

The Classical Surface in Modern Theories of Solid Surfaces: II. Subband Formalism and Dimensionality Theory

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In a previous paper [Chin. J. Phys. **29**, 49 (1991)], we found that in front of a classical surface, the dimensionality has some ambiguity. Because we treat the surface or interface as a classical surface for semiconductors, etc., we find some dimensionality discriminations in our theory. We study the one-dimensional energy to incorporate subbands, reduced from the three-dimensional space. Because the surface condition $\mu(z)$, as a one-dimensional-boundary condition is not mathematically compatible with the one-dimensional Schrödinger equation in 3D, the plane subband theory thus obtained is not the 2D Bloch theory of electrons. There are different structural formulation influences when reduced from 3D. They imply that we can have, for any one crystal energy, three different appearances and nature: a three-dimensional E_{3D} and two one-dimensional E_{zn}^a and $E_n^{(sl)}$. The latter two provide envelope functions, with reductions in dimensionality. This suggests a new picture having various dimensionalities for energy quanta packets. This implies that in the statistical method we have three different Fermi energies: from E_{3D} , $E_F^{(3D)}$; from E_{zn}^a , $E_{F1}^{(1D)}$; and from $E_n^{(sl)}$, $E_{F3}^{(1D)}$, for running waves. This also implies that the physical contents of the crystal momentum include (a) a complex nature to indicate the mean free path, and (b) an extension to other (extra or deviate) dimensionalities. The origins of the mobilities are mentioned and related to the electron scatterings with 2D structure from the $k_z^{(2D)}$, the $k_z^{(2D)}$ p_z -perturbations. They are related to some energy eigen-equation with energy value E_{zn}^a which has the peculiarities: (a) it is not exactly one-dimensional for the envelope function; and (b) the $k_z^{(2D)}$ p_z -perturbation for this E_{zn}^a for all kinds of perfect crystals with a plane-surface, has a peculiar $k_z^{(2D)}$ coming from the other dimensions (2D). This reveals a new dimension and is a dimensionality-breakthrough from 2D into 3D. One obvious reason for this dimensionality-breakthrough is the existence of lattice lateral-vibration dynamics on the static surface $\mu(z)$. This resolves the problem that subband theories are 2D, e.g., in the xy -plane while the surface equation is expressed in one-variable with one degree of freedom in variable-variations, such as $\mu(z)$. Consequently a two-dimensional plane, $\mu(z)$, is physically measurable in three-dimensional space, by a certain periodic potential condition in terms of the primitive vectors in an (xy) -plane. Contrary to mathematics, the area integral is immeasurable in the formulation of volume integrals in Riemann integral theory due to the lattice dynamics vibrating into new dimensions.

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PACS. 73.20.At – Surface state, band structure, electron density of states.

PACS. 71.18.+y – Fermi surface: calculations and measurements; effective mass, g factor.

I. Introduction

Investigations of the growth and the adsorption mechanisms of surfaces lead us [1] to understand that we must have a surface or interface of two-*dimensions* (geometrical) or two-*degrees of freedom* (lattice dynamical) (2D) (2D-xy-plane) to formulate an energy eigen-equation, which is eventually in 1D in computational physics at least, nowadays within computer capabilities. Based on the underlying concepts in Sec. II, eqn. (24a), which is an equation equating a constant to another constant, we have the following argument: First the adsorption process is mainly a 2D-surface penetrated into the third dimension by growth. To this 2D-surface, the subband energy is correlated to the growing third dimension in a realistic process, although the energy equation is finally only 1D. How to understand the physics on account of the dimensionality? We find that we incorporate the 1D in the energy equation as our third dimension (with adsorbate growth). However from (29), we find that there are quantities, as physical constants, i.e. L_z precisely, belonging to the (xy)-plane. Hence we discover the subband energy includes dynamical terms obtained from the 2D-xy-plane. Moreover this (xy)-plane is not precisely the xy-plane in 3D $\mathbf{r}$ -space. It penetrates from the (xy)-directions into z-dependency. This z-dependency forms a new dimension in (29). This point will be clearer in (29). The separability of the above 2D-x;y-plane and the 3D $\mathbf{r}$ -space is a kind of dimension theory discussed on p. 30 in Ref. [2] and verification was tried by metal gate-charges in MOSFET in the discussion below (29b). That means, we find, in the theoretical prediction framework of this paper, that this new dimension (z-dependency) is, in fact, not exactly the conventional third z-direction. What we mean by the theoretical framework is the periodic structure kinematics such as the crystal periodic structures in the Bloch electron theory for energy band calculations. Intuitively the statement above is clear when we have a semi-infinite medium with periodic structure (occupying $z \geq 0$) vs. vacuum space (with $z < 0$). Physically the half-space $z > 0$ is entirely different from the other half-space $z < 0$. Mathematically there are no differences for the whole z-axis, since it is only along a 1D axis. In this paper, the above physical distinguishability, for $z < 0$ and $z > 0$, makes us to deduce and to induce some dimensional ‘consequences’ such that for $z > 0$ and $z < 0$ there are some physical ways to provide two different measures along this one single axis. These measures make it possible for us to reveal some new dimension (like surface charges), mathematically along the z-axis (similar to volume charges). However this new dimension is only for some ‘thickness-in-z-direction’ decided by the geometry of the xy-plane (e.g. a quantum size effect of the metal gate in MOSFET, etc.) (eqns. (29), (29a) below).

