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Theory of the Okorokov effect

S. Shindo and Y. H. Ohtsuki
Department of Physics, Waseda University, Nishi-Ohkubo 4, Tokyo, Japan

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A kinematical and a dynamical theory of the Okorokov effect are developed by time-dependent perturbation theory. The peak profile of the coherent resonant excitation is calculated in detail for He$^+$ ions. We show that the peak profile changes very strongly for the various channeling conditions. In almost all cases the half-width of the peak is comparable with the difference of the higher harmonics position in the Okorokov condition.

I. INTRODUCTION

In recent years, there has been a growing interest in what is called the "Okorokov effect," that is a coherent resonant excitation of the electrons bound in the ion by the periodic Coulomb interaction with the crystal lattice. The ion moving with velocity v along the atomic row of lattice constant d is excited at the condition

$$\omega_{n0} = 2\pi v/d$$

where $\hbar\omega_{n0}$ is the excitation energy of the ion.

Experimentally, Okorokov's group[1] and Lyon's group[2] have reported that a few peaks appear in the radiation yield emitted from the excited He$^+$ ion. However, few other groups[3] have given negative conclusions. They could not detect any peaks near the Okorokov condition.

On the other hand, Okorokov *et al.*[1] have developed a theory of the coherent excitation by ordinary diffraction method. Kondo[4] has given an expression of the excitation probability by Bloch's theory of the band calculation.

However, at this moment, we have no exact expression for the peak profile of the coherent excitation. Especially, it will be pointed out that the coherent excitation probability depends strongly on the impact parameter, then the channeling condition could contribute very strongly to the peak profile.

Here, we give a kinematical and a dynamical theory of the Okorokov effect for ions in a channeling condition. We use the time-dependent perturbation theory with a two-state approximation.

II. KINEMATICAL THEORY

We expand the static (periodic) Coulomb potential $V(\vec{R})$ in Fourier series with the reciprocal-lattice vector $\vec{g}$,

$$V(\vec{R}) = \sum_l V_a(\vec{R} - \vec{R}_l) = \sum_{\vec{g}} V_{\vec{g}} \exp(-i2\pi\vec{g}\cdot\vec{R}), \tag{1}$$

where $V_a(\vec{R} - \vec{R}_l)$ means the Coulomb potential due to the atom at the position $\vec{R}_l$. The coordinate of the incident ion is assumed to be determined by the classical trajectory,

$$\vec{R}_0(t) = \vec{b} + \vec{v}t, \quad \vec{b}\perp\vec{v}, \quad \vec{R} = \vec{R}_0(t) + \vec{r}, \tag{2}$$

where $\vec{v}$ is the ion velocity and $|\vec{b} - \vec{R}_{l\perp}|$ means the impact parameter which is independent of t [see Fig. (1)].

The coordinate of an electron bound in the ion is given by $\vec{R} = \vec{R}_0(t) + \vec{r}$ which is inserted into (1), and we obtain

$$V(\vec{R}_0(t) + \vec{r}) = \sum_{\vec{g}_\perp,}\sum_{g_z} V_{\vec{g}_\perp, g_z} \exp(-i2\pi\vec{g}_\perp\cdot\vec{b}) \times \exp(-i2\pi g_z v t) \exp(-i2\pi\vec{g}\cdot\vec{r}), \tag{3}$$

where $\vec{g}_\perp$ and g_z are transversal and incident-beam direction components of $\vec{g}$, respectively, (see Fig. 1).

If we consider a periodic atom in the z direction with spacing d, g_z is represented as $g_z = m/d$ ($m = 0, 1, 2, \ldots$), and we may obtain from (3)

$$V = i\hbar \sum_m F^{(m)} \exp\left(-i\frac{2\pi m v}{d}\right), \tag{4}$$

where

$$F^{(m)} = \frac{1}{i\hbar} \sum_{\vec{g}_\perp} V_{\vec{g}_\perp, 2\pi m/d} \exp(-i2\pi\vec{g}_\perp\cdot\vec{b}) \times \exp(-i2\pi\vec{g}_\perp\cdot\vec{r}_\perp - i2\pi m z/d). \tag{5}$$

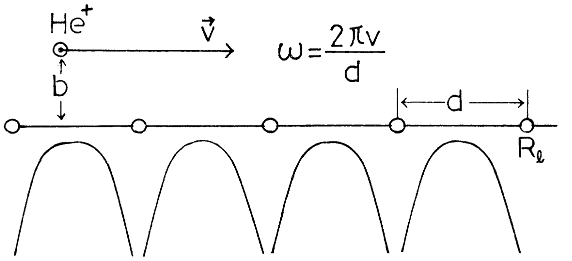

FIG. 1. Indication of passing through of He$^+$ ions along the periodic static potentials with lattice spacing d.

