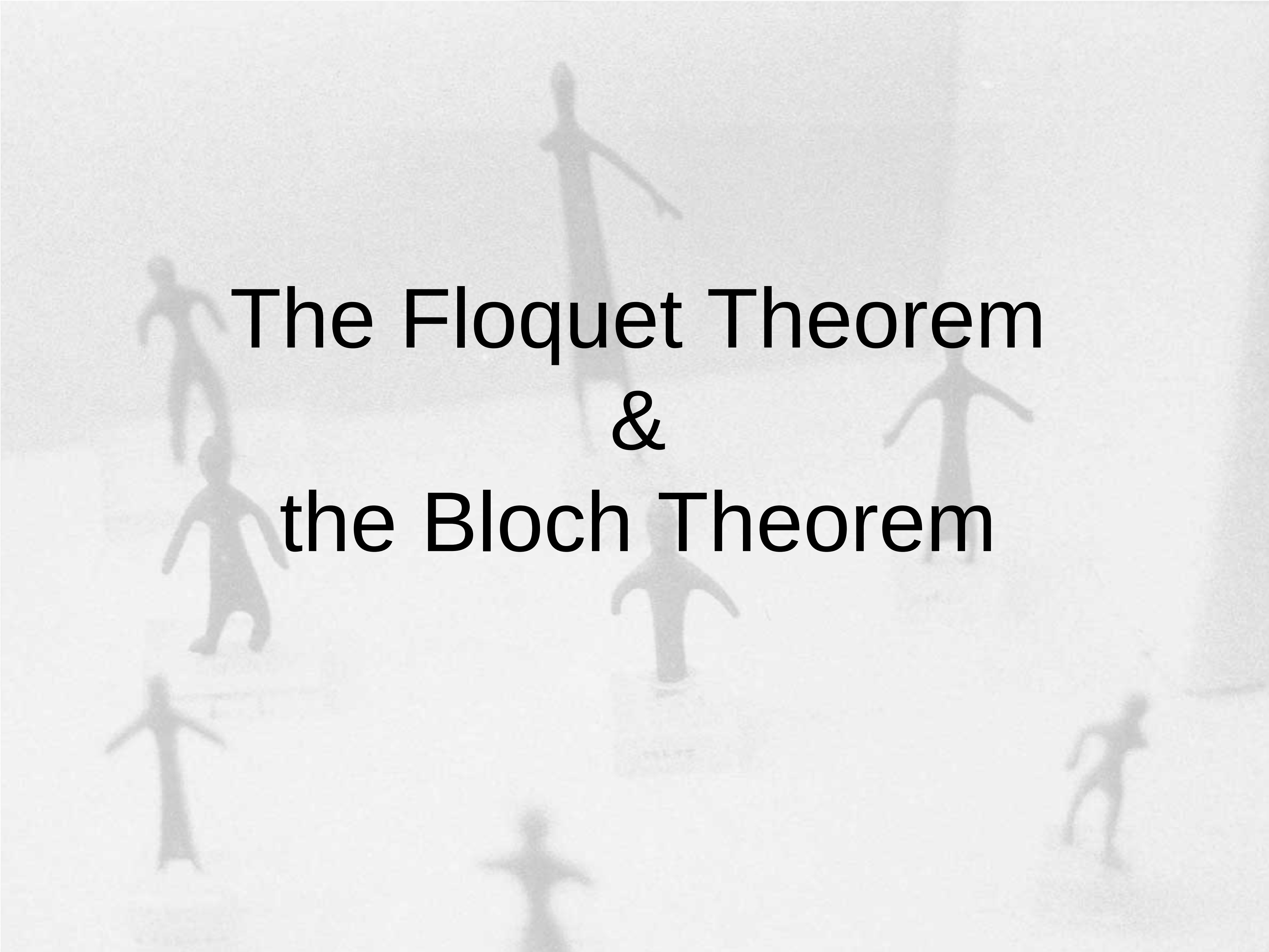

The Floquet Theorem
&
the Bloch Theorem

ANNALES

SCIENTIFIQUES

DE

L'ÉCOLE NORMALE SUPÉRIEURE,

PUBLIÉES SOUS LES AUSPICES

DU MINISTRE DE L'INSTRUCTION PUBLIQUE,

PAR

UN COMITÉ DE REDACTION COMPOSÉ DE MM. LES MAITRES DE CONFÉRENCES DE L'ÉCOLE.

