

On an Illustrative Example of the Theory of Bloch Waves*

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The Lamé equation $d^2\psi/dz^2 - (h + 2p(z))\psi = 0$ is interpreted as the Schrödinger equation of a particle in a one dimensional periodic potential and the corresponding band structure is discussed.

Interpreta-se a equação de Lamé $d^2\psi/dz^2 - (h + 2p(z))\psi = 0$ como equação de Schrödinger para uma partícula em um potencial periódico unidimensional e discute-se a estrutura de faixas correspondentes.

1. INTRODUCTION AND CONCLUSION

There is no doubt the usefulness of examples illustrating general theories even if the examples are constructed in a somewhat artificial way. One dimensional models have always been used to demonstrate the fundamental properties of solids for example, long before highly anisotropic material have been studied as realizations of such models. The model of Kronig and Penney for electrons in a one dimensional conductor is an example which is well known. It seems to have been unnoticed for a long time that the solution of the Lamé equation, first given by Hermite³, also provides a beautiful illustration of Bloch's theory of elec-

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trons in a lattice. Recently it appeared in the context of the Korteweg-de Vries equation for nonlinear waves in weakly dispersive systems⁴. The far reaching generalization of the formulas which are used in this paper can be found there and they can be used to approximate any arbitrary one dimensional potential⁵.

It seems useful to present the interpretation of the Lamé equation as a Schrödinger equation here in more detail because the material is rather dispersed in mathematical papers on the aforementioned topic. The prerequisite knowledge on Elliptic Functions we shall need⁶ does not prevent the educational use of our example and the exploration of it in this sense is our objective.

The plan of this paper is the following: Starting from the Lamé equation and its explicitly given solution we show how the Lamé operator can be interpreted as Schrödinger operator. The dispersion relation is derived easily for Bloch waves. The density of states and the effective masses are given. The band structure is highly degenerate because it contains only one gap. In respect to this we refer to some results in connection with the Inverse Problem. We then discuss the limiting cases of nearly free and tightly bound electrons. Using a representation of the potential by the superposition of local "atomic" potentials, the asymptotic behaviour of these "atomic" potentials, of the wavefunction of their bound states and finally of the corresponding Wannier functions is given.

2. THE LAMÉ EQUATION INTERPRETED AS SCHRÖDINGER EQUATION

Though being complex, the Lamé equation given by

$$\frac{d^2 \phi}{dz^2} - \{h + n(n+1)p(z)\} \phi = 0 \quad (1)$$

with h a parameter, n an integer and p the Weierstrassian Elliptic Function is apparently of the same form as the Schrödinger equation of a particle in a one dimensional potential written in atomic units ($\hbar = e = m = 1$)

$$-\frac{1}{2} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \quad (2)$$

To interpret the Weierstrassian p -Function as a potential we have to restrict their invariants to be real. To exclude the unphysical singularities of the order two from the potential function one has to take pure real and pure imaginary periods $2\omega_1$ and $2\omega_3$. On the straight line $z = x + \omega_3$, p is then real and free from singularities. For simplicity's sake we will also restrict the parameter n of eq. (1) to one. Choosing for the potential

$$V(x) = p(x + \omega_3)$$

which has the real period $2\omega_1$ as lattice constant and writing the energy eigenvalue E in terms of the notation of (1)

$$E = -\frac{1}{2} \hbar$$

the Schrödinger equation (2) is seen to be equivalent to the Lamé equation (1) restricted to the line $z = x + \omega_3$, $2\omega_3$ being the imaginary period of p .