Now, we calculate the excitation transition probability $P(t)$ from the 0 state to the nth excited state with the energies E_0 and E_n, respectively;

$$P(t)=\left| -\frac{i}{\hbar}\int_0^t V_{n0}\exp\left(i\frac{E_n-E_0}{\hbar}t\right)dt\right|^2, \tag{6}$$

where V_{n0} is the matrix element of (4) for this excitation. Inserting (4) and (5) into (6), we obtain

$$P(t)=\left|\sum_m \frac{\exp[i(\omega_{n0}-2\pi m v/d)t]-1}{\omega_{n0}-2\pi m v/d}F_{n0}^{(m)}\right|^2$$
$$=\sum_m |F_{n0}^{(m)}|^2 t^2 \delta_{\omega_{n0},2\pi m v/d}, \tag{7}$$

where $\omega_{n0}=(E_n-E_0)/\hbar$, and $F_{n0}^{(m)}$ means the matrix element of (5).

From (7), we get the Okorokov condition,

$$\omega_{n0}=(2\pi m/d)v. \tag{8}$$

We note that $P(t)$ does not give any condition like

$$\omega_{n0}=(2\pi v/d)(1/m) \tag{9}$$

which is used, for example, by Okorokov *et al.*[1] and Lyon's group.[2]

When we consider the thermal vibration, $F_{n0}^{(m)}$ in (7) is replaced by

$$F_{n0}^{(m)}\to F_{n0}^{(m)}\,e^{-M}, \tag{10}$$

where the Debye-Waller coefficient M is given by

$$M=\tfrac{1}{6}(2\pi m/d)^2\langle u_z^2\rangle; \tag{11}$$

$\langle u_z^2\rangle$ being the thermal average of squared displacement in the z direction.

III. DYNAMICAL THEORY

We start from the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t}=(H_0+V)\psi, \tag{12}$$

where H_0 and V are the unperturbed and the interaction Hamiltonians, respectively. The explicit expression for V is given by (4).

The wave function ψ is expanded by

$$\psi(t)=\sum_k a_k(t)\psi_k\exp(iE_kt/\hbar),$$
$$H_0\psi_k=E_k\psi_k. \tag{13}$$

Inserting (13) into (12), we obtain

$$\frac{d}{dt}a_n=\sum_k\sum_m F_{nk}^{(m)}\exp(i\epsilon_{nk}^{(m)}t)a_k, \tag{14}$$

where

$$\epsilon_{nk}^{(m)}=(E_n-E_k)/\hbar-(2\pi v/d)m \tag{15}$$

First, we take a "two-state approximation," which means that we may consider only 0 and n states,

$$\frac{d}{dt}a_n=F_{n0}^{(m)}\exp(i\epsilon_{n0}^{(m)}t)a_0,$$
$$\frac{d}{dt}a_0=F_{n0}^{(m)*}\exp(-i\epsilon_{n0}^{(m)}t)a_n. \tag{16}$$

Solving (16), we can get excitation probability at the initial condition $a_0(0)=1, a_n(0)=0$.

$$P(t)=|a_n(t)|^2=\frac{1}{1+|\epsilon_{n0}^{(m)}|^2/4|F_{n0}^{(m)}|^2}$$
$$\times\sin^2[\tfrac{1}{2}(|\epsilon_{n0}^{(m)}|^2+4|F_{n0}^{(m)}|^2)^{1/2}t]. \tag{17}$$

In the case of very small t, (17) coincides with (7), the kinematical excitation probability. Further, (17) corresponds to the expression first given by Kondo[4] by the formal Bloch theory. However, we note that the matrix element $F_{n0}^{(m)}$ is different from that of Kondo, which we show in more detail.