DEUXIÈME SÉRIE.

TOME DOUZIÈME. — ANNÉE 1883.

PARIS,

GAUTHIER-VILLARS, IMPRIMEUR-LIBRAIRE

DE L'ÉCOLE POLYTECHNIQUE, DU BUREAU DES LONGITUDES,

SUCCESSEUR DE MALLET-BACHELIER,

Quai des Augustins, 55.

1883

SUR LES

ÉQUATIONS DIFFÉRENTIELLES LINÉAIRES

A COEFFICIENTS PÉRIODIQUES,

PAR M. G. FLOQUET,

PROFESSEUR A LA FACULTÉ DES SCIENCES DE NANCY.

Je considère, dans ce travail, une équation différentielle linéaire homogène

$$P(y) = \frac{d^m y}{dx^m} + p_1 \frac{d^{m-1} y}{dx^{m-1}} + p_2 \frac{d^{m-2} y}{dx^{m-2}} + \ldots + p_m y = 0,$$

Ann.Sci.Ec.Norm.Sup.Paris **12**, 47 (1883)

Über die Quantenmechanik der Elektronen in Kristallgittern.

Von **Felix Bloch** in Leipzig.

Mit 2 Abbildungen. (Eingegangen am 10. August 1928.)

Die Bewegung eines Elektrons im Gitter wird untersucht, indem wir uns dieses durch ein zunächst streng dreifach periodisches Kraftfeld schematisieren. Unter Hinzunahme der Fermischen Statistik auf die Elektronen gestattet unser Modell Aussagen über den von ihnen herrührenden Anteil der spezifischen Wärme des Kristalls. Ferner wird gezeigt, daß die Berücksichtigung der thermischen Gitterschwingungen Größenordnung und Temperaturabhängigkeit der elektrischen Leitfähigkeit von Metallen in qualitativer Übereinstimmung mit der Erfahrung ergibt.

Z.Physik **52**, 555 (1928)

$$a\,G_1 = K, \quad b\,G_2 = L, \quad c\,G_3 = M,$$

so wird aus (6)

$$\psi_{klm} = e^{2\pi i\left(\frac{kx}{K} + \frac{ly}{L} + \frac{mz}{M}\right)} u_{klm}(x\,y\,z). \tag{6a}$$

Über die spezielle Form der Funktion u_{klm} ist nichts ausgesagt. Diese hängt natürlich davon ab, wie das Potential im einzelnen verläuft, und außerdem kann sie außer von den Zahlen k, l, m noch sehr wohl von anderen Quantenzahlen abhängen.

Die Tatsache, daß sich von den Eigenfunktionen nach (6a) stets ein Faktor $e^{2\pi i\left(\frac{kx}{K} + \frac{ly}{L} + \frac{mz}{M}\right)}$ abspalten läßt, wobei der Rest nur noch die Periodizität des Gitters aufweist, läßt sich anschaulich so formulieren, daß wir es mit ebenen de Broglie-Wellen zu tun haben, die im Rhythmus des Gitteraufbaus moduliert sind*.