3. THE DISPERSION RELATION

The solution of the Lamé equation are wellknown⁷. Defining by $p(a) = \hbar$, the solutions are given by

$$\phi(z) = e^{\mp z \zeta(a)} \frac{\sigma(z \pm a)}{\sigma(z)} \quad (3)$$

this can be easily verified with the aid of the definitions of the Weierstrassian ζ - and σ -Functions and of the addition theorems. The wavefunctions $\phi(z)$ are already almost explicitly in the form of Bloch waves, consequently the wavevector k can be extracted from them in the following way. By the quasi-periodicity of σ a shift of ϕ by one lattice constant $2\omega_1$ results in

$$\phi(z + 2\omega_1) = e^{\mp 2\omega_1 \zeta(a)} e^{\pm 2\eta_1 a} \phi(z)$$

with $\eta_1 = \zeta(\omega_1)$. Comparing with the phase vector $e^{-\sqrt{-1} 2\omega_1 k}$, which results from the Bloch theorem for the same shift, we can determine the wavevector:

$$k = \mp \sqrt{-1} \left(\zeta(\alpha) - \frac{\eta_1}{\omega_1} \alpha \right) \quad (4)$$

Together with $E = \frac{1}{2} p(\alpha)$ this establishes a parametric representation of the dispersion relation. Using the Inversion of the p-Function, which leads to the integral formula of p and a similar formula of ζ which are the Weierstrassian Normal Elliptic integrals of the first and second kind we can rewrite the dispersion relation as

$$k(E) = \pm \sqrt{-1} \left\{ - \int_{-2E_0}^{-2E} \frac{4dy}{\sqrt{4y^3 - g_2y - g_3}} + \zeta[p^{-1}(-2E_0)] - \frac{\eta_1}{\omega_1} \int_{-2E_0}^{-2E} \frac{dy}{\sqrt{4y^3 - g_2y - g_3}} - \frac{\eta_1}{\omega_1} p^{-1}(-2E_0) \right\}$$

with the usual invariants g_2, g_3 and $-2E_0$ arbitrary. A convenient choice of E , and therefore the integration constants will be given below. It is now advantageous to factorize the polynomial $4y^3 - g_2y - g_3$ in the usual way into $4(y - e_1)(y - e_2)(y - e_3)$ where e_1, e_2, e_3 obey the relations $e_1 > e_2 > e_3$ and $e_1 + e_2 + e_3 = 0$. With the choice $-2E_0 = e_3$ the integration constants above result in $-\frac{1}{\omega_1} \sqrt{-1} \frac{\pi}{2}$ by Legendre's relation. The final form of the dispersion relation is then given by

$$k(E) = \mp \left\{ \frac{\pi}{2\omega_1} + \int_{2E}^{-e_3} \frac{\left(y - \frac{\eta_1}{\omega_1}\right) dy}{\sqrt{4(y + e_1)(y + e_2)(y + e_3)}} \right\} \quad (5)$$

A graph of the dispersion relation for a special choice of parameters is given in Fig. 1.