IV. CALCULATION OF THE MATRIX ELEMENTS

We calculate the matrix elements in detail for the He$^+$ ion excitation from the 1s state to the 4p state, which corresponds to Okorokov's experiments. We take an assumption that electron orbit-range is smaller than the lattice constant, and

$$\exp(-i2\pi\vec{g}\cdot\vec{r})\cong 1-i2\pi\vec{g}\cdot\vec{r}. \tag{18}$$

Inserting (18) into (15), the matrix element becomes

$$F_{n0\parallel}^{(m)}=\frac{i}{\hbar}\frac{2\pi}{d}\left[\frac{1}{d}\int V(b,z)\exp\left(i\frac{2\pi m}{d}z\right)dz\right]$$
$$\times\int\psi_n z\psi_0\,d\vec{r}, \tag{19}$$

for the $s-p$ $(m=0)$ transition, and

$$F_{n0\perp}^{(m)}=\frac{i}{\hbar}\frac{\partial}{\partial\vec{b}}\left[\frac{1}{d}\int V(b,z)\exp\left(i\frac{2\pi m}{d}z\right)dz\right]$$
$$\times\int\psi_n\vec{r}_\perp\psi_0\,d\vec{r}, \tag{20}$$

for the $s-p$ $(m=\pm 1)$ transitions, where m is the magnetic quantum number. Thus we obtain

$$|F_{n0}^{(m)}|^2=|F_{n0\parallel}^{(m)}|^2+|F_{n0\perp}^{(m)}|^2. \tag{21}$$

For the Bohr potential, (21) is rewritten as

$$|F_{n0}^{(m)}|^2 = \sum_l \left(\frac{2\pi m}{d}\right)^2 \left(\frac{Ze^2}{d}\right)^2 4K_0^2 \left\{ b_l \left[\left(\frac{2\pi m}{d}\right)^2 + \left(\frac{1}{a_B}\right)^2\right]^{1/2} \right\} \langle z\rangle^2$$
$$+ \sum_l \left[\left(\frac{2\pi m}{d}\right)^2 + \left(\frac{1}{a_B}\right)^2\right] \left(\frac{Ze^2}{d}\right)^2 4K_1^2 \left\{ b_l \left[\left(\frac{2\pi m}{d}\right)^2 + \left(\frac{1}{a_B}\right)^2\right]^{1/2} \right\} (\langle x\rangle^2 + \langle y\rangle^2); \tag{22}$$

on the other hand, for the Moliere potential

$$|F_{n0}^{(m)}|^2 = \sum_l \left(\frac{2\pi m}{d}\right)^2 \left(\frac{Ze^2}{d}\right)^2 4 \left| \sum_i \alpha_i K_0 \left\{ b_l \left[\left(\frac{2\pi m}{d}\right)^2 + \left(\frac{\beta_i}{a}\right)^2\right]^{1/2} \right\} \right|^2 \langle z\rangle^2$$
$$+ \sum_l \left(\frac{Ze^2}{d}\right)^2 4 \left| \sum_i \left[\left(\frac{2\pi m}{d}\right)^2 + \left(\frac{\beta_i}{a}\right)^2\right]^{1/2} \alpha_i K_1 \left\{ b_l \left[\left(\frac{2\pi m}{d}\right)^2 + \left(\frac{\beta_i}{a}\right)^2\right]^{1/2} \right\} \right|^2 (\langle x\rangle^2 + \langle y\rangle^2). \tag{23}$$

In above, a_B and a are the Bohr's screening length and Thomas-Fermi radius, respectively, $\langle \cdots \rangle$ means the dipole moment, and $\langle z\rangle^2 = \langle x\rangle^2 + \langle y\rangle^2$. The coefficients α_i, β_i in (23) are the constants appearing in the Moliere potential. K_0 and K_1 are the modified Bessel function of the second kind, and $b_l = |\vec{b}_l - \vec{R}_{l\perp}|$.

