curves were calculated by assuming the same values of activation energy, temperature, frequency factor and β-parameter.

The concentration of trapped charges and, therefore, the associated PIP electric field are approximately constant for time intervals which are greatly reduced with the decrease in initial filling, in agreement with the experimental data in fig. 3.

4. – Conclusions.

The decay of the PIP electric fields associated with the charges trapped in discrete levels at the surfaces of anthracene crystals has been studied.

The experimental data show that the PIP electric fields are constant during definite time intervals. The intervals depend on the temperature and on the initial concentration of charges trapped.

A model for the emptying kinetics of a single superficial trapping level has been developed: the computed decay curves show a dependence on the temperature and on the initial filling which is in agreement with the experimental data.

● RIASSUNTO

La cinetica di svuotamento dei livelli superficiali di intrappolamento in cristalli di antracene è stata studiata per mezzo di segnali di fotocorrente pulsata. È stata messa in evidenza una forte dipendenza dalla temperatura e dalle condizioni iniziali di riempimento dei livelli. È stato sviluppato un modello cinetico in buon accordo con i risultati sperimentali.

Резюме не получено.

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Rotation Symmetry in the Hamiltonian Dynamics.

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Summary. — The motion of a mass point in a central potential is considered. It is usually assumed that the projection of the angular momentum on the radius vector is equal to zero. It is shown that, if this assumption is relaxed, the angular part of the Hamiltonian becomes identical to the angular part of the monopole Hamiltonian given by Dirac.

1. – Introduction.

Let us consider the classical motion of a mass point in a central potential $U(r)$. In spherical co-ordinates the Hamiltonian can be written as

$$\mathscr{H} = \frac{I^2}{2mr^2} + \frac{P_r^2}{2m} + U(r)\,, \tag{1}$$

where $\boldsymbol{I} = \boldsymbol{L} = [\boldsymbol{r} \times \boldsymbol{p}]$ is the orbital angular momentum. Expression (1) might at first seem to be the most general Hamiltonian quadratic in momentum which possesses spherical symmetry. This is not, however, the case. There are nontrivial generalizations of $\mathscr{H}$ which describe motion under spherically symmetric conditions though they are far from being invariant under rotations. We discuss in some detail an important modification of $\mathscr{H}$ which is of this type.

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Let us denote the Poisson bracket of u and v by (u, v) and the components of $\boldsymbol{r}$ by x_i. Since

$$(I_i, x_j) = \varepsilon_{ijk} x_k , \tag{2}$$

$$(I_i, I_j) = \varepsilon_{ijk} I_k , \tag{3}$$

the components of $\boldsymbol{I}$ can be considered as infinitesimal generators of rotations. From (3) it follows that $(I_i, I^2) = (I_i, \mathscr{H}) = 0$; therefore, the Hamiltonian (1) is rotationally invariant, *i.e.* it describes motion under isotropic conditions.

The Hamiltonian (1) is consistent with the constraint $r = \text{const}$. The first term of $\mathscr{H}$ is equal to the kinetic energy of motion on a sphere and I^2 can be considered as the Hamiltonian H of a spherical pendulum with the moment of inertia equal to $\frac{1}{2}$:

$$H = I^2 .$$

Our choice of $\boldsymbol{L}$ for $\boldsymbol{I}$ leads to the constraint

$$\boldsymbol{In} = 0 , \tag{4}$$

where $\boldsymbol{n} = (1/r)\boldsymbol{r}$ and it is this relation which can be generalized. Let us assume that relations (1)-(3) hold, but (4) is not valid. We show in sect. **3** that $\boldsymbol{In}$ may be at most a constant which will be denoted by $\frac{1}{2}\sigma$. Thus, instead of (4), we require

$$\boldsymbol{In} = \tfrac{1}{2}\sigma . \tag{5}$$

As a consequence of (2) and (3), $\mathscr{H}$ continues to describe motion under spherically symmetric conditions and it remains consistent with the constraint $r = \text{const}$. When the latter is imposed, $\mathscr{H}$ is equal to the kinetic energy up to a constant term $\sigma^2/8r^2$ which can be absorbed into $U(r)$. Indeed,

$$\dot{\boldsymbol{r}} = \left(r, \frac{I^2}{2mr^2}\right) = \frac{1}{mr^2}[\boldsymbol{I}\times\boldsymbol{r}] ,$$

and, using (5), we have

$$\frac{I^2}{2mr^2} = \frac{1}{2mr^4}\left(I^2r^2 - (\boldsymbol{Ir})^2\right) + \frac{\sigma^2}{8r^2} = \frac{1}{2}m\left(\frac{1}{mr^2}[\boldsymbol{I}\times\boldsymbol{r}]\right)^2 + \frac{\sigma^2}{8r^2} = \frac{1}{2}m\dot{\boldsymbol{r}}^2 + \frac{\sigma^2}{8r^2} .$$

This relation shows that $H = I^2$ can be considered as the Hamiltonian of a kind of spherical pendulum (with the moment of inertia equal to $\frac{1}{2}$) even when $\sigma \neq 0$. The question arises: what will be the expression for $\boldsymbol{I}$ which

replaces the relation $\boldsymbol{I} = [\boldsymbol{r}\times\boldsymbol{p}]$ when $\sigma \neq 0$? In order to answer this question one has to solve (1)-(3) and (5) for $\boldsymbol{I}$ in terms of the canonical variables $\boldsymbol{r}$ and $\boldsymbol{p}$. The solution is expected to be essentially unique since energy and angular-momentum conservation completely determine the motion and the defining relations (1)-(3), (5) do not contradict these conservation laws.

The expression for $\boldsymbol{I}$ will be derived in sect. **3**. The Hamiltonian $H = I^2$ will turn out to be identical to the angular part of the Hamiltonian for the motion of an electrically charged particle in the field of a massive magnetic monopole which was first obtained by DIRAC [1].