The subband energy, or the subband ladder energy, or subband bottom energy, is usually in the free particle form, $E_{3D} \approx E_{zn}^0 = \hbar^2(k_1^2 + k_2^2)/2m^*$ as in (24a) below. We find in this paper that the remaining 1D in the 3D-space with an energy $E_{3D} \approx E_{zn}^0$ in (24a), is actually determined, in part, by some quantities from other dimensions. This is the main theoretical subject of study in Sec. II, after eqn. (24a).

In recent discoveries and the current treatment of the surface growth process [1], we find that the surface plays the dominate role, physically and mathematically. This is because, by physical methods, the detectable thickness from the surface top into the bulk is limited anyhow, say from a few to less than 100 layers due to multiple scattering losses. More than 100 layers below the surface or interface, we really do not know its chemical composition, and its lattice structure in form and in magnitude, the electron-form-factors, even the matter densities, etc. This point is judged by the coverage increased to $\mu \gg 100$, and/or moderate high pressure measurements. Up

to the present, this point is determined by the structures near the surface and those ‘atoms’ located well inside the bulk, cf. e.g. [3] by a synchrotron light source, etc. These recent studies are in addition to the traditional LEED, x-ray measurements, etc. and are prepared for the verification of future near-field optic-measurements and femtosecond laser physics results.

We believe that the whole bulk or 3D properties are essentially determined by the ‘near-surface-few-hundred-layers’. Structural distinctions, from single-layer delta-doped quantum wells (as characterized by the layer-localized or surface- or interface-*localized phonons* [4]) to a surface or interface of a semi-infinite medium (as characterized by the *bulk-surface phonons*, as given in nearly all current textbooks, such as in the electron-energy-loss-spectroscopy (EELS) [5]), etc. are subjects of minor importance. In fact, the relevant common property is only that they have the subband energy structure on or near the surface or interface relative to the 2D incorporation. The difference is the results from one-layer or from a hundred layers. The realistic dominating factor derived from these considerations is that ‘geometric-flatness’, determined by the crystallographical Miller indices, impurities, foreign contaminations, defects, missing row, cracks and vacancies, etc., does really lead us to decide to choose some kind of physics ruling the way to prescribe our theories, and leave the strain-stress problems apart. A viewpoint of this kind is explained by an example below:

Current existing debate about the high Miller indices: For stepped surfaces of high Miller’s indices, e.g. $W(750)$, we have a more than usual Laue diffraction pattern, viz., there are *extra* diffraction spots due to the lateral steps of $W(750)$ [6] apart from those spots existing due to the ordinary regular net of the upmost layer of terrace platform. Directly from p. 166, Fig. 2.9 in [6], we have two extra spots for $W(750)$ than is common in $W(110)$. Usually we consider that a (110)-surface is a 2D plane. For $W(750)$ described in [6], it is determined by measurements: a terrace width $12.6 \pm 0.1 \text{ \AA}$, and a step height $2.19 \text{ \AA}$. $W(750)$ is typically a 2D surface plus a third penetrated direction. From Fig. 2.9(b), the two extra spots for $W(750)$ are on the same 2D plane which shows the LEED pattern of (11) and (20), etc. for $W(110)$. Therefore we have 2D-reciprocal-momentum-space patterns to exhibit diffraction patterns from *both* a 2D-crystal surface *and* a (2D-terrace + a third penetrated direction)-stepped-surface, typically 3D appearance (stepped) surface. We can not trust that “seeing is believing”. Here we think that both the 3D ‘stepped-surface’ and the 2D-plane-surface make diffraction patterns on the same 2D $\mathbf{k}$ -plane(s). There is a dimensionality-transformation or a breakthrough in dimensionality from the 2D $\mathbf{k}$ -plane into the 3D stepped-surface in reality! Experiments of this kind made us believe that the mathematical surface formed by the outmost steps (750) is our standard “surface” existing in nature for minerals or for growth after deposition processes, etc. We illustrate in Fig. 1(a): a mathematical surface of such a kind, not for (750) but for (110). By ‘mathematical surface’, we mean surfaces existing by Miller indices predictions. They are a kind of “natural” surfaces existing themselves in nature without any artificial processes. They do not include the polished surfaces, capped surfaces and special cut-surfaces [7], etc.

