

THE SCHROEDINGER EQUATION AND MOMENTUM TRANSFER IN CRYSTALS

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Abstract—The differential equation recently proposed by Fitzgerald in connection with momentum transfer and non-elastic deformation in crystalline solids is shown to be an alternative form of the time-dependent Schroedinger equation which applies generally to periodic structures such as crystals. The physical significance of the momentum transfer equation is not clear when it is presented solely as a form of the Schroedinger equation and hence the new formulation adds little to an understanding of the momentum transfer process in crystal lattices. On the other hand, some increased understanding of the Schroedinger equation itself appears to be possible as a result of the ideas discussed here.

INTRODUCTION

FITZGERALD [1, 2] has recently described an alternate interpretation of the wave or wave function, ψ , which is to be associated with moving particles according to the de Broglie relation. A real-property (momentum) wave, $\psi_n = mv_n$, was postulated to exist in addition to (or in place of) the Born probability waves of orthodox wave mechanics, and a differential equation for momentum transfer in periodic structures was adduced as an alternative to the Schroedinger equation. Fitzgerald's equation has the form

$$\frac{\partial(mv_n)}{\partial t} = \frac{i\hbar}{2d^2}(v_{n+1} + v_{n-1} - 2v_n) \quad (1)$$

where \hbar is Planck's constant/ 2π , v_n is the velocity of a general n th mass (atom) as a result of a particle momentum wave propagating in a lattice with atom masses m , in a direction with spacing, d . From this equation and its solutions a number of macroscopic mechanical properties of crystalline solids can be successfully described and some mechanical quantities can be calculated directly from fundamental atomic constants. These include transition velocities observed in impact experiments, the threshold velocity for cratering or phonon fission in crystals, non-elastic resonance frequencies, characteristic stresses associated with plastic deformation, and coefficients of sliding friction [2]. The equation thus has considerable practical value, but like all postulated relationships, its existence is justified only by its success.

The purpose of this article is to demonstrate a close connection between Fitzgerald's postulated momentum transfer equation for crystals and Schroedinger's (also postulated) time dependent wave equation. In fact, the Fitzgerald equation can be considered to be an *alternative form* of the Schroedinger equation which applies to non-continuous, periodic structures such as crystals. In order to show this, however, it is necessary to retain Fitzgerald's concept that a real-property wave (i.e., a momentum wave) can be associated with moving particles. Neither the de Broglie relation nor the Schroedinger equation in themselves define or in any way determine the exact nature of the waves to be associated with

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moving particles [2]. The probability interpretation of ψ was advanced separately by Born [3] and, of course, is the currently accepted view, in spite of conceptual difficulties in connection with particle diffraction by crystals [2] and various philosophical objections [4].

In considering a momentum wave to be associated with moving particles it is not necessary to exclude the coexistence of Born probability waves. Rather, it is simply more convenient in certain circumstances to consider only the momentum waves. It may well turn out that in other instances it is useful or even necessary to consider both types of waves.

1. THE SCHROEDINGER EQUATION FOR AN ATOM IN A ONE-DIMENSIONAL LATTICE

Consider a one-dimensional (row) lattice of point masses, m , and regular spacing, d , as shown in Fig. 1. The point masses, m , are further assumed to be in equilibrium at the

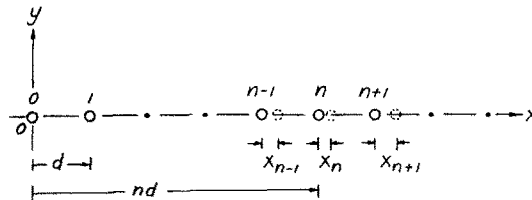


FIG. 1. Schematic drawing of a one-dimensional (row) lattice of equal point masses. Solid circles represent equilibrium positions of masses; the dashed circles, the positions of deflected or displaced masses (atoms). In the text a velocity interaction and momentum transfer between adjoining masses is discussed in terms of the Schroedinger equation.

lattice points as a result of the existence of a periodic potential energy distribution $V(x)$ such that

$$V(x) = V(x+d) \tag{2}$$

throughout the lattice. The absolute value of the potential energy is arbitrary and is here selected so that the potential is zero at the lattice points $n-1, n, n+1$ etc. That is,

$$\dots V_{n-2} = V_{n-1} = V_n = V_{n+1} = V_{n+2} \dots = 0 \tag{3}$$

where $V_n = V(x_n)$, etc.