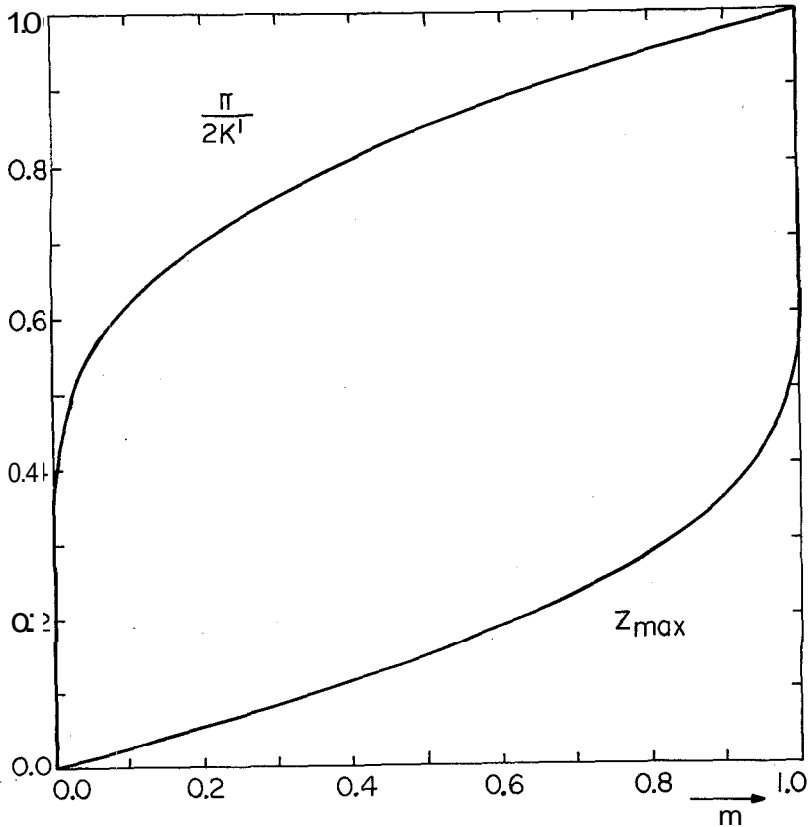


Fig.1 - The dispersion relation in a scaled plot ($\omega_3 = i \omega_1, \dots$) corresponds to the equivalent relation for a free particle to compare to the case $2\omega_1=1$.

4. THE BAND STRUCTURE

With the aid of the formula (5) the band structure can be discussed. The integrand is real for all energies $E > -e_3/2$ and so is the wavevector for infinitely wide energy band. On the contrary, in the region $-e_3/2 > E > -e_2/2$ the integrand is imaginary, so that the wavevector is becoming complex. This corresponds to a gap. Specifically

$$k(-\frac{e_2}{2}) = k(-\frac{e_3}{2}) = \pm \frac{\pi}{2\omega_1}$$

which can be obtained by the integral formulas of the half periods. Because of this, the wavevector returns to real values for the finite al-

lowed energy band - $e_2/2 > E > -e_1/2$. Finally in the region - $e_1/2 > E$ there are no real wavevectors. So the band structure is highly degenerated and has only one gap as can be seen also in Fig.1. An explanation of this is given below in section 7.

Because our model is one dimensional it is easy to derive from our dispersion relation the density of states and from this the effective masses.

A differentiation of the wavevector with respect to the energy provides the density of states:

$$n(E) = \frac{2}{\pi} \frac{dk(E)}{dE} = \frac{4}{\pi} \sqrt{2} \frac{E - \frac{\eta_1}{2\omega_1}}{\sqrt{(E + \frac{e_1}{2})(E + \frac{e_2}{2})(E + \frac{e_3}{2})}} \quad (6)$$

This expression shows explicitly the singular behaviour of the density of states at the band edges - $e_3/2$, - $e_2/2$, - $e_1/2$.

In a similar way we have for the effective mass

$$\begin{aligned} m^* &= \frac{1}{\frac{d^2E}{dk^2}} = -\frac{4}{\pi} \frac{n^3}{\frac{dn}{dE}} = \\ &= 8 \left(E - \frac{\eta_1}{2\omega_1}\right)^3 \left\{ \left(E + \frac{e_1}{2}\right) \left(E + \frac{e_2}{2}\right) \left(E + \frac{e_3}{2}\right) \right. \\ &\quad \left. - \frac{1}{2} \left(E - \frac{\eta_1}{2\omega_1}\right) \left[\left(E + \frac{e_1}{2}\right) \left(E + \frac{e_2}{2}\right) \right. \right. \\ &\quad \left. \left. + \left(E + \frac{e_2}{2}\right) \left(E + \frac{e_3}{2}\right) + \left(E + \frac{e_1}{2}\right) \left(E + \frac{e_3}{2}\right) \right] \right\}^{-1} \end{aligned} \quad (7)$$

Specifically the effective masses at the band edges - $e_3/2$, - $e_2/2$, - $e_1/2$ are given by

$$\frac{8\left(e_3 + \frac{\eta_1}{\omega_1}\right)^2}{(e_1 - e_3)(e_2 - e_3)} \quad \left| \quad \frac{8\left(e_2 + \frac{\eta_1}{\omega_1}\right)^2}{(e_1 - e_2)(e_3 - e_2)} \quad \left| \quad \frac{8\left(e_1 + \frac{\eta_1}{\omega_1}\right)^2}{(e_2 - e_1)(e_3 - e_1)} \right.$$

respectively.