When we formulate our calculation framework, we think the surface of this kind is not only a standard but the only correct one to use everywhere. Furthermore it is the only one in the pattern of this kind by which we can have the Bloch theory of periodic structures presented in the solid state. Based on this conception, from the Bloch theory for 1D, the surface of this kind is the only one able to formulate and to become a 3D-Bloch theory. Actually there are other surfaces such as some classical surfaces, etc. which are applicable or also satisfied by the Bloch theory.

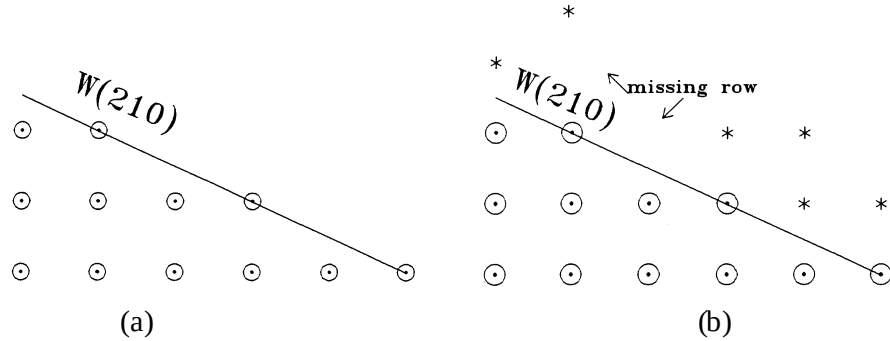


FIG. 1. Side views of tungsten with the stepped surface $W(210)$ shown. (a) $W(210)$ in a mathematical model. (b) $W(210)$ in a defect model.

We include the classical surfaces of this kind as “cut-surfaces” below.

A contrary viewpoint, started by Mullins, we call Mullins’ defect model [8]: a ‘high Miller indices surface’ is an irregular step surface, as shown in Fig. 1(b) with many additional adsorbates, as surface impurities. It can be a “classical surface” without regular or ‘flat’ Miller indices predictions. There can exist many missing rows or line defects with a deep crack possibly. If the surface, as shown in Fig. 1(b), is the one predicted by Mullins’ model as the outmost surface next to the vacuum space as a natural surface, we really do not know how to explain it by the periodic structure, as used in Bloch theory. Mathematically one of reasons that the subband ladder energy appeared here, instead of the simple parabolic band energy of free electrons, for a (semi-infinite) crystal structure, is the dominate role of the above ‘classical surface’ involved. This classical surface will change our mathematics related to dimensionality in both prediction and calculation. Similar properties were reported in our first paper [9] with a positronium in front of a classical surface and some charge density problems for image potentials.

As a theorist, for the subband manipulation for a metal cap structure, we would think the structure like the one shown in Fig. 1(a) was a proper one. After we introduce the *classical surface* for the cap or substrate, we find that the one shown in Fig. 1(b) is also a possible one, moreover it is more proper to have used Fig. 1(b) than the one given in Fig. 2. The reason, apart from experimental preparation ones, is given as follows: A 2D-surface in the form of a classical plane, such as $z = 0$ (46) below, is sometimes not a part of the description in the framework of a 3D perfect periodic solid crystal. This description (a) is not unique; and (b) does not include the whole content inside which $z = 0$ say, does exist. It forms a breakthrough to break the above ‘incomplete description’, in fact the 3D perfect periodic structures, as defined by the kinetic energy in (45); meanwhile the potential energy being (45a), splits the total-periodicity in (49b). The mathematical reason, for the non-existence of a $z = 0$ plane inside the perfect periodic structure, is that a 2D-plane has “zero measure” inside a 3D volume and aside from the measures of a periodic potential, etc. We might think that a 3D perfect crystal is some ‘volume’ mathematically 3D with the coexistence of many 2D-planes. This intuitive viewpoint has been changed for a crystal either with a periodic structure or with a plane surface below. Putting both the periodic structure and the plane surface together in a consistent theory is the subject of this paper. A surface or interface is 2D, thus of zero measure, similar to a surface integral equal to a

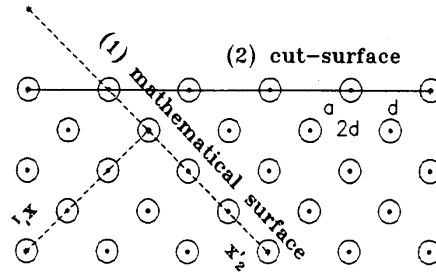


FIG. 2. A two-dimensional illustration of surfaces for $V(z)$ and $V(x_1^0; x_2^0)$ in (47c). (1) A “mathematical surface” to express the perfect 3D crystal for $V(x_1^0; x_2^0)$ in (49) for some $C_+ A_+$, $C_i A_i$ and proper d_i in x_i^0 -directions. (2) A physical “cut-surface” for $V(z)$ for different d in the z -direction.

volume integral of zero thickness, and has various uncertain influences on the 3D energy calculations. Between the whole-2D-plane and whole-3D-volume, stepped surfaces, as an interface between the material and the vacuum, are subjects for testing influences of this kind. From the viewpoints above, our decompositions into $\mathbf{f}, \mathbf{a}, \mathbf{b}, \mathbf{C}, \mathbf{g}$ primitive translations in (21) below, fit the experimental set-ups in order to fit our “classical surface”.