DIRAC derived his H starting from electrodynamics, *i.e.* within the context of a definite dynamics. We will obtain the same H from (1)-(3) and (5) without any special dynamical assumption. This means that the monopole Hamiltonian has to be applied whenever a constant nonzero angular momentum acts along the radius vector and the particle, moving in the potential $U(r)$, has no degrees of freedom other than the position.

The Hamiltonian H is not manifestly invariant under rotations. In the derivation given by DIRAC this fact appears as a consequence of the nonexistence of a vector potential defined everywhere when a magnetic charge is present. In our treatment notions like magnetic charge and vector potential do not arise and the necessity for the violation of manifest rotation invariance emerges in a rather different way.

2. – Note on dynamical gauge transformations.

It is well known that relations of the type $p = \partial L/\partial\dot{q}$ or $\dot{q} = \partial H/\partial p$ connecting velocities and momenta cannot be tested experimentally since there is no way to measure momenta independently of the velocities. These relations, therefore, serve to define momenta through velocities. When a total derivative is added to L, the dynamical content of the theory remains the same but the expression of p as a function of $\dot{q}$ usually changes its form. There is no unique way to assign definite momenta to a given state (*i.e.* given positions and velocities) since they depend on the Lagrangian which is defined only up to a total derivative.

In the canonical description the generator function

$$\Phi = \sum_r q_r p'_r + \omega(q_1, \ldots, q_n, t)$$

(1) P. A. M. DIRAC: *Proc. Roy. Soc.*, **133** A, 60 (1931).

leads to the canonical transformation

$$q_r \to q'_r = q_r\,,$$
$$p_r \to p'_r = p_r - \frac{\partial \omega}{\partial q_r}\,,$$
$$H(q,p) \to H'(p,q) = H\left(p - \frac{\partial \omega}{\partial q}, q\right) + \frac{\partial \omega}{\partial t}\,.$$

The Hamiltonians H' and H describe the same dynamics in the following sense: if initial data are given in terms of positions and velocities, then the positions and the velocities will be the same at any moment if either H or H' is used to calculate trajectories. The momenta will be different for the two cases, but they are not measurable quantities.

Canonical transformations of this kind, leaving the dynamics unchanged, will be called *dynamical gauge transformations*. Their existence makes it possible to include the interaction of charged particles with the electromagnetic field in the canonical framework. If—for example—H contains the vector potential $\boldsymbol{A}$ and the momenta only in the combination $\boldsymbol{p} - (e/c)\boldsymbol{A}$, then an electrodynamical gauge transformation $\boldsymbol{A} \to \boldsymbol{A}' = \boldsymbol{A} + \nabla\chi$ can also be viewed as a dynamical gauge transformation with $\omega = (e/c)\chi$. Since the latter does not lead to any observable dynamical effect, the unobservability of the electrodynamical gauge transformations through the particle motion is ensured. We emphasize, however, that dynamical gauge transformations represent a purely dynamical concept. In defining them there is no need to make any reference to electrodynamics.

In quantum mechanics the problem of measurability of different physical quantities is much more complicated than in classical mechanics. Nevertheless, if we assume, relying on experience, that the vector potential is not measurable and the interaction between matter and electromagnetic field is of the usual gauge-invariant form, then canonical momentum is not a measurable quantity in quantum mechanics either. This is equivalent to the assumption that wave functions which differ from each other in a *local* phase factor alone cannot be distinguished by any measurement.

In quantum mechanics there is a special restriction on ω. Namely $\exp[(i/\hbar)\omega]$ must be single valued. If this is the case, the eigenfunctions of any two operators $O(q,p)$ and $O(q,p')$, where $p'_r = p_r - \partial\omega/\partial q_r$, differ from each other only in this local phase factor which is not measurable. Let us assume now that $\exp[(i/\hbar)\omega]$ is not single valued. If ψ is some eigenfunction of $O(q,p)$, then $\exp[(i/\hbar)\omega]\psi$ is not single valued and cannot be considered as an eigenfunction of $O(q,p')$ since—according to basic postulates of quantum mechanics —only single-valued functions are acceptable as solutions of eigenvalue equations. In this case the true eigenfunction of $O(q,p')$ will differ from ψ more significantly than just in a phase factor and this can lead to observable physical effects.

An immediate consequence is that in quantum theory two vector potentials which differ from each other in a gauge function χ may be distinquished if $\exp[(ie/\hbar c)\chi]$ is multivalued. A famous example is the Aharonov-Bohm effect.

Our subsequent considerations are strongly based on dynamical gauge transformations. We hope that this short summary will help to avoid misunderstandings.

3. – The classical case.

We look for $\boldsymbol{I}$ in the form

$$I = \boldsymbol{L} + \boldsymbol{S} = [\boldsymbol{r}\times\boldsymbol{p}] + \boldsymbol{S}\,. \tag{6}$$

According to (2) $\boldsymbol{S}$ must not depend on $\boldsymbol{p}$, it may be a function of $\boldsymbol{r}$ alone and thus $(S_i, S_j) = 0$.

Let us denote the scalar product of $\boldsymbol{I}$ and $\boldsymbol{r}$ by f: $\boldsymbol{Ir} = \boldsymbol{Sr} = f$. It follows from (3) that f may depend only on r. From $(\mathscr{H}, \boldsymbol{I}) = 0$, we have $(p_r^2, \boldsymbol{I}) = (p_r^2, \boldsymbol{S}) = 0$, which holds if $(\boldsymbol{rp}, \boldsymbol{S}) = 0$. Multiplying this by $\boldsymbol{r}$, we get $(\boldsymbol{rp}, \boldsymbol{Sr}) - (\boldsymbol{rp}, \boldsymbol{r})\boldsymbol{S} = 0$, which can be written as $(f, \boldsymbol{rp}) = f$ or $r(\mathrm{d}f/\mathrm{d}r) = f$. The function $f(r)$ is, therefore, proportional to r and (5) is the only possible generalization of (4).

