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Transfer matrix in one dimensional problems

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Résumé. — La méthode de la matrice de transfert à une dimension est étendue à une large classe de problèmes. Nous présentons des solutions pour les équations de Schrödinger et Dirac, ainsi que pour le modèle à deux bandes de Kane. Dans le cas d'un potentiel périodique, $E(k)$ est obtenue par diagonalisation de la matrice de transfert, et les solutions des équations décrites plus haut peuvent alors être mises sous la forme $\cos(kd) = d(E)$.

Abstract. — The transfer matrix in one dimension is generalized in order to treat a wide class of problems. Solutions involving the Schrödinger and Dirac equations as well as the Kane two band model are presented. In the case of a periodic potential $E(k)$ is obtained by diagonalizing the transfer matrix and solutions of the above equations yield a dispersion relation which can be written as $\cos(kd) = f(E)$.

1. Introduction.

In this article we attempt to set up in a rigorous manner the transfer matrix in order to treat a wide class of one-dimensional problems. We refer the reader to the book of one-dimensional physics by Lieb and Mattis [1] for a general introduction to this subject.

Examples of one-dimensional problems that can be easily solved using the transfer matrix are;

A) solutions of the Schrödinger equation for a one band model [2];

B) solutions of the Kane two band model dealing with a coupled system of two first order equations [3];

C) solutions of the Dirac equation involving two coupled first order equations as in case B [4];

D) solutions of a three band model dealing with 3 second order equations [5];

E) solutions of graded structures with variable effective mass using a second order Schrödinger equation [6].

In part one of this paper we present a general mathematical description of the transfer matrix. In part two we treat the problem of two different but contiguous

intervals, while part three deals with periodic potentials where the dispersion relation for cases A, B and C takes on the form $\cos(kd) = f(E)$. Lastly we give specific examples of this theory as applied to cases A, B and C.

2. Transfer matrix.

Let us examine the system of ordinary linear homogeneous differential equations :

$$\sum_{j=1}^n \sum_{l=1}^{m+1} A_{ijl}(z) \varphi_j^{(l-1)}(z) = 0 \quad i = 1, 2, \dots, n \quad (1)$$

where the superscript indicates the order of differentiation. Using the restriction

$$A_{ijm+1}(z) \equiv \delta_{ij} \quad (2)$$

allows us to always reduce our equations to 1st order without much loss of generality.

Let $\psi(z)$ be a column vector with $N = nm$ components representing the functions $\varphi_j^{(l-1)}(z)$. This definition allows us to rewrite (1) in the form of a system

of N first order differential equations

$$\frac{d\psi}{dz}(z) = P(z) \psi \tag{3}$$

where P is an $N \times N$ matrix which may be written in a block form :

$$P(z) = \parallel R_{qr}(z) \parallel \quad q, r = 1, 2, \dots, n \tag{4a}$$

with

$$R_{qr} = \begin{pmatrix} 0 & \delta_{qr} & 0 & \dots & 0 \\ 0 & 0 & \delta_{qr} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -A_{qr1} & -A_{qr2} & -A_{qr3} & \dots & -A_{qrm} \end{pmatrix} \tag{4b}$$

If $\{ h_v(z), v = 1, 2, \dots, N \}$ is a set of linearly independent solutions of (3), then :

$$\psi(z) = \sum_{v=1}^N c_v h_v(z). \tag{5}$$

Moreover if $\{ h_v \}$ is a canonical basis in z_0 , i.e. :

$$h_{uv}(z_0) = \delta_{uv} \tag{6}$$

where u represents a particular component, and v represents a particular vector in the basis, we obtain

$$c_v = \psi_v(z_0) \tag{7}$$

and

$$\psi(z) = M(z, z_0) \psi(z_0) \tag{8}$$

where we have introduced the transfer matrix $M(z, z_0)$ which connects the values of ψ at z_0 and z , i.e. :