Primitive and non-primitive cells in crystal structures: The above discussion is conventional. For a pictorial interpretation, refer to the figures in Kittel’s ISSP [7], Figs. 14, 15 in Ch. 1, conventional non-primitive cells or Bravais or space lattices are given in Fig. 11. All simple cubic, body-centered cubic (bcc), and face-center-cubic (fcc) are given for a lattice constant a . Their corresponding primitive cells are all simple cubic in form and are given in Figs. 12, and 13. Recall that these simple cubics have entirely different oriented faces or surfaces with respect to conventional cell surfaces! They are not oriented in the way of “cut-surfaces”. The periodicity lengths are $\sqrt{3}a=2$ for bcc and $a=\sqrt{2}$ for fcc. When we talk about a (classical cut) surface which has a metal cap (which are mostly a surface after it has been polished or laser-evaporated), it is a surface faced on the conventional cell faces, not on the primitive cell faces. While the latter is mostly the Miller indices surface, because we apply to this primitive cell surface the crystal periodic boundary condition in Bloch theory. It must be a ‘mathematical surface’ defined as the right one for Bloch theory. The discussion here shows that Fig. 1(a) is a primitive or Miller indices ‘mathematical surface’ while Fig. 1(b) and Fig. 2 are capped surfaces.

The crystal structure for some currently used surface: Contrary to the above discussion, in many semiconductor heterostructures, we cut a surface which makes a few degrees (say, $2^\pm$) with the conventional surface [10, 11]. The technique substantially extends the scope of our discussion above. For the present author, we should consider that they are classical surfaces. Furthermore they fall into the category of Mullins’ defect model (for surfaces) from an argument of realistically experimental preparations. In experiments, say in [11], we may use $\text{Al}_{0.7}\text{Ga}_{0.3}\text{As}$. It seems that it is similar to a simple-metallic surface of Mullins’ model. On the theoretical side, we can have quantum transport due to lower gap-energies for X and L points thereby having indirect transitions involving phonon processes. Further there may be uncertainties of energy entering the quantum transport regime, cf. p. 175 in [12]. It is natural to include umklapp processes according to the

reciprocal lattice vector space formulation. However it makes the PL peak intensity increase, say by 10 times as in [11].

Current Fermi-Dirac statistics applied in physics: We introduce the relevant current theoretical quotations on various topics we need to use in the following for the total value of a dynamical variable $A(E)$, as a function of E . Then the total value of this A over the occupied energy levels labelled by $\hbar$ of $E_{\hbar}$ is

$$\langle A(E) \rangle = \sum_{\hbar} A(E_{\hbar}) P(E_{\hbar}) \quad (1)$$

for a (normalized) population (or probability) $P(E_{\hbar})$. For many electron systems, we use Fermi-Dirac statistics with the distribution function $f^{(FD)}(E)$ for some energy value E . Hence, with the density of states (DOS) $D(E)$, we have

$$\langle A(E) \rangle = \frac{\int D(E) dE A(E) f^{(FD)}(E)}{\int D(E) dE f^{(FD)}(E)}. \quad (2)$$

Current Fermi levels of 3D and 1D in statistics from a periodic structure: (I) For exact 3D systems, we replace (1) by changing $\hbar$ in the summation to $(n_x; n_y; n_z) \rightarrow n$ which appeared in the crystal momentum $k = n^{2/4}L$. We then have (1) becoming

$$\sum_n \left(\frac{L^3}{(2^{1/4})^3} \int dk \right) \left(\frac{L^3}{(2^{1/4})^3} \int_0^{E_F^{(3D)}} \frac{4^{1/4} (2E_{3D}) d^3 p}{2E_{3D}} \right) \quad (3)$$

for 3D $E_{3D} = k^2/2$, without counting the spins. Here $E_F^{(3D)}$ is the usual “3D Fermi energy in 3D systems”. The necessity of (3) is also required for the band energy calculations for crystals when they are of three dimensions, not the one in the Bloch theory of 1D as say in the Kronig-Penney model, for which we have many debates about the changing from 1D to 3D.