From (5) we have

$$\boldsymbol{Sn} = \tfrac{1}{2}\sigma\,, \tag{7}$$

while (3) leads to the relation

$$(L_i, S_j) + (S_i, L_j) = \varepsilon_{ijk} S_k\,. \tag{8}$$

Let us assume that $\boldsymbol{S}$ is a *dynamical vector* under which we mean that it transforms as a vector when the co-ordinate system is rotated and, in addition, it obeys the relation

$$(I_i, S_j) = \varepsilon_{ijk} S_k\,, \tag{9}$$

which is the analogue of (2).

In this case (8) reduces to $(S_i, L_j) = 0$ and for an arbitrary unit vector $\boldsymbol{\varkappa}$ we have $(\boldsymbol{\varkappa S}, \boldsymbol{L}) = 0$. Hence $\boldsymbol{\varkappa S} = c(r)$ and, since $\boldsymbol{\varkappa}$ is arbitrary, we obtain $c = 0$, $\boldsymbol{S} = 0$ and $\sigma = 0$.

We have, therefore, to assume that though $\boldsymbol{S}$ is a *geometrical vector* (*i.e.* it transforms as a vector when the co-ordinate system is rotated) it is *not* a dynamical vector since it must not obey (9).

Let us write the condition (9) in the form

$$(\boldsymbol{L\varkappa}, \boldsymbol{S}) = [\boldsymbol{S}\times\boldsymbol{\varkappa}]\,, \tag{10}$$

where $\boldsymbol{\varkappa}$ is an arbitrary unit vector. As indicated above, $\boldsymbol{S}$ must not satisfy (10) for all possible $\boldsymbol{\varkappa}$, but there may exist linear subspaces of $\boldsymbol{\varkappa}$'s for which (10) is fulfilled. Such a subspace may be a plane, a line or it may happen that there are no $\boldsymbol{\varkappa}$ satisfying (10) at all. Now these three cases will be treated separately.

a) Let us assume that (10) is satisfied for $\boldsymbol{\varkappa}$'s which are orthogonal to some unit vector $\boldsymbol{e}$. For these $\boldsymbol{\varkappa}$'s we have from (8) $(\boldsymbol{\varkappa S}, \boldsymbol{L}) = 0$ and this leads to $\boldsymbol{\varkappa S} = c(r)$. The direction of the $\boldsymbol{\varkappa}$'s is arbitrary in the plane orthogonalto $\boldsymbol{e}$. Hence, the function $c(r)$ must vanish and we obtain that $\boldsymbol{S}$ is parallel to $\boldsymbol{e}$. From (7) we get

$$\boldsymbol{S} = \frac{\sigma}{2(\boldsymbol{en})}\boldsymbol{e}\,.$$

This expression contradicts (8) and, therefore, (10) cannot be satisfied by vectors $\boldsymbol{\varkappa}$ lying in a plane.

b) We assume that (10) is fulfilled only if $\boldsymbol{\varkappa}$ is equal to some given unit vector $\boldsymbol{e}$:

$$(\boldsymbol{Le}, \boldsymbol{S}) = [\boldsymbol{S}\times\boldsymbol{e}]\,. \tag{11}$$

This will be the case if $\boldsymbol{S}$ is a geometrical vector depending on $\boldsymbol{r}$ and $\boldsymbol{e}$. The latter is a numerical vector which has zero Poisson bracket with both $\boldsymbol{r}$ and $\boldsymbol{p}$. But then one has to ensure that the dynamics will be independent of the direction of $\boldsymbol{e}$ since the latter cannot be identified with any physical degree of freedom. This will indeed be true if any change of $\boldsymbol{e}$ turns out to be equivalent to a dynamical gauge transformation the condition for which can be formulated as follows.

Let $\boldsymbol{S}$ correspond to $\boldsymbol{e}$ and $\boldsymbol{S}'$ correspond to some $\boldsymbol{e}'$ different from $\boldsymbol{e}$. The change $\boldsymbol{e} \to \boldsymbol{e}'$ is equivalent to a dynamical gauge transformation if

$$[\boldsymbol{r}\times\boldsymbol{p}] + \boldsymbol{S}' = [\boldsymbol{r}\times(\boldsymbol{p} - \nabla\omega)] + \boldsymbol{S}$$

or

$$\boldsymbol{S}' - \boldsymbol{S} = [\nabla\omega\times\boldsymbol{r}] \tag{12}$$

with some function $\omega = \omega(\boldsymbol{e}, \boldsymbol{e}', \boldsymbol{r})$.

We show that, if $\boldsymbol{S}$ is a geometrical vector, satisfying (8), then (12) is automatically fulfilled.

To see this let us consider first an infinitesimal rotation of the co-ordinate system around the unit vector $\boldsymbol{k}$ by an angle $\delta\alpha$. Since $\boldsymbol{S}$, $\boldsymbol{r}$ and $\boldsymbol{e}$ are geometrical vectors, they change by an amount

$$\begin{cases} \delta\boldsymbol{S} = [\boldsymbol{k}\,\delta\alpha\times\boldsymbol{S}]\,, \\ \delta\boldsymbol{r} = [\boldsymbol{k}\,\delta\alpha\times\boldsymbol{r}]\,, \\ \delta\boldsymbol{e} = [\boldsymbol{k}\,\delta\alpha\times\boldsymbol{e}]\,. \end{cases} \tag{13}$$