$$M(z, z_0) = \parallel h_{uv}(z) \parallel. \tag{9}$$

In general using a basis $\{ f_v(z) \}$, and defining

$$N(z) \parallel f_{uv}(z) \parallel \tag{10}$$

it is not difficult to show that :

$$M(z, z_0) = N(z) N^{-1}(z_0). \tag{11}$$

In the particular case of constant coefficients A_{ijl} , P will be a constant matrix having an explicit solution [11] of the form :

$$M(z, z_0) = e^{P \cdot (z - z_0)}. \tag{12}$$

3. Complex structures.

Usually the analytical properties of the coefficients A_{ijl} assures us of the continuity of any solution $\psi(z)$. Knowing the transfer matrix in two contiguous intervals allows us to determine the complete transfer matrix. In other words, if

$$\psi(z) = M_0(z, z_0) \psi(z_0) \quad z_0 \leq z \leq z_1 \tag{13a}$$

and

$$\psi(z) = M_1(z, z_1) \psi(z_1) \quad z_1 \leq z \leq z_2 \tag{13b}$$

then

$$\psi(z) = M(z, z_0) \psi(z_0) \quad z_1 \leq z \leq z_2 \tag{14}$$

where

$$M(z, z_0) = M_1(z, z_1) M_0(z_1, z_0) \tag{15}$$

and likewise for any other contiguous intervals. This is an interesting situation that arises frequently in the analysis of complex structures composed of different layers [7].

In other cases [6, 12] some components of $\psi(z)$ have a steplike behaviour at a point, say z_1 , where the limiting values to the left and right sides of this point are connected by a linear expression

$$\psi(z_{1+}) = C(z_1) \psi(z_{1-}). \tag{16}$$

If this is the case, we write :

$$M(z, z_0) = M_1(z, z_1) C(z_1) M_0(z_1, z_0). \tag{17}$$

4. Periodic potentials.

If the coefficients A_{ijl} are periodic, with periodicity d , then the P matrix is periodic. Floquet [13] has demonstrated that in this case there are solutions that satisfy the condition

$$\psi_\lambda(z + d) = \lambda \psi_\lambda(z) \tag{18}$$

where λ is a complex number called the Floquet multiplier. Writing :

$$\lambda = e^{ikd} \tag{19}$$

and imposing the periodic boundary condition, we get $-\pi/d \leq k < \pi/d$, and $\psi_\lambda(z)$ may be written as :

$$\psi_k(z) = e^{ikz} U_k(z) \tag{20}$$

$U_k(z)$ being periodic :

$$U_k(z + d) = U_k(z). \tag{21}$$

Rewriting (18) in terms of the transfer matrix we have :

$$M(z + d, z) \psi_k(z) = e^{ikd} \psi_k(z). \tag{22}$$

In other words : The Floquet solutions in z are the eigenfunctions of the transfer matrix that connects the two ends of the unit cell $(z, z + d)$. Furthermore, since $M(z + d, z)$ depends on all the parameters in the original system (1), in particular the energy, the diagonalization procedure gives us the dispersion relation $E = E(k)$. This simplifies the results for the cases A, B, C, where $N = 2$. The eigenvalues $\lambda_1 = e^{ik_1d}$, $\lambda_2 = e^{ik_2d}$ are the solutions of

$$\lambda^2 - \text{Tr } M(z + d, z) \lambda + \det M(z + d, z) = 0 \tag{23}$$

or, alternatively,

$$\lambda_1 + \lambda_2 = \text{Tr } M \tag{24a}$$

$$\lambda_1 \lambda_2 = \det M. \tag{24b}$$

In these three cases the $\det M(z + d, z) = \det M(z, z) = 1$ (due to the absence of certain terms in (1)). Then $\lambda_2 = 1/\lambda_1$ and, from (24a),

$$\cos(kd) = f(E) = \frac{1}{2} \text{Tr } M. \tag{25}$$

This is the general form that the dispersion relation takes in cases A, B, C, for any one dimensional periodic potential. This result is well known for the Schrödinger equation (14) and has been obtained for several other particular cases [3, 4, 6, 7, 8, 9].