The general time-dependent Schroedinger equation for one of the masses (atoms) of the row lattice of Fig. 1 has the well-known form [5]

$$\frac{\partial^2 \psi}{\partial x^2} - \frac{2m}{\hbar^2} V\psi + \frac{2im}{\hbar} \frac{\partial \psi}{\partial t} = 0 \tag{4}$$

where V in this case is the periodic potential given by equation (2). If ψ is a continuous function of x , then the second differential operator has its common meaning that

$$\frac{\partial^2 \psi}{\partial x^2} = \lim_{\Delta x \rightarrow 0} \frac{\Delta^2 \psi}{\Delta x^2} = \lim_{\Delta x \rightarrow 0} \frac{\Delta \left(\lim_{\Delta x \rightarrow 0} \frac{\Delta \psi}{\Delta x} \right)}{\Delta x} \tag{5}$$

since ψ is defined everywhere in the interval Δx . However, if ψ is to be a real-property of the type that can be defined in the vicinity of a mass point in a lattice but not elsewhere [1, 2], then a different meaning must be attached to the second derivative operator $\partial^2\psi/\partial x^2$. Fortunately an appropriate interpretation has already been provided by Leibnitz as discussed, for example, by Courant [6].

According to Leibnitz the second derivative can be thought of as the limit of the "second difference quotient" as follows. We consider values of the function ψ at three points, $x, x+a, x+2a$ and then take the second difference quotient as

$$\frac{1}{a} \left(\frac{\psi_2 - \psi_1}{a} - \frac{\psi_1 - \psi}{a} \right) = \frac{1}{a^2} (\psi_2 + \psi - 2\psi_1) \tag{6}$$

where $\psi = \psi(x); \psi_1 = \psi(x+a); \psi_2 = \psi(x+2a)$.

Hence if $a = \Delta x, \psi_2 - \psi_1 = \Delta\psi_1$, and $\psi_1 - \psi = \Delta\psi$ then the numerator in equation (6) becomes

$$\Delta\psi_1 - \Delta\psi = \Delta(\Delta\psi) = \Delta^2\psi \tag{7}$$

while the denominator is $(\Delta x)^2$, i.e. the square of Δx . For situations where it may not be possible to make Δx arbitrarily small, it is worthwhile to fashion a variation of Leibnitz's second difference quotient by considering values of the function ψ at x and on either side of x ; i.e., at $x-a, x$, and $x+a$. Then the second difference quotient may be written as

$$\frac{1}{a} \left(\frac{\psi_+ - \psi}{a} - \frac{\psi - \psi_-}{a} \right) = \frac{1}{a^2} (\psi_+ + \psi_- - 2\psi) \tag{8}$$

where $\psi = \psi(x); \psi_- = \psi(x-a); \psi_+ = \psi(x+a)$. In this case the second difference quotient will yield a better "mean" value for $\partial^2\psi/\partial x^2$ at x under circumstances where $a = \Delta x$ becomes very small but does not actually approach zero.

In the row lattice of Fig. 1 we have just such a case where a cannot be arbitrarily small, but has the limiting value d . In this case, therefore, an appropriate meaning for $\partial^2\psi/\partial x^2$ at a general n th mass (atom) of the lattice becomes

$$\left. \frac{\partial^2\psi}{\partial x^2} \right|_{x=x_n} = \frac{\partial^2\psi_n}{\partial x^2} = \frac{1}{d^2} (\psi_{n+1} + \psi_{n-1} - 2\psi_n) \tag{9}$$

where $\psi_n = \psi(x_n)$, etc. and d is the lattice spacing. With the substitution of equation (9) for the second partial derivative, the Schroedinger equation for a real-property wave, ψ_n , associated with a general n th mass of the row lattice of Fig. 1 takes the form,

$$\begin{aligned} \frac{1}{d^2} (\psi_{n+1} + \psi_{n-1} - 2\psi_n) - \frac{2m}{\hbar^2} V_n \psi_n + \frac{2im}{\hbar} \frac{\partial \psi_n}{\partial t} &= 0 \\ \frac{\partial \psi_n}{\partial t} &= \frac{i\hbar}{2d^2 m} (\psi_{n+1} + \psi_{n-1} - 2\psi_n) - \frac{i}{\hbar} V_n \psi_n. \end{aligned} \tag{10}$$

With the further substitution of linear momentum for ψ_n as proposed by Fitzgerald, equation (10) becomes

$$\frac{\partial(mv_n)}{\partial t} = \frac{i\hbar}{2d^2} (v_{n+1} + v_{n-1} - 2v_n) \tag{11}$$

where $\psi_n = mv_n$ and $V_n = 0$ as specified in equation (3). Hence the form of periodic potential present in the lattice does not have any effect on momentum wave propagation in the lattice. The product $V\psi$ is, in fact zero everywhere in the lattice for real-property waves. That is, values of ψ exist only in the vicinity of the mass points where V is zero; where V is not zero, ψ is zero.