(II) For the 1D case of standing waves, in the zero temperature formalism for a convention, we change the label $\hbar$ in (1) to a 1D crystal vector (in the standing wave) $E_{\hbar} \rightarrow E(k)$ with $k = k_m = m^{1/4}L$, $m = 1, 2, \dots$ for a length L of the 1D periodic structure. (2) becomes

$$\langle A(E) \rangle = \frac{\int D(E(k_m)) dE(k_m) A(E(k_m)) f^{(FD)}(E(k_m))}{\int D(E(k_m)) dE(k_m) f^{(FD)}(E(k_m))}. \quad (4)$$

Here the DOS $D(E(k_m))$ is calculated by the counting of m instead of $\hbar$ as (in atomic units: $\hbar = m_e = |e| = a_{Bohr} = 1$ and, in the zero temperature formalism)

$$\sum_m \left(\frac{L}{1/4} \int dk_m \right) \left(\frac{L}{1/4} \int_0^{E_F^{(1D)}} \frac{d^3 p}{2E(k_m)} \right); \quad (5)$$

where “ $\dots$ ” means other functions included in the sum or in the integrand, as in (1) and (2), etc. For $D(E)$, we need to multiply by another factor 2 for counting the spin-occupations. The upper

limit $E_{F2}^{(1D)}$ in (5), the “1D Fermi energy in 1D systems” has many applications in solid surface theory [13].

As developed below in this paper for the first time, E_{3D} becomes E_{zn}^a in (26) or (24a), which is a 1D energy in a 3D system; (3) is calculated as for a given subband energy $(k_1^2 + k_2^2) = 2$,

$$\sum_n \left(\frac{L}{2^{1/4}} \int_0^{E_{F1}^{(1D)}} dk_n \right) \frac{L}{2^{1/4}} \int_0^{E_{F1}^{(1D)}} (2E_{zn}^a) d^3p \frac{1}{2E_{zn}^a} \quad (6)$$

for a 1D periodic running wave in a 3D system with crystal momentum $k_n = n2^{1/4}L$ for $E_{zn}^a = E_{zn}^a(k_n) = k_n^2 = 2$. The upper limit $E_{F1}^{(1D)}$ of the integral in (6) is *not* the same $E_{F2}^{(1D)}$ given in (5). However this E_{zn}^a -statistics is different from the Kronig-Penney model mentioned above.

(III) As a remark, $E_{F2}^{(1D)}$ in (5) is a different 1D Fermi energy (in a low-dimensional system) in comparison with the “1D Fermi energy (in lower-dimensional systems) in 3D systems” [14], as we shall suggest for the first time in this paper. The difference comes from (30) below for

$$E_{zn}^a = E_n^{(sl)} + \frac{\hbar^2}{2m_z} k_z^{(2D)2}. \quad (7)$$

Here both E_{zn}^a and $E_n^{(sl)}$ are 1D energies. The eigenvalue of E_{zn}^a indicates 3D energy quatum packet while that of $E_n^{(sl)}$ 1D energy packet. When we use either E_{zn}^a or $E_n^{(sl)}$, each of them can formulate a kind of statistical mechanics of its own. They can have their own Fermi energy. For instance, the Fermi energy of the E_{zn}^a -formalism is $E_{F1}^{(1D)}$, which is a lower-dimensional system including a term $\frac{\hbar^2}{2m_z} k_z^{(2D)2}$, which is in the z-direction mathematically but comes from other dimensions, viz., with k_1, k_2 from the x; y-dimensions physically. Therefore for $E_n^{(sl)}$ -statistics, we can have, similar to (6),

$$\sum_n \left(\frac{L}{2^{1/4}} \int_0^{E_{F3}^{(1D)}} dk_n \right) \frac{L}{2^{1/4}} \int_0^{E_{F3}^{(1D)}} (2E_n^{(sl)}) d^3p \frac{1}{2E_n^{(sl)}} \quad (8)$$

Here we have $E_{F3}^{(1D)}$ for a 1D Fermi energy, which is a (pure 1D) low-dimensional system, not a lower-dimensional system in 3D.

Conclusively for 1D Fermi energies: we have $E_{F1}^{(1D)}$ for E_{zn}^a -statistics, $E_{F2}^{(1D)}$ for standing wave $E(k_m)$ -statistics, and $E_{F3}^{(1D)}$ for $E_n^{(sl)}$ -statistics. The category-classification here has been applied to the free-electron-model for density-functional theories from Pauli paramagnetism [1, 15]. The main influence in setups is on the evaluation of the workfunctions ϕ_i . Here we have three different workfunctions for 1D-surface-systems, or the familiar lower-dimensional system of a solid surface of a crystal. From the above three kinds of statistics: explicitly

$$\phi_i = \text{vacuum level energy} - E_{Fi}^{(1D)}; \quad (9)$$

where $E_{Fi}^{(1D)}$ is the three values of the Fermi energies above. From the experimental side or instrument side, the Fermi level determination is a major subject in heterostructures [14]. The