A.A. Cottey, Am.J.Phys. 39,1235 (1971)

Canonical forms of translations

Suppose the time-independent **one-dimensional** Schrödinger equation is given by

$$\frac{d^2\psi(x)}{dx^2} + Q(x)\psi(x) = 0 \qquad ,$$

where

$$Q(x) = \frac{2m}{\hbar^2}(E - V(x)) \qquad ,$$

such that the potential function $V(x)$ is periodic in some constant a

$$V(x) = V(x+a) \quad , \quad \forall x \qquad .$$

The Schrödinger equation is an ordinary linear second order differential equation that has two linear independent solutions for each value of E such that a linear combination of these two solutions is also a solution of the eigenvalue problem.

It should be noted that for some values of E these solutions are not stable, i.e. there is no constant M such that

$$|\psi(x)| < M \quad , \quad \forall x \qquad .$$

The solutions $\psi(x)$ are contineous and can become unstable only by growing indefinitely at $x = \infty$, $x = -\infty$ or $x = \pm\infty$.

Suppose that for a given eigenvalue E, $\psi_1(x)$ and $\psi_2(x)$ are the two linear independent then $\psi_1(x+a)$ and $\psi_2(x+a)$ are also solutions of the Schrödinger equation, since this equation is unchanged if x is replaced by $x+a$:

$$\begin{aligned}&[d^2/dx^2 - V(x)]\,\psi_1(x) = \\ &= [d^2/d(x+a)^2 - V(x+a)]\,\psi_1(x+a) = \\ &= E\psi_1(x) \equiv E\psi_1(x+a)\end{aligned}$$

Using $\psi_1(x)$ and $\psi_2(x)$ as a basis,

$$\underline{v}(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix} \qquad ,$$

then obviously the following relation applies

$$\begin{aligned}\underline{v}(x+a) &= \begin{pmatrix} \psi_1(x+a) \\ \psi_2(x+a) \end{pmatrix} = \\ &= \underline{T}\underline{v}(x) = \underline{T}\begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix} \qquad ,\end{aligned}$$

where $\underline{T}$ corresponds to a linear operator, who-se matrix representative is of dimension two with in general complex matrix elements. $\underline{T}$ is the matrix representative of that operator, that corresponds to a translation by a.

A different combination of solutions can be obtained by a linear transformation $\underline{L}$

$$\underline{v}'(x) = \underline{L}\underline{v}(x) \quad , \quad \det(\underline{L}) \neq 0 \quad .$$

The translational properties are then given by

$$\begin{aligned} \underline{v}'(x+a) &= \underline{T}'\underline{v}'(x) \\ \underline{L}\underline{v}(x+a) &= \underline{T}'\underline{L}\underline{v}(x) \end{aligned}$$

i.e.,

$$\underline{L}\underline{v}(x+a) = \underline{T}'\underline{L}\underline{v}(x) \quad ,$$

or

$$\underline{v}(x+a) = \left(\underline{L}^{-1}\underline{T}'\underline{L}\right)\underline{v}(x) \equiv \underline{T}\underline{v}(x) \quad .$$

Obviously this is a similarity transformation for the matrix representative $\underline{T}$

$$\boxed{\underline{T}' = \underline{L}\underline{T}\underline{L}^{-1}} \quad .$$

The canonical form of the matrix $\underline{T}$ depends on its eigenvalues τ, i.e., depends on the solutions of the following system of equations

$$\boxed{\det(\underline{T} - \tau\underline{I}) = 0} \quad ,$$

It should be recalled that the eigenvalues of $\underline{T}$ remain unchanged by a similarity transformation. Since $\underline{T}$ and $\underline{I}$ are two-by-two matrices the eigenvalue equation corresponding to the last equation is quadratic in τ.