Equation (11) can be considered as the Schroedinger equation for an atom in a row lattice. It is seen to be identical with Fitzgerald's differential equation for momentum transfer which was developed along entirely different lines. In order to put the Schroedinger equation into the form given by equation (11) it must be emphasized that, first, the usual meaning of the second derivative operator was extended to allow its use in a discontinuous (but regular) medium such as a crystal lattice; and, second, that particle waves were taken to be momentum waves instead of the usual probability waves of contemporary wave mechanics.

2. MOMENTUM TRANSFER IN A CRYSTAL LATTICE

In order to understand the physical significance of equation (11) and its relation to momentum transfer in a lattice it is necessary to examine Fitzgerald's [1, 2] original methods for obtaining this equation. In the first place, the equation follows if an interaction or force between masses in a lattice is postulated in which the magnitude of the force depends on the relative *velocities* of the masses. That is, if we consider a general n th mass of the row lattice of Fig. 1, we postulate a force f_n on the mass given by

$$f_n = \frac{\partial(mv_n)}{\partial t} = -\mathbf{K}_p(v_n - v_{n-1}) - \mathbf{K}_p(v_n - v_{n+1}) \quad (12)$$

where v_n is the velocity of the n th mass, etc. and \mathbf{K}_p is some type of *velocity interaction constant*. This equation was suggested [1, 2] by analogy with the situation for elastic interaction forces between atoms in a lattice. For elastic interactions the force on a general n th mass (for nearest neighbors interactions only) depends on the relative *displacement* from equilibrium of the masses, viz.,

$$f_n = m \frac{\partial^2 x_n}{\partial t^2} = -K_e(x_n - x_{n-1}) - K_e(x_n - x_{n+1}) \quad (13)$$

where x_n is the displacement from equilibrium of the n th mass, etc., and K_e is an elastic interaction constant which depends on the periodic potential function $V(x)$.

A second basis for equation (12) arises if we consider that some type of *momentum transfer process* exists in the lattice for which the rate of momentum transfer depends on the velocity differences between neighboring masses. In this case we write equation (12) in the form

$$\frac{\partial(mv_n)}{\partial t} = \mathbf{K}_p(v_{n-1} - v_n) - \mathbf{K}_p(v_n - v_{n+1}) \quad (12')$$

and for momentum transfer from left to right in the row lattice of Fig. 1 we note that

$\frac{\partial(mv_n)}{\partial t}$	represents the net time rate of change of momentum at lattice point n .
$\mathbf{K}_p(v_{n-1} - v_n)$	is the rate of momentum transfer from point $n - 1$ to point n .
$\mathbf{K}_p(v_n - v_{n+1})$	is the rate of momentum transfer from point n to point $n + 1$.
\mathbf{K}_p	is the <i>momentum transfer constant</i> for the lattice.

Equation (12') in this view simply represents a continuity equation for momentum flow or transfer in the lattice, i.e., the physical basis for the equation is a statement of conservation of momentum between the three interacting masses in the lattice.

So far nothing can be said about the exact nature of the possibly complex momentum transfer constant \mathbf{K}_p . However it is possible to write a wave solution [1, 2] for v_n in equations (12 or 12') of the form

$$v_n = B e^{-i(2\pi\nu_p t - knd)} \tag{14}$$

where $k = 2\pi/\lambda$ is the wave vector, d is the lattice spacing, B is a constant, and the frequency ν_p is given by

$$\nu_p = \frac{-i2\mathbf{K}_p}{\pi m} \sin^2 \frac{kd}{2}. \tag{15}$$

Then if we associate a momentum wave ($\psi = mv$) with a particle, we expect that in the limit as $k \rightarrow 0$ (or $\lambda \rightarrow \infty$) the lattice of Fig. 1 should act as a field-free region to the wave.

That is, the closely spaced periodic variation of potential in the lattice cannot have any effect on a wave of very large wavelength. Thus, as shown by Fitzgerald [1, 2], we find that in the limit as $k \rightarrow 0$ the expression for the frequency, ν_p , of a particle momentum wave in a lattice (equation 15) must reduce to that for a free particle,

$$\lim_{k \rightarrow 0} \frac{-i2\mathbf{K}_p}{\pi m} \sin^2 \frac{kd}{2} = \frac{\hbar}{4\pi m} k^2 \tag{16}$$

where $\hbar k^2/4\pi m$ is the free-particle frequency obtained from the de Broglie relation and by setting $\hbar\nu = mv^2/2$.

At small values of k the sine can be replaced by its argument in equation (16), so we have

$$\mathbf{K}_p = i\hbar/2d^2. \tag{17}$$

Hence by this method a value for \mathbf{K}_p is determined by the physical boundary condition that at long wavelengths (small k) the variation of ν_p with k in a lattice must be the same as that for a free particle. Equations (12 and 12') thus are identical to equation (11) obtained from the Schroedinger equation.