Fermi levels are determined by the charge neutralization of donor N_D or/and acceptor densities N_A , i.e., for the electron density n and hole density p , we determine the Fermi levels by

$$n + N_A = p + N_D$$

for p-GaAs and N-Al_xGa_{1-x}As heterostructures. As to the built-in potential V_D , it determines the difference between the Fermi levels of the two sides of an interface of the heterostructure. Clearly this calculation is based on Fermi-Dirac statistics, with the proper chemical potential as the Fermi energy calculated from the total number of particles in the system. As a comment from the above results, we really do not know that the Fermi levels determined here are $E_F^{(3D)}$ or $E_{Fi}^{(1D)}$, since the dimensionalities of the particle numbers above are really relevant. The experimental setups or deposition designs of the electron density [14] are actually based on the formula of electron density n . The Fermi energy E_F , as a function of the conduction band bottom E_c for a setup-parameter N_c which is usually referred to 300 K, is

$$E_F = E_c + k_B T \ln \frac{n}{N_c} + 3.53553 \times 10^{-1} \frac{n}{N_c} + 4.95009 \times 10^{-3} \frac{n^2}{N_c} \\ + 1.48386 \times 10^{-4} \frac{n^3}{N_c} + 4.42563 \times 10^{-6} \frac{n^4}{N_c};$$

in which the Fermi energy we are referring to is really important! But we are not sure about which one of the above Fermi energies we are referring to, 3D or 1D?

To be explicit, our viewpoint or comments on the currently existing framework on semiconductor, such as (Al,Ga)As heterostructures, is as follows: The flat-band energy band diagrams show only incomplete 1D energy levels for interface physics with interface-barriers, such as the Schottky barriers, etc. in Ref. [14]. For 3D, energy value levels must be those in Ref. [16]. For GaAs with a surface or interface aside, we have energy diagrams with the Fermi-level (here the 3D Fermi energy in the 1D diagram) aligned, such as p. 209 in [14]. This way of treatment is perfectly alright. However current texts argue differently. They have stated some deviated applications followed by some deviated plots, such as a 3D Fermi energy for 1D plots in [14], which seem to lead us to arrive at conclusions in non-equilibrium viewpoints! For heterostructures, near the surface or the interface, we consider that it is at a j -point for a surface-plane [100] or [111] for GaAs. The system occupies $z > 0$, the semi-infinite medium. The energy-band diagram along the whole z -axis is plotted according to the j -point energy levels in the band structure. Far enough from the heterojunction plane of heterostructures, we have various flat-bands in various regions along the z -axis. The plot in this way is: (a) different from the usual band-energy diagram for bulk solid state materials in which it is plotted from X to j to L -points with high symmetries, but reducing its dimensionality, in $\mathbf{k}$ -space; and (b) not theoretically acceptable or explainable based on interface physics. However in the so-called flat-band regions, we can calculate the electron distributions in a statistical mechanics way, as on p. 203 in [14]. In this calculation, we claim usually that it is an energy-band application on the 'solid with surface' from current solid state physics, which treats *solids without surfaces*. In the author's opinion, it is not right since in practice, the semiconductor with surface or interface is only one-dimensional Fermi-Dirac statistics with $E_{Fi}^{(1D)}$, as in (8) pure 1D. Not the Fermi energy used in [14] in which $E_F^{(3D)}$ is supposed, such as in (3).

Furthermore in the discussion of the band-tail states from the DOS consideration [16], the present author tries to believe that this is a case of one-dimensional statistical mechanics instead of an interpretation in the energy-band picture. On many occasions, this is not related to the energy-band theories at all. In Kane's theory or the theory of Halperin and Lax say, we have energy-bands (tail) extensions in energy band diagrams, such as the exciton levels say, cf. p. 81 in Ref. [16]. The troublesome thing is the energy distribution extended from 0 (at E_c of the conduction band) to some negative energy values in the Fermi-Dirac distribution with a DOS $E^{-1/2}$. In this DOS, we are not able to write a real expression from $\int_{-\infty}^0 j(E) dE$. Here we have put zero energy at E_c whereas negative E means a level slighter lower than E_c , actually in donor states region. This DOS is expressible as a one-dimensional distribution in numerical continuation, with a deviation from the parabolic energy bands, cf. [16]. As given on p. 95 in [16] for nonradiative recombinations, say for CCCH Auger process, etc., the energy-band plot is different from the ones for the 'solid with surface', given above in the last paragraph and the 'flat-band plot' given throughout the plots in Ref. [14]. In Auger processes of this kind in [16], the energy-band is plotted from the Γ -point to the L-point, such as the one extended from the energy at Γ_6 (as the zero-value of E at E_c) to negative (exciton levels) values. They are for 3D bulk structures, as occurs in current solid state physics not in surface or interface physics. For the Fermi energy, the use of $E_F^{(3D)}$ must be a misuse. We need to use $E_{Fi}^{(1D)}$ in (9). The subject which needs to have deeper investigations is the same as above, viz., which one of $E_{Fi}^{(nD)}$ $n = 1$, or 3 or 2; $i = 1, 2, 3$? is proper in practice? The theory that needs to be studied is in what maximum compatible capabilities are we able to interpret and predict the physical properties of semiconductor systems when the energy-band theory and the one-dimensional-statistical theory are put together? Do not mix up the 1D systems and 3D systems!

