New Original Gapless Dispersion Surfaces instead of the Previous Erroneous Dispersion Ones

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Abstract. In almost all previous works, the hyperbolic dispersion surfaces of the central proper quadrics in the two wave approximation has been crudely derived from reduction of the degree of the bi-quadratic equation by use of roughly indefinable approximate relations. Moreover, neglecting the high symmetry of the hyperbola, both branches have been approximated on the asymmetric surfaces composed of a pair of a branch of the hyperbola and a vertex of the ellipse without showing any reasonable evidence. From the same X-ray propagation equation, a new original dispersion surfaces could be rigorously introduced without crude omission of even a term in the bi-quadratic equation based upon usual analogy with the band theory of the solid state physics as the close approximation to the truth.

1. Introduction.
It could be considered that the application of the usual dispersion surfaces by solid line in Fig. 1 [1] used in almost all works of the dynamical theory of X-ray diffraction (DTXD) [2-6], which were carefully drawn from the solutions of the secular equation only in the electron-diffraction [1], has prevented to foster greater understanding of DTXD. As well-known in the band theory of the solid state physics, the energy gap at the Brillouin zone boundary between the hyperbola and ellipse in Fig. 1 could be introduced as a perturbative effect of the Fourier component of the periodic potential in the crystal [7], which is the off-diagonal term in the secular equation. However, the off-diagonal terms of \( K^2 \chi_4 \) and \( K^2 \chi_6 \) from the X-ray propagation equation in the two wave approximation are composed of the wave number, the polarization factor and the Fourier component of polarizability. All of the factors for X-rays are transparent to contrary to the potential for electron, and therefore cannot construct the forbidden band as the Bragg gap in Fig. 1.

Secondly, the hyperbolic dispersion surfaces in DTXD have been allocated at the Lorentz point \( L_D \) in an unwarranted gap between the hyperbola and ellipse in Fig. 1. The hyperbola is point symmetry about the center. However, the gap in Fig. 1 is composed of the arc from the ellipse and the branch of the hyperbola. Therefore, the latter has two asymptotes that cannot exist in the former. Let it be ever so infinitesimal line elements in each, ellipse and hyperbola are invariably ellipse and hyperbola, respectively. Generally, approximation can round off magnitude of the quantity but cannot change the plus and minus signs and the geometrical symmetry as the characteristic nature. Therefore, the ellipse could not transform into the hyperbola by approximation.
Fig. 1. The popular dispersion surfaces with gap in DTXD, which are composed of pair of the oval and the
cocoon-shaped curves constricted in the middle by solid line from the two dotted Laue spheres $O$ and $G$.

Fig. 2. A new gapless dispersion surfaces, which are drawn from the same two dotted Laue spheres $O$ and $G$
in Fig. 1 by use of eq. (8) derived from the same propagation equation by the close approximation to the truth.

This report could be an extended work of our previous works [8-10], at least surpassing the
above two erroneous points the rightly reasonable dispersion surfaces are carefully described based
upon the band theory in the solid state physics[3] as the closest approximation to the truth [11]

2. The new dispersion surfaces based upon the band theory of the solid state physics [11]

The vector propagation equation of electro-magnetic wave by the electric displacement $d$ in
a medium with a periodic polarizability $\chi(\mathbf{r})$ has been represented by

$$\Delta \mathbf{d} + K^2 \mathbf{d} + \mathbf{rot} \cdot \mathbf{rot} \chi \mathbf{d} = 0.$$  

From the equation, the two wave propagation equations from the Bloch waves of $d_o$ and $d_g$ by

$$d(\mathbf{r}) = d_o \exp(-i\mathbf{k}_o \cdot \mathbf{r}) + d_g \exp(-i\mathbf{k}_g \cdot \mathbf{r})$$

could be derived as follows,

$$(k^2 - k_o^2)d_o - K^2 C \chi_g d_g = 0$$  \hspace{1cm} (1a)

and

$$K^2 C \chi_o d_o - (k^2 - k_g^2)d_g = 0,$$  \hspace{1cm} (1b)

in which $k$ is the wave number in the crystal, $K$ that in vacuum defined by $k = K(1 + \chi_o/2) = nK$,
where $n$ the refraction index, $C$ the polarization factor and $\chi_{o,g}$ Fourier components of the
polarizability, in which $\chi_g = \chi_g^2$ from $\chi_g = \chi_g^2$ by neglecting the absorption. In order to
solve the two wave propagation equations of eqs. (1a) and (1b), which could be represented by the
simultaneous linear equations with two unknowns, the necessary and sufficient condition satisfied
for existence of solutions in the elementary algebra [6] could be represented by

$$[S_{ij}] = \begin{vmatrix} k^2 - k_o^2 & K^2 C \chi_o \\ K^2 C \chi_g & k^2 - k_g^2 \end{vmatrix} = k^4 - (k_o^2 + k_g^2)k^2 + k_o^2 \cdot k_g^2 - K^4 C^2 \chi_o^2 = 0.$$  \hspace{1cm} (2)