Canonical type I

If both eigenvalues of $\underline{T}$ are different, $\tau_1 \neq \tau_2$, then $\underline{T}'$ is diagonal:

$$\underline{T}' = \begin{pmatrix} \tau_1 & 0 \\ 0 & \tau_2 \end{pmatrix} \quad .$$

Canonical type II

If $\tau_1 = \tau_2$ and

$$\underline{T} \neq \begin{pmatrix} \tau_1 & 0 \\ 0 & \tau_1 \end{pmatrix} \quad ,$$

then $\underline{T}'$ is of the form:

$$\underline{T}' = \begin{pmatrix} \tau_1 & 0 \\ 1 & \tau_1 \end{pmatrix} \quad .$$

Canonical type III

If $\tau_1 = \tau_2$ and

$$\underline{T} = \begin{pmatrix} \tau_1 & 0 \\ 0 & \tau_1 \end{pmatrix} \quad ,$$

then

$$\underline{T} = \underline{T}' \quad , \quad \forall \underline{L} \quad .$$

For a further evaluation of the eigenvalues τ_1 and τ_2 one can make use of the fact that $\det(\underline{T}) = 1$. In order to show that this is indeed the case, one picks two linear independent solutions $\psi_1(x)$ and $\psi_2(x)$ of the Schrödinger equation and constructs the following matrix:

$$\underline{W}(x) = (\underline{v}(x), \frac{d\underline{v}(x)}{dx}) = \begin{pmatrix} \psi_1(x) & d\psi_1(x)/dx \\ \psi_2(x) & d\psi_2(x)/dx \end{pmatrix} \qquad .$$

Since $\psi_1(x)$ and $\psi_2(x)$ are solutions of the Schrö-dinger equation to one and the same eigenvalue E,

$$\frac{d^2\psi_1(x)}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\psi_1(x) = 0 \qquad ,$$

$$\frac{d^2\psi_2(x)}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\psi_2(x) = 0 \qquad ,$$

one can multiply the first of these two equations with $\psi_2(x)$ and the second with $\psi_1(x)$. Subtracting now the first equation from the second equation yields

$$\psi_1(x)\left(\frac{d^2\psi_2(x)}{dx^2}\right) - \psi_2(x)\left(\frac{d^2\psi_1(x)}{dx^2}\right) = 0 \qquad .$$

This in turn implies that $\det(\underline{W})$, the so-called **Wronski determinant** is a constant:

$$\det(\underline{W}) = \psi_1(x)\,(d\psi_2(x)/dx) - \psi_2(x)\,(d\psi_1(x)/dx)$$
$$= const \qquad .$$

Considering now the translational properties of $\psi_1(x)$ and $\psi_2(x)$,

$$\underline{v}(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix} \qquad ,$$

$$\frac{d\underline{v}(x)}{dx} = \begin{pmatrix} d\psi_1(x)/dx \\ d\psi_2(x)/dx \end{pmatrix} \qquad ,$$

$$\frac{d\underline{v}(x+a)}{dx} = \underline{T}\left(\frac{dv(x)}{dx}\right) \qquad ,$$

for the matrix $\underline{W}(x+a)$,

$$\underline{W}(x+a) = \begin{pmatrix} \psi_1(x+a) & d\psi_1(x+a)/dx \\ \psi_2(x+a) & d\psi_2(x+a)/dx \end{pmatrix} \qquad ,$$

one obtains the following translational property

$$\underline{W}(x+a) = \underline{TW}(x)$$

and therefore

$$\det(\underline{W}(x+a)) = \det(\underline{T})\det(\underline{W}(x)) \qquad .$$

However, since

$$\det(\underline{W}(x+a)) = \det(\underline{T})\,\det(\underline{W}(x)) = const \quad ,$$

it follows immediately that

$$\det(\underline{T}) = 1 \qquad .$$

Furthermore, since - as is well-known - the determinant is unchanged by a similarity transformation, i.e.,

$$\det(\underline{T}') \equiv \det(\underline{T}) \qquad ,$$

this implies for the eigenvalues τ_1 and τ_2 that

$$\boxed{\tau_1 \tau_2 = 1 \quad or \quad \tau_1^2 = 1} \qquad .$$

Finally one can use the fact that the trace (tr) of the matrix $\underline{T}'$ has to be real. This again is easily understood from the Schröd-inger equation. Since all quantities in this equation are real, also the solutions $\psi_1(x)$ and $\psi_2(x)$ can be chosen to be real in the interval $-\infty < x < \infty$. Quite clearly then also the solutions $\psi_1(x+a)$ and $\psi_2(x+a)$ are real,