This same change of $\boldsymbol{S}$ can also be expressed as

$$\delta S_i = \sum_j \frac{\partial S_i}{\partial e_j}\,\delta e_j + \sum_j \frac{\partial S_i}{\partial x_j}\,\delta x_j = \sum_j \frac{\partial S_i}{\partial e_j}\,\delta e_j + \sum_j \frac{\partial S_i}{\partial x_j}\,(x_j, \boldsymbol{kL}\,\delta\alpha)\,, \tag{14}$$

where the relation $\delta\boldsymbol{r} = (\boldsymbol{r}, \boldsymbol{kL}\,\delta\alpha)$, following from (2) and (13), was used. Since

$$\sum_j \frac{\partial S_i}{\partial x_j}\,(x_j, \boldsymbol{kL}\,\delta\alpha) = (S_i, \boldsymbol{kL}\,\delta\alpha)\,,$$

(14) can also be written as

$$\delta S_i = \sum_j \frac{\partial S_i}{\partial e_j}\,\delta e_j + (S_i, \boldsymbol{kL}\,\delta\alpha)\,,$$

or, by using (13),

$$\sum_j \frac{\partial S_i}{\partial e_j}\,\delta e_j + (S_i, \boldsymbol{kL}\,\delta\alpha) = [\boldsymbol{k}\,\delta\alpha\times\boldsymbol{S}]_i\,. \tag{15}$$

Let us multiply (8) by $k_j\,\delta\alpha$ and sum over j. We get

$$(L_i, \boldsymbol{kS}\,\delta\alpha) + (S_i, \boldsymbol{kL}\,\delta\alpha) = [\boldsymbol{k}\,\delta\alpha\times\boldsymbol{S}]_i\,. \tag{16}$$

Subtracting (16) from (15), we arrive at the expression

$$(\boldsymbol{L}_i, \boldsymbol{kS}\,\delta\alpha) = \sum_j \frac{\partial S_i}{\partial e_j}\,\delta e_j\,. \tag{17}$$

Since $\boldsymbol{S}$ does not depend on $\boldsymbol{p}$, we can write

$$(\boldsymbol{L}_i, \boldsymbol{kS}) = \sum_j (L_i, S_j)k_j = \sum_{j,k} k_i \frac{\partial S_j}{\partial x_k}(L_i, x_k) = \sum_{j,k,l} k_j \frac{\partial S_j}{\partial x_k}\varepsilon_{ikl}x_l = [\nabla(\boldsymbol{kS})\times\boldsymbol{r}]_i\,.$$

Putting this into (17), we have

$$\sum_j \frac{\partial S_i}{\partial e_j}\,\delta e_j = [\nabla(\boldsymbol{kS}\,\delta\alpha)\times\boldsymbol{r}]_i\,, \tag{18}$$

where $\delta\boldsymbol{e}$ is given by (13). This relation is valid for arbitrary unit vector $\boldsymbol{k}$ and parameter $\delta\alpha$.

Let us turn to the transformation $\boldsymbol{e} \to \boldsymbol{e}'$. We will consider infinitesimal transformations, therefore $\boldsymbol{e}' = \boldsymbol{e} + \Delta\boldsymbol{e}$. Then the condition for this to be a dynamical gauge transformation can be written as (see (12))

$$\sum_j \frac{\partial S_i}{\partial e_j} \Delta e_j = [\nabla\omega \times \boldsymbol{r}]_i \,. \tag{19}$$

Now the most general infinitesimal transformation $\boldsymbol{e} \to \boldsymbol{e}'$ is a rotation about some axis $\boldsymbol{k}$ by an amount $\delta\alpha$. Therefore, $\Delta\boldsymbol{e} = \delta\boldsymbol{e}$ and a comparison with (18) shows that (19) is fulfilled with

$$\delta\omega = \boldsymbol{k}\boldsymbol{S}\,\delta\alpha \,.$$

The explicit form of $\boldsymbol{S}$ can be obtained in the following way. Multiplying (8) by e_i, summing over i and using (11), we see that $(\boldsymbol{e}\boldsymbol{S}, L_i) = 0$. Hence,

$$\boldsymbol{e}\boldsymbol{S} = c(r) \,, \tag{20}$$

where c is an arbitrary function of r.

Let us now take the scalar product of (8) with x_i. Since $\boldsymbol{r}\boldsymbol{L} = 0$, the first term does not contribute and we get

$$(\boldsymbol{r}\boldsymbol{S}, L_j) - S_i(x_i, L_j) = [\boldsymbol{S} \times \boldsymbol{r}]_j \,.$$

This equation is fulfilled as a consequence of (7) and (2).

Now we can see that (8) is always satisfied if (7) and (20) do so. Indeed, we take an arbitrary vector $\boldsymbol{a}$, multiply (8) by a_i and sum over i. The vector $\boldsymbol{a}$ can be written as a linear combination of $\boldsymbol{e}$, $\boldsymbol{r}$ and $[\boldsymbol{e}\times\boldsymbol{r}]$. As we have just seen, the terms proportional to $\boldsymbol{e}$ and $\boldsymbol{r}$ do not contribute and we obtain

$$[\boldsymbol{e}\times\boldsymbol{r}]_i \{(L_i, S_j) + (S_i, L_j) - \varepsilon_{ijk} S_k\} = 0 \,.$$

Now we can take another vector $\boldsymbol{b}$, multiply this expression by b_j and sum over j. The vector $\boldsymbol{b}$ can also be expressed as a combination of $\boldsymbol{e}$, $\boldsymbol{r}$ and $[\boldsymbol{e}\times\boldsymbol{r}]$. Again terms containing $\boldsymbol{e}$ and $\boldsymbol{r}$ vanish and we get

$$[\boldsymbol{e}\times\boldsymbol{r}]_i [\boldsymbol{e}\times\boldsymbol{r}]_j \{(L_i, S_j) + (S_i, L_j) - \varepsilon_{ijk} S_k\} = 0 \,.$$

But this condition is satisfied due to the antisymmetry of the expression in the curly bracket.

Since $\boldsymbol{a}$ and $\boldsymbol{b}$ were arbitrary vectors, this consideration shows that eq. (8) is indeed satisfied as a consequence of (7) and (20).