Furthermore on the physics side, we need to pay much attention to our theory of semiconductors. There are investigations to fulfill the interpretations of theory, such as the flat-band concept. Recent attacks of the same author are: (i) From discussion in Refs. [1, 14, 26], it is more natural to interpret the space charge layers near the interfaces by the charge-transfer of semiconductor materials, such as III-V compounds. By an interpretation of this kind, we can have the "flat-band" charge distributions in the flat band regions. This leads us to have Fermi-Dirac statistics for the carrier, hole and electron distributions in place of a pure energy band theory as concluded below. Many of them are discussed in this paper. For a Thomas-Fermi study of this flat-band problem, we have results in x[3.4] and p. 32 in Ref. [2]. (ii) For adsorption theory in front of a surface for charge transfer to an adatom, we have results in [26]. But for the bulk-charge transfer for a semiconductor, which implies experimental results displaying the bulk-space charge near interfaces, we are intensively studying their peculiarities.

Because we have various energies in various dimensions as discussed above, we have some correction to their derived quantities, such as the effective mass definition. In eqn. (4.1) on p. 289 in Ref. [2], we have derived the effective mass for an isotropic material. $1/m^* = (1/3) r_k^2 E(k)$ instead of the usual value $1/m^* = \partial^2 E(k)/\partial k^2$. This is clear from the definition of the reciprocal effective mass tensor in (16) below. Generally the correct effective mass for isotropical materials should be derived from the radial part of the Laplacian r_r^2 , viz., $1/m^* = (1/3) r_k^2 E(k)$, not from the wrong expression: borrowed from $\partial^2 = \partial^2/\partial r^2$ which corresponding to the current value $1/m^* = \partial^2 E(k)/\partial k^2$.

The surface state from the complex k of Kohn: From an analytical function theory for Bloch electrons of periodic potentials for 3D perfect crystals, in Ref. [17], Kohn introduced the complex crystal momentum and concluded that, for pure imaginary crystal momentum k , the band energy $E_{n;k}$ is inside the energy gaps between the bands or the allowed ranges of $E_{n;k}$. The Wannier function is the subject to be studied, particularly for surface states. In Refs. [18, 19], the authors formulated a basis from the “generalized Wannier functions” $a_n(x)$. In turn, a_n is expanded in terms of $g_{n^0}(x; n^0)$, the Gaussian distribution functions at various lattice points, $x = n^0$. In these references, this group obtained some surface state above or below the lowest band, just like the acceptor or donor states, inside the band energy gap, which is along one particular direction in crystal momentum space and is essentially 1D *in a statistical sense, the same as $E_{F1}^{(1D)}$* . Therefore it is natural to have some imaginary part for the crystal momentum. This quotation is from a background of Gaussian-distribution-bases which had been applied to magnetic field systems extensively in these years. They are always referred to as the localized-states. For dynamical Wannier functions, see eqns. (4.2.6) and (4.3.14) in Ref. [12] for quantum transport in semiconductors.

Resolution of new-dimension hidden coincidently along the z-axis by complex k : From the conclusion (29b) below, 2D behaviours such as subbands, etc. are considered as a $k_z^{(2D)}$ in the z-direction, to have its new dimensionality because it is derived from the x;y-plane quantities, i.e. the constants $k_x; k_y$ from the x;y-dimensions. The dimensionality is thus conceptually extended to some *abstract or implicit* dimensions. In the other version, it may be considered as a way to include the complex momenta. For a complex extension of a real physical quantity, such as k above, we can have the real axis together with an imaginary axis. It is thus a possibility to make a *breakthrough* to break into physical configurations, such as from the bulk crystal (wave function) to be extended to include a surface (envelope function), for bulk material (a 3D volume) and a surface (a 2D envelope). We have a detailed dimension theory in [2]. They are separated in measure theory, such as in the Riemann integral theory in which the 2D-plane is immeasurable in the 3D volume integral for a simplified version of the mathematical origin. For this we can have an x;y;z-axes for the 3D material (such as volume-charges) while there are x;y-coordinates for a 2D surface (such as surface-charges, with zero thickness in the z-direction). Another example is that the complex k may provide a complex $E(k)$ whose imaginary part is related to the lifetime, etc. cf. p. 247 in [2]. All of them exhibit a new extension to various new directions, or degrees of freedom or dimensionality, such as surface charge distributions wrapping a volume charge. Further it incorporates surface behaviour (in surface localized-state conceptions in a delta doped layer) together with 2D peculiarities, one of them for the surface of semi-infinite structures. It is directly related to the mean free path λ , cf. p. 247 in Ref. [2], by

$$k_I = \frac{1}{2\lambda} \quad \text{in } k = k_R + ik_I : \quad (10)$$

It is usual that the plane wave wave function will be changed to

$$\tilde{A} \gg e^{ikx} = e^{ik_R x} e^{i k_I x} \quad (11)$$

with decreasing length $\lambda = 1/k_I$. Their applications to mobilities through either Kohn’s way discussed above, or through (10), as given in Ref. [2], will be given with a physical implication in (29a), or (29b).