$$\underline{T} real \underbrace{\begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix}} = real \underbrace{\begin{pmatrix} \psi_1(x+a) \\ \psi_2(x+a) \end{pmatrix}} \qquad ,$$

which implies that $\underline{T}$ has only real matrix elements, i.e.,

$$tr(\underline{T}) \equiv tr(\underline{T}') \equiv real \qquad ,$$

$$\boxed{\tau_1 + \tau_2 = real \quad or \quad \tau_1 = real} \qquad .$$

Writing therefore the eigenvalues τ_1 and τ_2 of the canonical forms of $\underline{T}'$ as the following unit roots

$$\boxed{\tau = \exp(i\kappa a) = \exp(ika)\exp(-\mu a)} \quad ,$$

$$\boxed{\kappa = k + i\mu} \quad ,$$

$$\boxed{Im(k) = Im(\mu) = 0} \quad ,$$

the various canonical forms can be classified according to the (real) numbers k and μ such that $\det(\underline{T}') = 1$ and $Im[tr(\underline{T}')] = 0$.

Floquet theorem

Solutions of the Schrödinger equation with the property

$$\psi(x+a) = \tau\psi(x) \qquad ,$$

are called *Floquet functions* or *Floquet solutions*. There exist two linear independent solutions of the Schrödinger equation if and only if $\underline{T}$ has two different eigenvalues ($\tau_1 \neq \tau_2$), which is the case for the **canonical type I** or if $\underline{T} = \pm\underline{I}$ (unit matrix), which is the case for **canonical type III**.

If $\underline{T}$ has a double degenerated eigenvalue ($\tau_1 = \tau_2 = \pm 1$) and is **not** of the form $\underline{T} = \pm\underline{I}$ (**canonical type II**) then there exists a Floquet solution $\psi_1(x)$ of the Schrödinger equation such that the corresponding linear independent solution $\psi_2(x)$ has the pro-perty

$$\psi_2(x+a) = \tau_1\psi_2(x) + \psi_1(x) \qquad .$$

Remark 1: The Floquet theorem follows immediately from the possible canonical forms of $\underline{T}$ and the properties

$$\det(\underline{T}) = 1 \text{ and } Im[tr(\underline{T})] = 0.$$

Remark 2: Suppose $g(x)$ is a general solution of the Schrödinger equation

$$g(x) = \alpha\psi_1(x) + \beta\psi_2(x) \quad ,$$

$$g(x+a) = \alpha\psi_1(x+a) + \beta\psi_2(x+a) \quad ,$$

$$Im(\alpha) = Im(\beta) = 0 \quad ,$$

then one can see that since for

$$\textbf{type I}: \quad g(x+a) = \tau_1\alpha\psi_1(x) + \tau_2\beta\psi_2(x)$$

$$\textbf{type II}: \quad g(x+a) = \tau_1 g(x) + \beta\psi_2(x)$$

$$\begin{aligned} \textbf{type III}: \quad g(x+a) &= \tau_1\left(\alpha\psi_1(x) + \beta\psi_2(x)\right) \\ &= \tau_1 g(x) \end{aligned}$$

only in the case of **canonical type III** the general solution of the Schrödinger equation is also a Floquet solution.

Remark 3: A Floquet solution can always be written in the following form

$$\psi(x+a) = e^{i\kappa x} u(x) \qquad ,$$

where

$$u(x) = u(x+a) \qquad .$$

The function $u(x)$ and the (complex) number κ are **not** uniquely determined by the equation

$$\psi(x+a) = \tau\psi(x) \qquad ,$$

since all κ' and $u'(x)$ of the form

$$\kappa' = \kappa + (2\pi n/a) \qquad ,$$

$$u'(x) = \exp(-2\pi i n x/a) u(x)$$

$$n = 0, \pm 1, \pm 2, \cdots$$

also satisfy the requirements for a Floquet solution.