We look for $\boldsymbol{S}$ in the form

$$\boldsymbol{S} = \alpha\boldsymbol{r} + \beta\boldsymbol{e} + a[\boldsymbol{e}\times\boldsymbol{r}] \tag{21}$$

and put this expression into (7) and (20). We get

$$\alpha(\boldsymbol{e}\boldsymbol{r}) + \beta = c(r) \,, \qquad \alpha r^2 + \beta(\boldsymbol{e}\boldsymbol{r}) = (\sigma/2)\, r \,,$$

from which we obtain

$$\alpha = \frac{(\sigma/2)r - (\boldsymbol{e}\boldsymbol{r})c}{r^2 - (\boldsymbol{e}\boldsymbol{r})^2} \,, \qquad \beta = \frac{cr^2 - (\sigma/2)r(\boldsymbol{e}\boldsymbol{r})}{r^2 - (\boldsymbol{e}\boldsymbol{r})^2} \,.$$

We substitute this into (21) and write $\boldsymbol{S}$ in the form

$$\boldsymbol{S} = \frac{\sigma}{2r}\boldsymbol{r} + a\boldsymbol{V} - \frac{\sigma}{2}\left\{\frac{1}{r}\frac{1}{r - (\boldsymbol{e}\boldsymbol{r})} + \frac{b(r)}{r^2 - (\boldsymbol{e}\boldsymbol{r})^2}\right\}\boldsymbol{W} \,, \tag{22}$$

where

$$\boldsymbol{V} = [\boldsymbol{e}\times\boldsymbol{r}] \,, \qquad \boldsymbol{W} = [\boldsymbol{r}\times\boldsymbol{V}] \,, \qquad c(r) = -\frac{\sigma}{2}(1 + b(r)) \,, \tag{23}$$

and a is an arbitrary function of r and $(\boldsymbol{e}\boldsymbol{r})$. Notice that, though relations (2), (3), (5), defining $\boldsymbol{S}$, contain partial derivatives of $\boldsymbol{S}$, we have obtained (2) without actually solving differential equations.

Now we will show that different choices for a and b—where a is a function of r and $(\boldsymbol{e}\boldsymbol{r})$ and b is a function of r—correspond to dynamical gauge transformations.

Let us use the notation $\boldsymbol{S}'$ when some a' and b' are chosen instead of a and b. Then

$$\boldsymbol{S}' - \boldsymbol{S} = A\boldsymbol{V} - \frac{B}{r^2 - (\boldsymbol{e}\boldsymbol{r})^2}\boldsymbol{W} \,, \tag{24}$$

where

$$A = a' - a \,, \qquad B = \frac{\sigma}{2}(b' - b), \tag{25}$$

A is a function of r and $(\boldsymbol{e}\boldsymbol{r})$, B is a function of r.

By means of (23) and (24), eq. (12) can be written as

$$\left[\left(A\boldsymbol{e} + \frac{B}{r^2 - (\boldsymbol{e}\boldsymbol{r})^2}\boldsymbol{V}\right)\times\boldsymbol{r}\right] = [\nabla\omega\times\boldsymbol{r}] \,. \tag{26}$$

The transformation $a,\ b \to a',\ b'$ is equivalent to a dynamical gauge transfor-

mation if (26) is satisfied with some suitably chosen ω.

From (26) we have

$$\nabla\omega = A\boldsymbol{e} + \frac{B}{r^2-(\boldsymbol{e}\boldsymbol{r})^2}\boldsymbol{V} + C\boldsymbol{r}\,, \tag{27}$$

where C is an arbitrary scalar function of $\boldsymbol{r}$.

Without losing generality, we can choose $\boldsymbol{e}=(0,0,1)$. Then $A=A(r,\cos\theta)$, $B=B(r)$, $C=C(r,\cos\theta,\varphi)$. In polar co-ordinates,

$$V_r = V_\theta = 0\,, \quad V_\varphi = r\sin\theta\,, \quad e_r = \cos\theta\,, \quad e_\theta = -\sin\theta\,, \quad e_\varphi = 0$$

and (27) can be written as

$$\frac{\partial\omega}{\partial r} = A\cos\theta + Cr\,, \tag{28}$$

$$\frac{\partial\omega}{\partial\theta} = -Ar\sin\theta\,, \tag{29}$$

$$\frac{\partial\omega}{\partial\varphi} = B\,. \tag{30}$$

We have three integrability conditions. The condition

$$\frac{\partial^2\omega}{\partial\varphi\,\partial\theta} = \frac{\partial^2\omega}{\partial\theta\,\partial\varphi}$$

is fulfilled automatically, while the other two lead to the equations

$$\frac{\mathrm{d}B}{\mathrm{d}r} = r\frac{\partial C}{\partial\varphi}\,, \tag{31}$$

$$\frac{\partial A}{\partial(\cos\theta)}\cos\theta + \frac{\partial C}{\partial(\cos\theta)}r = \frac{\partial A}{\partial r}r\,. \tag{32}$$

From (31) we have

$$C = \varphi\frac{1}{r}\frac{\mathrm{d}B}{\mathrm{d}r} + D(r,\cos\theta)\,, \tag{33}$$

where D is an arbitrary function. Substituting this into (32), we get

$$\frac{\partial D}{\partial(\cos\theta)} = \frac{\partial A}{\partial r} - \frac{1}{r}\frac{\partial A}{\partial(\cos\theta)}\cdot\cos\theta \equiv F(r,\cos\theta)\,.$$

From here

$$D = \int^{\cos\theta}\mathrm{d}\eta\cdot F(r,\eta) + E(r)$$

and C is defined up to an arbitrary E. With this C (27) can be integrated to yield ω which generates a dynamical gauge transformation equivalent to a, $b \to a', b'$.