5. Examples.

(A) SCHRÖDINGER EQUATION. — Here we have $n = 1, m = 2, N = 2$ and equation (1) becomes

$$\psi''(z) + 2 \mu/\hbar^2 [E - V(z)] \psi(z) = 0. \tag{26}$$

Repeating the general procedure

$$\psi(z) = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} \psi \\ \psi' \end{pmatrix} \tag{27}$$

and

$$P(z) = \begin{pmatrix} 0 & 1 \\ -2 \mu/\hbar^2 [E - V(z)] & 0 \end{pmatrix} \tag{28}$$

Let $g_1(z)$ and $g_2(z)$ be two linearly independent solutions of (26). Then

$$N(z) = \begin{pmatrix} g_1(z) & g_2(z) \\ g_1'(z) & g_2'(z) \end{pmatrix} \tag{29}$$

$$M(z, z_0) = \frac{1}{\Delta} \begin{pmatrix} g_2'(z_0) g_1(z) - g_1'(z_0) g_2(z) & g_1(z_0) g_2(z) - g_2(z_0) g_1(z) \\ g_2'(z_0) g_1'(z) - g_1'(z_0) g_2'(z) & g_1(z_0) g_2'(z) - g_2(z_0) g_1'(z) \end{pmatrix} \tag{30a}$$

where

$$\Delta = g_1(z_0) g_2'(z_0) - g_1'(z_0) g_2(z_0). \tag{30b}$$

In the interval where the potential is constant we get using equation (30) or equation (12)

$$M(z, z_0) = \begin{pmatrix} \cos [p(z - z_0)] & \frac{1}{\theta} \sin [p(z - z_0)] \\ -\theta \sin [p(z - z_0)] & \cos [p(z - z_0)] \end{pmatrix} \quad (31a)$$

where

$$\theta = p = \sqrt{2\mu/\hbar^2[E - V]}. \quad (31b)$$

(B) KANE'S TWO BAND MODEL [3]. — The wave function $\psi(z) = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$ satisfies equation (3) with

$$P = \begin{pmatrix} 0 & \frac{1}{\rho} \left[V(z) - \left(E + \frac{E_{\text{eff}}}{2} \right) \right] \\ -\frac{1}{\rho} \left[V(z) - \left(E - \frac{E_{\text{eff}}}{2} \right) \right] & 0 \end{pmatrix} \quad (32a)$$

and where

$$\left(\frac{E_{\text{eff}}}{2} \right)^2 = \left(\frac{E_g}{2} \right)^2 + \rho^2 K^2 \quad (32b)$$

and

$$K^2 = k_x^2 + k_y^2 \quad (32c)$$

E_g is the energy gap; k_x, k_y are transverse momenta; and ρ is a parameter of the order of 10^{-8} eV-cm.

This example is similar to the previous one. However we note that the second component of ψ , ψ_2 is not obtained from the first component by derivation, but in a more complex manner as given by equation (3) and equations (32a-c). For a constant potential the transfer matrix $M(z, z_0)$ is exactly the same as (31a), but now

$$p = \frac{1}{\rho} \sqrt{\left[V - \left(E + \frac{E_{\text{eff}}}{2} \right) \right] \left[V - \left(E - \frac{E_{\text{eff}}}{2} \right) \right]} \quad (33a)$$

$$\theta = \frac{\rho p}{\left[V - \left(E + \frac{E_{\text{eff}}}{2} \right) \right]}. \quad (33b)$$