5. ON THE INVERSE PROBLEM

The Inverse Problem consists in determining the potential from a given band structure. From this point of view we could have started from a formula for band structures with only a finite number of gaps given by Hochstadt⁸ and would have got our expression of the dispersion relation without any other knowledge than that of the three band edges $-e_3/2$, $-e_2/2$, $-e_1/2$. Hochstadt too has given a differential equation⁹ for the potential in the case of band structures with only one gap. From this differential equation we can reconstruct our potential $p(x + \omega_3)$ without any additional knowledge. Only the band structures with no or one band gap correspond uniquely to one potential as is known from the theory of this Inverse Problem¹⁰.

This allows a naive study of the potential starting from the parameters of the band structure. The three parameters e_1, e_2, e_3 used above are not independent. If b denotes the width of the finite allowed band and R the width of the gap, then the ratio

$$\frac{e_2 - e_3}{e_1 - e_3} = \frac{R}{\ell + b} = m \quad (8)$$

gives m , the square of the modulus which occurs in the Jacobian Elliptic Functions. From the modulus the ratio of periods can be calculated:

$$\frac{\omega_3}{\omega_1} = \frac{-\sqrt{-1}}{\pi} \ln q(m)$$

with the well known parameter q named nome. The lattice constant is determined by

$$2\omega_1 = \sqrt{\frac{2}{\ell+b}} K(m) \quad (9)$$

with the Complete Elliptic Integral of the first kind K . These formulas give just a solution of the Inverse Problem associated with Weierstrassian Elliptic Functions. Finally we express the potential with the aid of Jacobian sine amplitude sn :

$$V(x) = p(x + \omega_3) = -\frac{2}{3} (2\ell + b) + 2\ell \operatorname{sn}^2(\sqrt{2(\ell+b)} x)$$

6. THE LIMITING CASES

It is instructive to visualize the potential in the limiting cases of small gap and of small finite band. In the limit of a small gap we have a modulus near zero and the potential is approximately given by (using formula 127.01 of reference 11)

$$V(x) \approx -\frac{2}{3} b - \ell \cos(2\sqrt{2b} x) \quad (10)$$

The Schrödinger equation in this approximation is of the Mathieu type. And the model is that of nearly free electrons.

The opposite limit of small band corresponds to a modulus near one and the approximation is (using formula 127.02 of reference 11)

$$V(x) \approx \frac{2}{3} \ell - \frac{2\ell}{\cosh^2(\sqrt{\ell}x)} \quad (11)$$

This is a so called Pöschl-Teller potential hole¹² which is characterized by a vanishing reflection coefficient and only one bound state. This model corresponds to that of tightly bound electrons for the finite band and nearly free electrons for the infinite band.

In conclusion, the Lamé operator can interpolate continuously the models of nearly free and strongly bound electrons, but only if the relation between the parameter of the band structure and the lattice constant given above by eq.(8) and (9) holds. Let us restrict further to neutral potentials i.e. potentials, whose mean second derivative in one lattice cell is zero. This gives the condition $1 + b = 1/2$ as can be easily verified. By this we have a one parameter set of potentials with a minimal lattice constant $2\omega_1 = \pi$. The gap is now a unique function of the lattice constant. Approximations of this function for nearly free and strongly bound electron are given by (using formulas 900.000 and 112.01 of reference 11.)

$$2\omega_1 \approx \pi \left(1 + \frac{1}{2} \ell\right) \quad \ell \ll 1$$

$$2\omega_1 \approx 2 \ell n \frac{4}{\sqrt{1-2\ell}} \quad 1-2\ell \ll 1$$

7. THE ASYMPTOTIC BEHAVIOUR OF THE WANNIER FUNCTIONS

Let us return to formula (11). The small band degenerates in the limit: to the bound state of the Pöschl-Teller potential hole. Because of the vanishing reflection coefficient of the latter the electrons with energies above the gap are transmitted unhindered, so that there can be no higher gaps. This simple understanding of the basic features of our band structure can be extended to arbitrary b and l . Using a well known series expansion of p in terms of \csc^2 (Ref.7) it can be shown by simple calculations that the potential $p(x+\omega_3)$ can be represented by a superposition of "atomic" potentials centered at the lattice points, plus a constant. These "atomic" potentials are, always reflectionless Pöschl-Teller potentials with only one bound state given by

$$\frac{\frac{\pi}{2|\omega_3|}}{\cosh^2 \frac{\pi}{2|\omega_3|} (x-x_0)} \quad (12)$$