The simplest choice for a and b is $a=b=0$. The function $\boldsymbol{S}$, corresponding to this choice, will be denoted by $\boldsymbol{S}^{\mathrm{D}}$ since $\boldsymbol{L}+\boldsymbol{S}^{\mathrm{D}}$ is equal to $\boldsymbol{I}^{\mathrm{D}}$, the angular momentum in Dirac's theory of the monopole. This can be proven by substituting the vector potential of the monopole

$$\boldsymbol{A} = \frac{g}{r}\frac{[\boldsymbol{r}\times\boldsymbol{e}]}{r-(\boldsymbol{e}\boldsymbol{r})}$$

into $[\boldsymbol{r}\times(\boldsymbol{p}-(e/c)\boldsymbol{A})]+(\sigma/2r)\boldsymbol{r}$ and taking into account the relation $\frac{1}{2}\sigma = (1/c)\,eg$.

We have, therefore, shown that in classical mechanics conditions (1)-(3), (5) lead to Dirac's form of the angular momentum independently of any model.

c) In the third case there is no unit vector $\boldsymbol{\varkappa}$ for which (10) is satisfied. We will not consider this case in any detail, but confine ourselves to some remarks.

It is easy to see that this case is not empty. Let $\boldsymbol{S}^0(\boldsymbol{e}_i)$ be functions which satisfy (10) for $\boldsymbol{\varkappa}=\boldsymbol{e}_i$, (7) for $\sigma=1$ and obey (8) as well. Then

$$\boldsymbol{S} = \sum_i \sigma_i \boldsymbol{S}^0(\boldsymbol{e}_i)$$

is a solution of (7) and (8) provided $\sum_i \sigma_i = \sigma$. It is obvious that, for this solution, (10) is not satisfied by any $\boldsymbol{\varkappa}$. An arbitrary change $\Delta\boldsymbol{e}_i = [\boldsymbol{k}_i\,\delta\alpha_i\times\boldsymbol{e}_i]$ in $\boldsymbol{e}_i$ is equivalent to a dynamical gauge transformation with $\omega = \sum_i \boldsymbol{k}_i\boldsymbol{S}(\boldsymbol{e}_i)\,\delta\alpha_i$.

The sum can be extended to an integral

$$\boldsymbol{S} = \int\boldsymbol{S}^0(\boldsymbol{e}(\eta))\,\mathrm{d}\sigma(\eta)\,,$$

where $\boldsymbol{e}(\eta)$ is—for $0\leqslant\eta\leqslant1$—a curve on the unit sphere. Looking at the expression for $\boldsymbol{S}^0$ (eq. (22) with $\sigma=1$), we see that $\boldsymbol{S}$ is singular on a surface containing the origin and the directions $\boldsymbol{e}(\eta)$. In particular, when $\boldsymbol{e}(\eta)$ is a closed curve, $\boldsymbol{S}$ is singular on a cone.

4. – The quantum case.

In quantum mechanics only those dynamical gauge transformations are allowed for which $\exp[(i/\hbar)\,\omega]$ is single valued and we have to clarify restrictions imposed by this requirement on σ and $\boldsymbol{I}$.

First we have to investigate the ω function which corresponds to a finite change $\boldsymbol{e} \to \boldsymbol{e}'$. Since, according to (22), $\boldsymbol{S}$ is singular on the line $r^2 = (\boldsymbol{er})^2$, there must exist a term in ω which through (12) corresponds to this singularity. We choose $\boldsymbol{e} = (0, 0, 1)$ and denote the singular part of $\boldsymbol{S}$ by $\boldsymbol{s}$:

$$s_x = \frac{\sigma}{2}\left(\frac{x}{r-z} + \frac{b(r)xz}{r^2-z^2}\right), \qquad s_y = \frac{\sigma}{2}\left(\frac{y}{r-z} + \frac{b(r)yz}{r^2-z^2}\right), \qquad s_z = 0\,.$$

In the neighbourhood of the $+z$–semi-axis,

$$s_x = \sigma\left(1 + \frac{1}{2}b(z)\right)\frac{z\cdot\cos\varphi}{\varrho}\,, \qquad s_y = \left(1 + \frac{1}{2}b(z)\right)\frac{z\cdot\sin\varphi}{\varrho}\,, \tag{34}$$

where ϱ, φ, z are cylindrical co-ordinates. The cylindrical components are

$$s_\varrho = \sigma\left(1 + \frac{1}{2}b(z)\right)\frac{z}{\varrho}\,, \qquad s_\varphi = s_z = 0\,. \tag{35}$$

The singular part of ω, corresponding to (35), is of the form

$$\omega = g(z)\,\varphi\,. \tag{36}$$

Then

$$\nabla\omega = \frac{1}{\varrho}\,g(z)\,\boldsymbol{e}_\varphi + g'(z)\varphi\boldsymbol{e}_z\,,$$

where $\boldsymbol{e}_\varrho, \boldsymbol{e}_\varphi, \boldsymbol{e}_z$ are the local unit vectors of the cylindrical–co-ordinate system. Since $[\boldsymbol{e}_\varphi \times \boldsymbol{e}_z] = \boldsymbol{e}_\varrho$ we have in the neighbourhood of the $+z$–semi-axis

$$[\nabla\omega \times \boldsymbol{r}] = \frac{1}{\varrho}\,zg(z)\,\boldsymbol{e}_\varrho\,. \tag{37}$$

Putting (35) and (37) into (12), we get

$$-\sigma\left(1 + \frac{1}{2}b(z)\right)\frac{z}{\varrho} = \frac{1}{\varrho}\,zg(z)\,, \qquad g(z) = -\sigma\left(1 + \frac{1}{2}b(z)\right)$$

and

$$\omega = -\sigma\left(1 + \tfrac{1}{2}b(z)\right)\cdot\varphi \qquad (z > 0)\,. \tag{38}$$