Since the complex number κ was given by

$$\boxed{\kappa = k + i\mu} \quad ,$$

its real part k can be restricted to the interval

$$\boxed{-(\pi/a) \leq k \leq (\pi/a)} \quad ,$$

whereby the values $\pm(\pi/a)$ are equivalent to each other.

Remark 4: For a canonical type II Floquet solution $\psi_1(x)$ there exists a linear independent function $\psi_2(x)$, which can be written as

$$\psi_2(x) = \phi_2(x) + \frac{x}{a\tau_1}\psi_1(x)$$

with

$$\psi_2(x) = \tau_1\psi_2(x) + \psi_1(x) \qquad ,$$

such that

$$\phi_2(x+a) = \tau_1\phi_2(x) \qquad .$$

In this case, however, $\phi_2(x)$ is not a solution of the Schrödinger equation.

Remark 5: Floquet solutions are stable if and only if

$$Im(k+i\mu) = 0 \quad ,$$

since for $\mu \neq 0$

$$\exp\left((ik-\mu)x\right) u(x)$$

grows indefinitely for $x \to \pm\infty$. In the case of canonical type II the corresponding linear independent function $\psi_2(x)$ becomes singular for $x = \infty$ or $x = -\infty$.

Type	Canonical form	k	μ	Stab.
I^s	$\begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix}$	$\neq \frac{n\pi}{a}$	$= 0$	$\forall$ s.
I^+	$\begin{pmatrix} e^{\mu a} & 0 \\ 0 & e^{-\mu a} \end{pmatrix}$	$= \frac{2n\pi}{a}$	$\neq 0$	$\forall$ u.
I^-	$\begin{pmatrix} -e^{\mu a} & 0 \\ 0 & -e^{-\mu a} \end{pmatrix}$	$= \frac{(2n+1)\pi}{a}$	$\neq 0$	$\forall$ u.
II^+	$\begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$	$= \frac{2n\pi}{a}$	$= 0$	ψ_1 s. ψ_2 u.
II^-	$\begin{pmatrix} -1 & 0 \\ 1 & -1 \end{pmatrix}$	$= \frac{(2n+1)\pi}{a}$	$= 0$	ψ_1 s. ψ_2 u.
III^+	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$= \frac{2n\pi}{a}$	$= 0$	$\forall$ s.
III^-	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$= \frac{(2n+1)\pi}{a}$	$= 0$	$\forall$ s.

Bandstructure

Since the eigenvalues τ of the canonical forms of $\underline{T}'$ were written as

$$\tau = \exp(ika)\exp(-\mu a) = \exp(i\kappa a) \quad ,$$
$$Im(k) = Im(\mu) = 0 \quad ,$$

one can plot the possible eigenvalues E of the Schrödinger equation versus κ. In this case one gets a separation of the energies E into **bands**, namely a **one-dimensio** whereby the $\pm$ sign indicates that $\exp(ika) = \pm 1$.

$$\mu \neq 0 \text{ if and only if } k = 0, \pm\frac{\pi}{a} \quad .$$

The possible energy eigenvalues E fall then in the following intervals

$$E_0^+ < E_1^- \leq E_2^- < E_1^+ \leq E_2^+ < E_3^- \leq E_4^- \cdots \quad ,$$

whereby the $\pm$ sign indicates that $\exp(ika) = \pm 1$.