Here, heads of $k_o$ and $k_g(= k_o + g)$, where $g$ is the reciprocal lattice vector) in Figs. 1 and 2 lie
at the point $O$ and $G$ and their initial common point $D$.

The diagonal terms of $S_{11}$ and $S_{22}$ in eq. (2) represent the two same radius circles intersected
at two points in Figs 1 and 2. The roots $X(= k^2 \geq 0$, positive definite) in eq. (2) can be given by
Accurately, eq. (2) could not be a form of the orthodox secular equation but has been frequently impressed as the secular equation in some references [2, 3, 6 etc.].

Assuming that two intersected circles with the same radii in eq. (3) are shown in Figs. 1 and 2. If the magnitudes of \( k_o \) and \( k_g \) are close to each other, then the term of \( 4K^2C^2\chi_{g}^2 \) cannot be neglected. Thus, the amplitude of neither plane wave is negligible. When \( |k_o| = |k_g| \), eq. (3) becomes \( X = k_o^2 \pm K^2C\chi_g \) and the ratio of \( d_o \) to \( d_g \), determined from eq. (2) is \( K^2C\chi_g \). Hence, \( |d_o|/|d_g| = 1:1 \). Assuming that \( \pm \) in the first term under the radical sign in eq. (3) in case of \( |k_o| \neq |k_g| \), \( X \) can be expanded to be,

\[
X = \pm \sqrt{(k_o^2 + k_g^2) + 4K^2C^2\chi_{g}^2}
\]

When \( k_o \) is large compared with the first term under the radical sign in eq. (3) in case of \( |k_o| \neq |k_g| \), \( X \) can be expanded to be,

\[
X = \frac{1}{2}(k_o^2 + k_g^2) \pm K^2C\chi_g \pm \left(\frac{(k_o^2 - k_g^2)^2}{8K^2C\chi_g}\right)^{1/2}.
\]

(4)

If we translate the origin of \( k \) by \(- g/2\) and consider the vector \( g + \alpha \) if we denote by \( x \) the component of \( k \) parallel to \(- g \) and by \( z \) the normal component to \(- g \), then by using the following relations, after more elaborate vector analysis than it looks like,

\[
k_o^2 = k_x^2 + g + g = k_o^2 + 2(x + (x - g/2)): g + g^2 = k_o^2 + 2x \cdot g
\]

and

\[
k_g^2 = z^2 = (z - g/2)^2 = z^2 + x^2 - x \cdot |g| + |g|^2/4,
\]

a reasonable roots of \( X \) in eq. (3) from the 2nd and 3rd terms in eq. (4) can be rewritten as

\[
X = z^2 + x^2 + g^2/4 \pm \left[K^2C\chi_g \pm x^2/(2K^2C\chi_g)\right]^{1/2}.
\]

(5)

The 4th term in the brackets in eq. (5) could be the most important one expanded in series near the Brillouin zone boundary. As a result, the 4th term in eq. (5) could be indicated by

\[
y^2 = \left[K^2C\chi_g \pm \left(\frac{g^2x^2}{2K^2C\chi_g}\right)\right]^{1/2}.
\]

(6)

The expressions with the double sign in eq. (6) show the precisely canonical forms of the hyperbola and ellipse as

\[
y^2 = b^2 \pm (a^2/x^2)
\]

(7)

shown in Fig. 2, together with asymptotes labeled \( L_1 \) and \( L_2 \) in hyperbola. The constants \( a \) and \( b \) in eq. (7) can be given by eq. (6) as

\[
a = \sqrt{2K^2C\chi_g}/g
\]

(8a)

and

\[
b = K\sqrt{C}\chi_g.
\]

(8b)

Here, \( 2a = 2\sqrt{2K^2C\chi_g}/g \) and \( 2b = 2K\sqrt{C}\chi_g \) from eqs. (8a) and (8b) are the minor and major axes of the ellipse, respectively and the latter of \( 2b \) stands for the transverse axis of the hyperbola. Both of the hyperbola and ellipse could stand in a line without a gap as in Fig. 1. It can be proved that the Bragg gap in Fig. 1 between hyperbola and ellipse could not absolutely exist in eq. (6).