Similarly, on the negative z–semi-axis we have

$$s_\varrho = \frac{\sigma}{2}\,b(-z)\,\frac{z}{\varrho}\,, \qquad s_\varphi = s_z = 0\,.$$

Equation (37) remains true and we get

$$g(z) = -\frac{\sigma}{2}\,b(-z)\,, \qquad \omega = -\frac{\sigma}{2}\,b(-z)\varphi \qquad (z < 0)\,. \tag{39}$$

Let us fix $|z| = c$. In the neighbourhood of the point $z = c$ on the z-axis we have

$$\exp\left[\frac{i}{\hbar}\,\omega\right] \sim \exp\left[-\frac{i}{\hbar}\,\sigma\left(1 + \frac{1}{2}\,b(c)\right)\varphi\right]$$

($\sim$ means proportionality). This will be single valued only if

$$\frac{\sigma}{\hbar}\left(1 + \frac{1}{2}\,b(c)\right) = l = \text{integer}\,. \tag{40}$$

At the point $z = -c$,

$$\exp\left[\frac{i}{\hbar}\,\omega\right] \sim \exp\left[-\frac{i}{\hbar}\,\sigma\,\frac{1}{2}\,b(c)\,\varphi\right],$$

which is single valued if

$$\frac{\sigma}{\hbar}\cdot\frac{1}{2}\,b(c) = m = \text{integer}\,. \tag{41}$$

From (40) and (41) it follows that the necessary conditions for ω to describe a dynamical gauge transformation are

$$\frac{\sigma}{\hbar} = l - m = n = \text{integer} \tag{42}$$

and

$$b = 2\,\frac{m}{n} = \text{const}\,. \tag{43}$$

In writing down $\boldsymbol{s}$ we have assumed that the coefficient a in (22) is not singular on the z-axis.

Now we show that from the point of view of single valuedness around z the coefficient a does not play any role.

Cylindrical components of $\boldsymbol{V}$ are $V_\varphi = \varrho$, $V_\varrho = V_z = 0$. Hence the term $a\boldsymbol{V}$ in $\boldsymbol{S}$ changes only the φ-component of $\boldsymbol{s}$: $s_\varphi = (\sigma/2)\,a\varrho$ instead of being zero. According to (12) we have on the $+z$–semi-axis

$$-\frac{\sigma}{2}\,a\varrho = z[\nabla\omega \times \boldsymbol{e}_z]_\varphi\,, \tag{44}$$

which shows that $\nabla\omega$ must have a ϱ-component. We have to modify (36) to

$$\omega = g(z)\,\varphi + h(z,\varrho)\,. \tag{45}$$

The term h does not contribute to $[\nabla\omega\times\boldsymbol{e}_z]_\varrho$ and our previous considerations remain unaltered. But

$$[\nabla\omega\times\boldsymbol{e}_z]_\varphi = [(\nabla\omega)_\varrho\times\boldsymbol{e}_z]_\varphi = -\frac{\partial h}{\partial\varrho}$$

and (44) leads to $\frac{1}{2}\sigma a\varrho = z(\partial h/\partial\varrho)$, from which h can be determined. This shows that the additional term h in ω may indeed account for the term aV in $\boldsymbol{S}$. But h leads to a factor $\exp[(i/\hbar)\,h(z,\varrho)]$ in $\exp[(i/\hbar)\,\omega]$ which is single valued and does not lead to any new restriction connected with single valuedness.

Let us now investigate the transformations $a, b \to a', b'$, when the conditions (42), (43) necessary for the quantum description are fulfilled. The function ω is the solution of (28)-(30) with $B = \frac{1}{2}\sigma(b'-b)$. According to (42), (43) this can also be written as

$$B = \hbar(m'-m)\,, \tag{46}$$

where m and m' are connected with b and b' through $b = 2(m/n)$, $b' = 2(m'/n)$ (in the transformation $a, b \to a', b'$ σ and n remain unaltered).

The solution of (28)-(30) is of the form

$$\omega = B\varphi + q(r,\cos\theta)\,,$$

since $B = \text{const}$ and $C = D(r,\cos\theta)$. But then, owing to (46), $\exp[(i/\hbar)\,\omega]$ is single valued. This means that the necessary conditions (42), (43) are sufficient for the transformation $a, b \to a', b'$ to be a dynamical gauge transformation. We can, therefore, take $a = b = 0$ again and the Dirac expression $\boldsymbol{I}^{\mathrm{D}}$ is the unique solution of (1)-(3), (5) in the quantum case also.

The function ω, corresponding to a finite change $\boldsymbol{e} \to \boldsymbol{e}'$, has a simple geometrical meaning [2] when $a = b = 0$. In order to see this we integrate the relation $\delta\omega = \boldsymbol{k}\boldsymbol{S}\,\delta\alpha$:

$$\omega(\boldsymbol{r},\boldsymbol{e},\boldsymbol{e}') = \int_0^\alpha \boldsymbol{k}\boldsymbol{S}(\beta)\,\mathrm{d}\beta\,. \tag{47}$$

Here $\boldsymbol{S}(\beta) \equiv \boldsymbol{S}(\boldsymbol{e}(\beta),\boldsymbol{r})$, $\boldsymbol{e} = \boldsymbol{e}(0)$, $\boldsymbol{e}' = \boldsymbol{e}(\alpha)$ and $\boldsymbol{k}$ is a unit vector orthogonal to $\boldsymbol{e}(\beta)$. Using (22), we have for $a = b = 0$

[2] A. FRENKEL and P. HRASKÓ: *Ann. of Phys.*, **105**, 288 (1977).

$$\omega = \frac{\sigma}{2}\,\boldsymbol{r}\boldsymbol{k}\int_0^\alpha \frac{\mathrm{d}\beta}{r - \boldsymbol{e}(\beta)\boldsymbol{r}} = \frac{\sigma}{2}\,\boldsymbol{k}\left(\frac{\boldsymbol{r}}{r}\right)\int_0^\alpha \frac{\mathrm{d}\beta}{1-(\boldsymbol{r}/r)\,\boldsymbol{e}(\beta)}\,,$$

where $\sigma = \hbar n$. We notice that ω depends only on the direction of $\boldsymbol{r}$.

