\alpha\beta} \tag{3}$$

as $R = 0$ for this case. In the case of a cylindrically symmetric radial electrostatic field only F_{14} exists and we obtain from (3) that $T_3^3 + T_4^4 = 0$. Hence equation (2) gives $R_3^3 + R_4^4 = 0$. Therefore the line element (1) is reducible, under these circumstances, to Weyl's canonical form (Synge 1960)

$$ds^2 = -\exp(2\beta - 2\alpha)(dr^2 + dz^2) - r^2\exp(-2\alpha)\,d\phi^2 + \exp(2\alpha)\,dt^2. \tag{4}$$

The solution of the equation (2) gives in the case of the axially symmetric radial