(C) DIRAC EQUATION. — From a mathematical point of view the stationary one dimensional Dirac equation is a system of four differential equations which can be reduced by the unitary transformation

$$\Omega = U_1 A \quad (34a)$$

where

$$U_1 = \begin{pmatrix} 1 & 0 \\ 0 & i\sigma_3 \end{pmatrix} \quad (34b)$$

and

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (34c)$$

and

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (34d)$$

to a system of two coupled equations :

$$H_1 \Phi = E\Phi \quad (35a)$$

where

$$H_1 = \begin{pmatrix} V(z) + m_0 c^2 & -\Pi c - ic\hat{p}_z \\ -\Pi c + ic\hat{p}_z & V(z) - m_0 c^2 \end{pmatrix} \quad (35b)$$

and

$$\Pi^2 = p_x^2 + p_y^2 \tag{35c}$$

$$\hat{p}_z = -i\hbar \frac{d}{dz} \tag{35d}$$

$$\Phi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}. \tag{35e}$$

If we make the transformation

$$\psi(z) = U_2 \Phi \tag{36a}$$

with

$$U_2 = \frac{1}{\delta} \begin{pmatrix} \frac{1}{\alpha}(m_0 c^2 + \alpha) & \Pi c \\ -\Pi c & -\frac{1}{\alpha}(m_0 c^2 + \alpha) \end{pmatrix} \tag{36b}$$

and

$$\delta^2 = \frac{1}{4}(m_0 c^2 + \alpha)^2 + \Pi^2 c^2 \tag{36c}$$

and

$$\alpha = m_0 c^2(1 + 2\sqrt{1 + (\Pi/m_0 c)^2}) \tag{36d}$$

the system of equations takes the form (3) with

$$P = \begin{pmatrix} 0 & \frac{1}{\hbar c} \left[V(z) - \left(E + \frac{E_M}{2} \right) \right] \\ -\frac{1}{\hbar c} \left[V(z) - \left(E - \frac{E_M}{2} \right) \right] & 0 \end{pmatrix} \tag{37a}$$

where

$$\frac{1}{\alpha} E_M = [m_0 c^2 + \Pi^2 \xi/m_0]/(1 + \zeta) \tag{37b}$$

$$\xi = [1 + 2\sqrt{1 + (\Pi/m_0 c)^2}]/[1 + \sqrt{1 + (\Pi/m_0 c)^2}] \tag{37c}$$

$$\zeta = \frac{\Pi/m_0 c}{1 + \sqrt{1 + (\Pi/m_0 c)^2}}. \tag{37d}$$

It is evident that cases B and C are equivalent if we make the association $\rho \rightarrow \hbar c$ and $E_{\text{eff}} \rightarrow E_M$. The transfer matrix for a constant potential has the form (31a), p and θ being

$$p = \frac{1}{\hbar c} \sqrt{\left[V - \left(E + \frac{E_M}{2} \right) \right] \left[V - \left(E - \frac{E_M}{2} \right) \right]} \tag{38a}$$

$$\theta = \frac{\hbar c p}{V - \left(E - \frac{E_M}{2} \right)}. \tag{38b}$$

6. Conclusion.

We have attempted to show the power and generality of the transfer matrix method for solving a wide class of one dimensional problems. In particular formulae (9) and (11) demonstrate this generality. The method is exceptionally useful when the coefficients A_{ijl} have different analytical expressions in different intervals. This is the situation for graded structures (15). Equations (16) and (17) are useful when we wish to treat problems of variable mass, the simplest example of which is (see Ref. [6])

$$C(z_1) = \begin{pmatrix} 1 & 0 \\ 0 & \frac{m(z_{1+})}{m(z_{1-})} \end{pmatrix}$$

where $m(z_{1-})$ and $m(z_{1+})$ are the effective masses to the left and right of z_1 .

We have shown that the three important cases (A, B and C) have many common properties; in particular the transfer matrix for a constant potential has the same form (Eq. (31a)). In addition for a periodic potential the dispersion relation $\cos(kd) = f(E)$ where $f(E)$ is equal to half of the trace of the transfer matrix

for the unit cell, is the same. The method is particularly applicable to other problems such as bound states in quantum wells, transmission through barriers and evanescent states.

From a computational point of view, complicated potentials can be approximated stepwise in small intervals allowing for a simple algorithm.

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