CONCLUSIONS

It is possible to obtain Fitzgerald's differential equation for momentum transfer in a row lattice from the time-dependent Schroedinger equation for an atom of mass, m in the lattice. However, the physical significance of the equation (repeated below)

$$\frac{\partial(mv_n)}{\partial t} = \frac{i\hbar}{2d^2}(v_{n+1} + v_{n-1} - 2v_n) \quad (11)$$

is not clear when it is presented as a form of the Schroedinger equation. In particular, the term $i\hbar/2d^2$ has no obvious meaning. On the other hand, when this same equation is adduced by Fitzgerald's original methods [1, 2] several physical interpretations of $i\hbar/2d^2$ are immediately available; first, as a velocity interaction constant giving the relation between the force on a general n th mass of the lattice and the relative velocities of its nearest neighbors; second, as a momentum transfer constant for the lattice. In the latter case the equation can be put into a form where it becomes simply a statement of conservation of linear momentum between three interacting masses in the lattice. In this connection the assumption is made that momentum transfer can occur between equal masses only if their velocities differ.

The formulation of the momentum transfer equation from the Schroedinger equation thus adds little to an understanding of the momentum transfer process in a crystal lattice. On the other hand, there is a strong possibility that some increased understanding of the Schroedinger equation itself can be gained as a result of the formulation. For example, suppose that we are not considering a mass (atom) in a regular lattice with periodic potential $V(x)$ such that the term $V\psi$ is zero. Then the Schroedinger equation retains its usual form which can be written as

$$\frac{\partial\psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2\psi}{\partial x^2} - \frac{i}{\hbar} V\psi. \quad (18)$$

Now the question is, can a real-property such as the momentum (mv) of the mass be generally substituted for ψ ? The answer to this question must be negative since such a real property can be defined only in the vicinity of the mass, m , and not elsewhere. Hence ψ in this case can not be continuous and $\partial^2\psi/\partial x^2$ has no meaning. (For a regular lattice of spacing d we were able to find a reasonable special meaning for $\partial^2\psi/\partial x^2$, but this can not be done in general). We can, however, suggest that a velocity field, v , can be defined such that $P = mv$. Then the velocity field will be continuous in space even though the momentum, P , (because of the discrete location of masses) is not. Hence the "Schroedinger Equation" for such a velocity field can be written as:

$$\frac{\partial v}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 v}{\partial x^2} - \frac{i}{\hbar} Vv, \quad (19)$$

and the space dependence of $v(x)$ determined for a given $V(x)$, etc.

Further discussion of such "velocity fields" and other aspects of a possible reinterpretation of the Schroedinger equation will be given elsewhere.

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Résumé—L'équation différentielle proposée récemment par Fitzgerald relativement au transfert d'une quantité de mouvement et à la déformation non élastique dans des solides cristallins est présentée comme étant une forme alternative de l'équation dépendant du temps de Schroedinger qui s'applique généralement à des structures périodiques telles que des cristaux. La signification physique de l'équation du transfert d'une quantité de mouvement n'est pas claire lorsqu'elle est présentée uniquement comme une forme de l'équation de Schroedinger et par suite la nouvelle formulation aide peu à comprendre le processus du transfert de la quantité de mouvement dans des treillis cristallins. D'autre part, une compréhension quelque peu accrue de l'équation de Schroedinger elle-même paraît possible résultant des idées qui viennent d'être discutées.

Zusammenfassung—Die Differentialgleichung die kürzlich von Fitzgerald im Zusammenhang mit Impuls-Übertragung sowie nichtelastischer Verformung kristalliner Festkörper vorgeschlagen wurde; ist wie gezeigt wird eine Abart der zeitabhängigen Schrödinger'schen Gleichung die allgemein auf periodische Formen wie Krystalle angewandt werden kann. Die physikalische Bedeutung der Impulsübertragungs-Gleichung ist nicht klar wenn sie einfach als Form der Schrödinger'schen Gleichung gegeben wird, daher bietet die neue Form nicht viel zur Erklärung des Impulsübertragungs-Vorganges in Kristallgittern. Andererseits scheint es, dass die Schrödinger'sche Gleichung selbst als Resultat der Diskussionen jetzt besser verstanden wird.

Абстракт—Оказывается, что дифференциальное уравнение, выведенное недавно Фитцджералдом и относящееся к вектору передачи импульса и неупругой деформации в кристаллических твердых телах, является другим выражением зависящего от времени уравнения Шредингера, которое вообще говоря, пригодно для исследования таких периодических структур как кристаллы. Физический смысл уравнения вектора передачи импульса неясен в случае, когда оно представлено только в виде уравнения Шредингера. Следовательно новая формулировка приводит к некоторому выяснению картины вкорме передачи импульса в кристаллических решениях. С другой стороны, идеи обсуждаемые в настоящей статье помогают лучше понять смысл уравнения Шредингера.