The energy eigenvalue of the bound state is $-1/2 (\pi/2|\omega_3|)^2$. Asymptotically the potential falls off exponentially with the decay constant $\pi/|\omega_3|$ (Ref.12). It is interesting to compare this with the asymptotic behaviour of the Wannier function of the finite band. In his study of the analytic properties of Bloch waves and Wannier functions in one dimension¹³ Kohn has given a method to determine the asymptotic behaviour of the Wannier functions from the knowledge of the dispersion relation only. The decay constants are given by the maximal values of the imaginary part of the complex wavevector in the gaps. Consequently one has to calculate the wavevector where the imaginary density of states goes through zero. In our case this is $E_0 = \eta_1/2\omega_1$ and we have

$$\text{Im } K(E_0 = \frac{\eta_1}{2\omega_1}) = + \sqrt{-1} \int_{\frac{\eta_1}{\omega_1}}^{-e_3} \frac{(y - \frac{\eta_1}{\omega_1}) dy}{\sqrt{4(y+e_1)(y+e_2)(y+e_3)}} \quad (13)$$

If we denote with $K(m)$ and $E(m)$ the complete Elliptic Integrals of the first and second kind and with $Z(\beta, m)$ the Jacobian Zeta Function then we

can give the evaluation of the integral above by the following simple expression

$$\operatorname{Im} K\left(\frac{\eta_1}{2\omega_1}\right) = + \sqrt{2(\ell+b)} Z(\beta, m)$$

with

$$\beta = \arcsin \sqrt{\frac{1}{m} \left(1 - \frac{E(m)}{K(m)}\right)}$$

This β maximises the Zeta Function at fixed modulus (formula 141.25 of reference 11). If we represent the decay constant of the wavefunction of the bound state of the Pöschl-Teller potential as a function of the spectral parameters in an analogous manner as the lattice constant in formula (9) we obtain:

$$\frac{\pi}{2|\omega_3|} = \sqrt{2(\ell+b)} \frac{\pi}{2K'(m)}$$

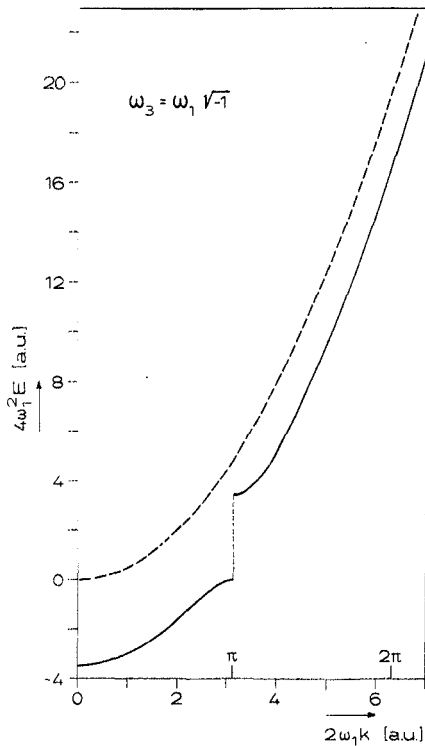


Fig.2 - Decay constants (Notation is explained in the text).

$K'(m)$ being $K(1-m)$. The factor $\sqrt{2(1+b)}$ occurs also in the expression of the decay constant of the Wannier function. This common factor corresponds to the decay constant of the Wannier functions in the tight-binding limit in the case where the bound state of the corresponding "atomic" potential lies at the energy $-e_1/2$ i.e. at the bottom of our finite band¹³. The different decay behaviour of the Wannier function and the wavefunction of the bound state is determined by the different factors Z_{\max} and $\pi/2K'$, respectively, which are shown in Fig.2.

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