### 3. On the crude approximation in the previous dispersion surfaces with the Bragg gap

According to the previous works [2-6], the dispersion surfaces in eq. (2) can be factorized as

\[
\begin{pmatrix}
k_o^2 - k^2 & K^2C\chi_g \\
K^2C\chi_g & k_g^2 - k^2
\end{pmatrix} = (k_o + k)(k_g + k)(k_o - k)(k_g - k) - K^4C^2\chi_{g}^2 = 0.
\]

(9)

In the previous works [2-6], by use of the numerically approximate relations of \( k_o + k \approx 2K \) and \( k_g + k \approx 2K = 2k \), the central proper bi-quadratic eq. (9) have been reduced to two quadratics as follows:

\[
(k_o + k)(k_g + k) - 4K^2 = 0
\]

(11a)

and

\[
(k_o - k)(k_g - k) - (K^2C^2\chi_{g}^2/4) = 0.
\]

(11b)

The factorization in eq. (9) is entirely impossible in the orthodox secular equation as proved [8].

Originally, the bi-quadratic dispersion surfaces in eq. (2) should be a composite form of the two central proper quadrics consisting of the hyperbola and ellipse including circle in eq. (5) and
easily understood from the intersected two spheres in Figs. 1 and 2. First, the central proper quadric of the hyperbola in eq. (11a), which could be given by replacing a very big product of $k_0 + k$ and $k_g + k$ with $4K^2$ by eq. (10), has been cut off and thrown away without any thought for the consequence. Secondly, although a product of terms of $k_a - k$ and $k_g - k$ has been approximated at zero by eq. (10), an order of magnitudes of eq. (11b) can be estimated to be

$$K^2C^2\chi^2 \gg K^2C^2\chi^2/4 \cong (C^2/4) \cdot 10^{2(9-10)} \cdot 10^{-5 \times 2} \cong (C^2/4) \cdot 10^{8 \times 10} \gg 1.$$  

This is tremendously huge number. The right reason of the omission of (11a) cannot be understood in the determinant of eq. (9). It is a wait-and-see way of thinking itself. These approximations are unmistakably self-contradictory and definitely break native goodness of the two central proper composite quadrics in eq. (2), which should be never allowed without rigorous verification.

It is apparent that eq. (11b) intuitively has at least two solutions. From the condition that the product of two variables is a constant of $C^2\chi^2$ in eq. (11b), a simple solution represents a rectangular hyperbola. However, this is not practically reasonable, considering the variations of the Bragg angle. In another, it could be understood from a attribute that the product of the two perpendiculars to the two asymptotes of the hyperbola from an arbitrary point on it is constant described by $\{a^2b^2/(a^2+b^2)\}$, which could be prove from the canonical form of eq. (11b) as

$$2/KC\chi \cdot (k_g^2 \cos^2 \theta_e - k_e^2 \sin^2 \theta_e) = 1.$$ 

The fitness of eq. (11b) of the hyperbola to the dispersion surfaces as the central point $L_D$ in Fig. 1 is out of the question, because that the surfaces compose of both of a hyperbolic branch and an elliptic arc near a vertex on the major axis side has not yet been correctly examined from a geometrical viewpoint to decide whether to support eq. (11b) on the principle of being fair and just. Superposition of the hyperbola over the gap between a branch of hyperbola and a vertex of ellipse in DTXD is a misapplication by a lighthearted interpretation.

4. Brief concluding remarks.

As a result, the new complete dispersion surfaces are composed of the continuous chain of hyperbola-ellipse-hyperbola string like a necklace without the Bragg gap in eq. (6) in Fig. 2. In the previous popular dispersion surfaces in Fig. 1, the concerned same central proper bi-quadratic in eq. (2) has been drastically reduced to the central proper quadratic eq. (11b) by omission of eq. (11a) by use of the crude approximated eq. (10). We attained a remark that there has been no presentation of evidence to support of this easily careless misapplication of the electron band gap in Fig. 1 to the dispersion surfaces in DTXD. Therefore, it is considered that the traditional crude approximations fail to discriminate good things from bad. Conclusively, it is important to promote that the above misapplication of Fig. 1 should be reasonably set to rights and validity of the new proposed dispersion surfaces in eq. 8 should be strictly examined by thorough investigations.

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