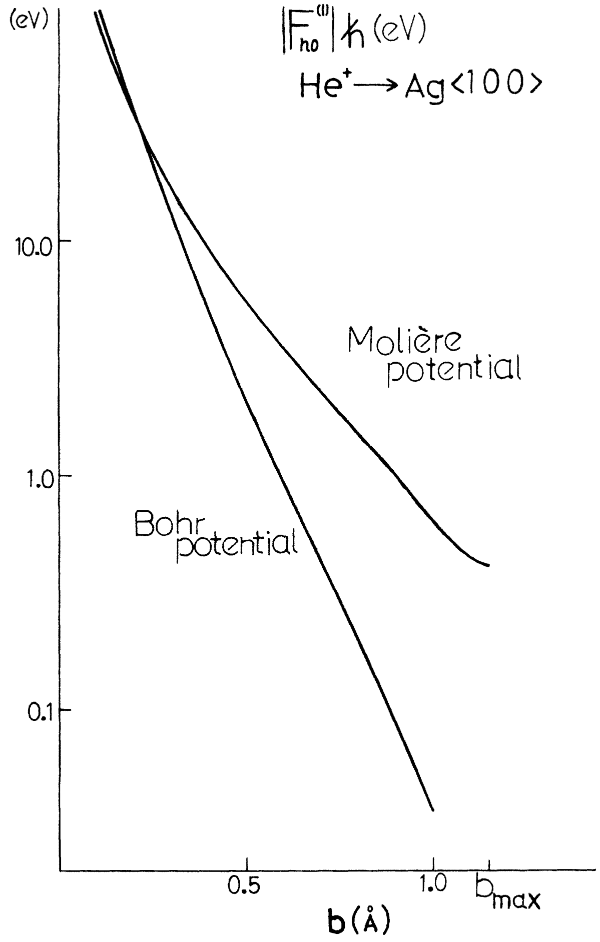

FIG. 2. Impact-parameter dependence of the matrix element $F_{n0}^{(1)}$ for the two model potentials.

In Fig. 2, we show the matrix element $F_{n0}^{(1)}$ for a different impact parameter b. We note the matrix element changes one or two orders of magnitude.

V. CHANNELING CONDITION AND NUMERICAL CALCULATIONS

For axial channeled particles, the impact parameter b is limited by $b > b_{\min}$, where $b_{\min}$ is decided as $U(b_{\min}) = E\varphi^2 = E_\perp$, φ beind the angle between atomic string and ion trajectory. U is the Lindhard's continuum potential. When $E_\perp$ is conserved, the impact-parameter-dependent physical quantity $f(b)$ is averaged along its trajectory by[5]

$$\langle f\rangle_{E_\perp} = \frac{1}{\pi(b_{\max}^2 - b_{\min}^2)} \int_{b_{\min}}^{b_{\max}} f(b)\nu(b)\,db, \tag{24}$$

where $\nu(b)$ is assumed as $2\pi b$ for the axial channeling case, and $\pi b_{\max}^2 = (Nd)^{-1}$ (N is the average number of atoms per unit volume).

Here we consider the transition probability $P(t)$

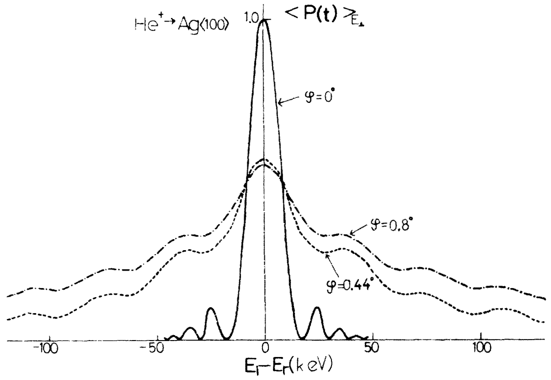

FIG. 3. Peak profile of the coherent resonant excitation $\langle P(t)\rangle_{E_\perp}$ for various channeling conditions (i.e., incident angle $\varphi = 0°$, 0.8°, and 0.44°) in the case of He$^+$ → Ag⟨100⟩. E_i is the incident energy and E_r is the resonant incident energy strictly corresponding to the Okorokov condition; in this case $E_r = 526$ keV.

for various channeling conditions. Then we obtain

$$\langle P\rangle_{E_\perp}=\frac{1}{\pi(b_{\max}{}^2-b_{\min}{}^2)}\int_{b_{\min}}^{b_{\max}} P(t)2\pi b\,db. \tag{25}$$

In Fig. 3 we show the $E_\perp$– dependent transition probability $\langle P(t)\rangle_{E_\perp}$ for various channeling conditions. It is worthy to note that the transition probability $\langle P\rangle_{E_\perp}$ depends strongly on the channeling condition. For example, the half-width of $\langle P\rangle_{E_\perp}$ changes for one order, which may include so many higher harmonics (i.e., $m=2,3,\ldots$).

VI. CONCLUDING REMARKS

A kinematical and a dynamical theory of the Okorokov effect were developed by time-dependent perturbation theory. The peak profile of the coherent resonant excitation was calculated in detail for He^+ ions in Ag⟨100⟩. The calculated peak profile is comparable with the difference of the higher-harmonics position in the Okorokov condition.

Our results suggest that the dynamical effect prevents finding the Okorokov peak for very "good" single crystals. So we have to use "bad" single crystals, for example, polycrystals. Another good means of detecting the Okorokov peaks is to take a hyperchanneling condition or semichanneling condition with the long impact parameter, in single crystals.

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