From this expression it can be deduced that ω satisfies the Laplace equation $\nabla^2\omega = 0$ since the integrand obeys this equation for any arbitrary $\boldsymbol{k}$ and $\boldsymbol{e}$.

From (38) we see that for $b = 0$ the change of ω under a complete revolution around the axis $\boldsymbol{e}$ is equal to $2\pi\sigma$. Evidently, the same is true for $\boldsymbol{e}'$ with the opposite sign (see (12)). Combining this with the equation $\nabla^2\omega = 0$, we conclude that ω is identical to the potential of a twofold layer in the $\boldsymbol{e}$, $\boldsymbol{e}'$ sector with a density equal to $\sigma/2$. But the latter is up to an arbitrary constant equal to $\sigma/2$ times the solid angle $\Omega(\boldsymbol{e},\boldsymbol{e}',\boldsymbol{r})$ of the sector $\boldsymbol{e}$, $\boldsymbol{e}'$ as seen from the point $\boldsymbol{r}$:

$$\omega(\boldsymbol{r},\boldsymbol{e},\boldsymbol{e}') = \frac{\sigma}{2}\,\Omega(\boldsymbol{e},\boldsymbol{e}',\boldsymbol{r}) + \text{const}\,. \tag{48}$$

This is the above-mentioned geometrical meaning of ω.

The components of $\boldsymbol{I}$ can be considered as generators of rotations. This possibility will be realized if one agrees to choose the arbitrary unit vector $\boldsymbol{e}$ always in the direction of the z–co-ordinate axis. Then the term $\boldsymbol{L}$ in $\boldsymbol{I}$ describes, as usual, the transformations $\psi(\boldsymbol{r}) \to \psi(R^{-1}\boldsymbol{r})$, while $\boldsymbol{S}$ generates a dynamical gauge transformation which rotates $\boldsymbol{e}$ from the old position of the z-axis into the new one. The complete transformation of the wave function is given, therefore, by the expression

$$\psi(\boldsymbol{r}) \to \exp\left[\frac{i}{\hbar}\,\omega_{\mathrm{R}}\right]\psi(R^{-1}\boldsymbol{r})\,. \tag{49}$$

The function ω_{R} is given by (48) if $\boldsymbol{e}$ and $\boldsymbol{e}'$ are identified with the direction of the z-axis before and after the rotation.

One might suppose that ω is equal to zero when R is a rotation around the z-axis ($\boldsymbol{e}' = \boldsymbol{e}$). However, the function $\boldsymbol{S}$ generates a nonzero exponent even in this case since, if we substitute $\boldsymbol{k} = \boldsymbol{e}$ into (47) and use (20) and (23) with $b = 0$, we get $\omega = -(\sigma/2)\,\alpha$. Now a general rotation R can be specified by the Eulerian angles φ, θ, ψ, the first and the third of which correspond to rotation around the z-axis. It is, therefore, convenient to choose the constant in (48) equal to $-(\sigma/2)(\varphi+\psi)$. With this choice (49) defines a representation of the rotation group the generators of which are given by the components of $\boldsymbol{I}$ [2].

One may now consider the function ω_{R} in (49) unspecified and try to determine it from the requirement that (49) be a representation of the rotation group. The generators of this representation are of the form $\boldsymbol{L} + \boldsymbol{S}$, where $\boldsymbol{S}$

does not depend on $\boldsymbol{p}$ and the problem is to find all possible functions $\boldsymbol{S}$. But it is just this problem we have solved above. Therefore, the expression $(1/\hbar)\,\omega_R = (n/2)(\Omega - \varphi - \psi)$ with an integer n is the unique function for which (49) defines a representation of the rotation group.

● KIVONAT

Tömegpont mozgását vizsgáljuk centrális potenciálban. Általában felteszik, hogy az impulzusmomentum vetülete a részecske helyzetvektorára zérus. Ha ezt nem tesszük fel, olyan Hamilton függvényre jutunk, amelynek szögrésze a monopólprobléma Dirac által adott Hamilton függvényének szögrészével egyezik meg.

● RIASSUNTO (*)

Si considera il moto di un punto di massa in un potenziale centrale. Si assume di solito che la proiezione dell'impulso angolare sul raggio vettore è uguale a zero. Si mostra che, se si abbandona questa ipotesi, la parte angolare dell'hamiltoniana diventa identica alla parte angolare dell'hamiltoniana di monopolo, data da Dirac.

(*) *Traduzione a cura della Redazione.*

Резюме не получено.

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Crystal Equilibrium and Lattice Dynamics of Vanadium (*).

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(ricevuto il 3 Gennaio 1978)

Summary. — A lattice-dynamical model which assumes short-range pairwise forces effective up to second nearest neighbours and the electron-ion interaction on the lines of Bhatia is considered to study the crystal dynamics of b.c.c. metals by using an appropriate value of the screening parameter. The volume force is averaged over the whole Wigner-Seitz sphere. The ionic lattice is in equilibrium in a medium of electrons. The present theory has been satisfactorily applied to compute the dispersion curves, the frequency spectrum, the lattice specific heat, the Debye characteristic temperature, the temperature dependence of the Debye-Waller factor, the X-ray Debye temperature and the mean-square displacement of the atoms of vanadium.

1. – Introduction.

Lattice vibrations play a dominant role in many solid-state phenomena. All those physical properties of a crystal which depend on the heat motion of the constituent particles require for their detailed explanation a knowledge of the actual form of the phonon spectrum. In recent years, several workers [1-14]

(*) To speed up publication, the authors of this paper have agreed to not receive the proofs for correction.

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