For each energy eigenvalue E within a **stable band** there exist two linear independent Floquet solutions. For each energy eigenvalue E within an **unstable band** there exist two linear independent Floquet of the type I such

that $Re(\kappa) = k = 0$ or $k = \pm\pi/a$. Within a band the function $E(\kappa)$ has the following important properties:

1.	$E(\kappa)$	is contineous
2.	$E(\kappa) = E(-\kappa)$	
3.	$dE(k)/dk = 0$	at a band edge

Bloch theorem

Let us return now to the Schrödinger equation and apply **cyclic boundary conditions for the wavefunctions**

$$x = x + Na \qquad ,$$

$$\underline{v}(x) = \underline{I} \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix} = \begin{pmatrix} \psi_1(x+Na) \\ \psi_2(x+Na) \end{pmatrix} = \underline{T}^N \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix} \qquad ,$$

where $\underline{I}$ again denotes a two-by-two unit matrix and $\underline{T}^N$ means that the translation matrix $\underline{T}$ is N times applied. Quite clearly the last equation can only be the case if and only if

$$\underline{T}^N = \underline{I} \qquad .$$

If one compares now this condition with the canonical forms of the matrix $\underline{T}$ discussed previously, one obtains the following relations:

Canonical type I

$$\underline{T}^N = \begin{pmatrix} \exp(i\kappa a) & \\ & \exp(-i\kappa a) \end{pmatrix}^N = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad ,$$

compatible with cyclic boundary conditions if and only if

$$\boxed{\mathrm{Im}(\kappa)=0 \quad , \quad \mathrm{Re}(\kappa)=2\pi \mathrm{m}/\mathrm{Na}}$$

m integer number

Canonical type II

$$\underline{T}^N = \begin{pmatrix} \pm 1 & 0 \\ 1 & \pm 1 \end{pmatrix}^N \neq \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad ,$$

not compatible with cyclic boundary conditions!

Canonical type III

$$\underline{T}^N = \pm \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}^N = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad ,$$

compatible with cyclic boundary conditions if and only if

$$N \text{ even } (+) \text{ or } N \text{ odd } (-) \qquad .$$

The last equations imply that all canonical solutions of the Schrödinger equation **compatible with cyclic boundary** conditions are **stable Floquet solutions.**

Bloch condition

The famous **Bloch theorem** can therefore now be stated as follows: **a general, not trivial solution of** the Schrödinger equation **satisfying cyclic boundary conditions is a combination of two stable Floquet solutions.**

Surface tates, thin film states

For a physical system with "perfect periodicity" for the potential function $V(x)$,

$$V(x) = V(x+a) \quad , \quad -\infty < x < \infty \qquad ,$$

only stable Floquet solutions (**Bloch functions**) refer to acceptable wave-functions.

If, however, the periodicity of $V(x)$ is only **semi-infinite**

$$V(x) = V(x+a) \quad , \quad -\infty < x < 0 \qquad ,$$

and for $x > 0$ the potential $V(x)$ decays rapidly enough to zero, then the case can arise that a **canonical type I** solution corresponding to a particular energy E in an unstable band can be matched contineously to a solution of the Schrödinger equation for $x > 0$ such that the total wavefunction is normalizable in the interval $-\infty < x < \infty$.

If this is indeed the case, then this energy E refers to a "**surface state**" and its wavefunction is well-behaved in the interval $-\infty < x < \infty$.

Canonical type II solutions diverge for $x \to \infty$ as well as $x \to -\infty$. For a semi-inifinte system this kind of solutions is always unphysical. Suppose, however, that $V(x)$ is periodic only in a finite interval

$$V(x) = V(x + a) \quad , \quad 0 < x < L \qquad ,$$

where L is sufficiently small like in a thin film, and $V(x)$ decays rapidly enough for

$$-\infty < x < 0 \quad and \quad L < x < \infty$$

Under certain conditions **canonical type II** solutions of the Schrödinger equation in the interval $0 < x < L$ can be matched to solutions of this equation in the intervals $-\infty < x < 0$ and $L < x < \infty$ such the resulting total wavefunction is normalizable in the interval $-\infty < x < \infty$.

If this is the case the corresponding energy E would then refer to a **"<u>thin-film</u>"-state**, namely to a **"surface"-state caused by the presence of two surfaces!** For an illustration of a typical "thin-film"-state see

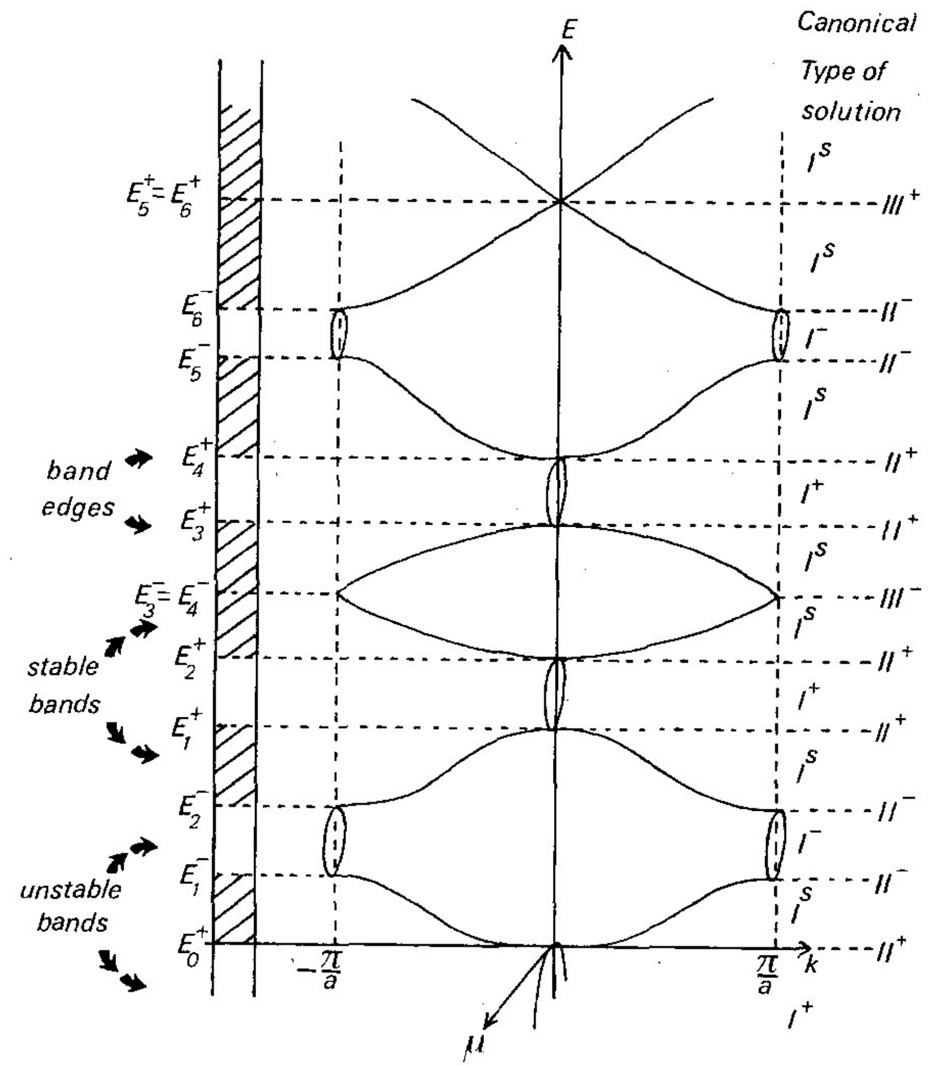

FIG. 2. The band structure in one dimension: E as a function of $\kappa(=k+i\mu)$; μ can be $\neq 0$ only when $k=0$ or $\pm\pi/a$. The superscript s is for "stable," and the superscripts $\pm$ are used when $\exp(ika)=\pm 1$.