Mobility for intrinsic semiconductors: Currently subband theory is extensively applied, e.g. related to mobility problems, such as microscopic mobility, Hall mobility etc., incorporating two-dimensional behaviour [20, 21] and/or high magnetic fields. Historically, from Seitz's result of the mobility for intrinsic semiconductors [7], it is related to the collision with phonons and is related to kinetic energy in its formalism in the initial equations. It is related to the so-called $\mathbf{k} \cdot \mathbf{p}$ -perturbation for the intraband calculation. Originally the $\mathbf{k} \cdot \mathbf{p}$ -perturbation was for the $u_{\mathbf{k}}(\mathbf{r})$ of the Bloch function $b_n = u_{\mathbf{k}} \exp i\mathbf{k} \cdot \mathbf{r}$ in the Schrödinger equation. It is a kind of scattering interaction with phonons inside the particular kind of structure. This can be seen from the band electron (i.e., with its motional momentum $\mathbf{p}$) interacting with the phonon (i.e. with the crystal momentum $\mathbf{k}$ evaluated from a given structural framework). Or we can see it from

$$\begin{aligned} \frac{\hbar^2}{2m} \int d\mathbf{r} |\nabla u_{\mathbf{k}}|^2 &= \frac{\hbar^2}{2m} \int d\mathbf{r} |\nabla b_n|^2 + \frac{\hbar^2 k^2}{2m} + \frac{2}{\hbar} \text{Re} \int d\mathbf{r} b_n^*(\mathbf{r}) (\mathbf{k} \cdot \mathbf{p}) b_n(\mathbf{r}) \\ &= K^{(B)} + K^{(class)} + \frac{2}{\hbar} \mathcal{E} \quad \text{Real part of } \mathbf{k} \cdot \mathbf{p}\text{-expectation} \end{aligned} \quad (12)$$

in the formula in Ref. [7]. The classical nature of kinetic energy $K^{(class)}$ is given on p. 347 in Ref. [2]. In view of (12) for the periodic $u_{\mathbf{k}}(\mathbf{r})$, the kinetic energy appeared twice, once in the quantum form of the Bloch function and another as a classical form. From the concepts of deriving the dimensionality of classical generalized coordinates in classical mechanics, the kinetic energy appears twice (and in different forms) so this must have the degrees of freedom = 6, twice as many as the one particle freedom = 3 in the kinetic part. This is to be understood in the following:

Resolution of a new-dimension by direct addition of the new dimension: This is familiar in molecular physics [15] for a diatomic molecular system. Below 1000 K, the heat capacity shows 3 translational motional degrees of freedom. Near 2000 K and below 3000 K, the rotational motions enter, so that the total degrees of freedom becomes 5. Higher than 3000 K, the vibrational motions enter so that the total degrees of freedom become 6, 7, or more. When we write the Schrödinger equation for this diatomic molecule, the dimensionality changes from 3 to 5 to 6, 7, or more in the above order for various temperatures. We see that, when the temperature increases in molecular physics and thermodynamics, we have to increase the dimensionality for the same molecule. This illustrates that we can add directly the new-dimensions to our system quite naturally and with nearly no limitations.

For the extension of atomic or molecular vibrations on a surface, we see that the vibration frequencies on a surface do not depart from the free status very much. For instance, a CO-molecule on Cu(111) shows a C–O vibration with frequency 2074 cm^{-1} (coverage < 0.33) [22]. This can happen in a wall-collision of CO on a Cu-wall, stuck or adsorbed, and detached. From a standard table, the vibrational frequency of gaseous-phase C–O is $2169.8233 \text{ cm}^{-1}$, not very different from that of the surface value. Because, as a picture, C is between O and the Cu surface, there are two harmonic potential energies acting on C, viz., one is the C–O bond V_{bond} and another is the whole CO inside a harmonic potential V_{CO} due to the surface. When written inside the system total Hamiltonian, the C is affected by two harmonic potentials, added together as $V_{\text{bond}} + V_{\text{CO=Cu}}$. However in a status of motion, we obtained the frequency of the C–O vibration which occurs for the so-called localized vibrations, cf. p. 346 in [22], not the localized phonon band of surface

[4], in a mode which is nearly not influenced by $V_{\text{CO}=\text{Cu}}$. Now we write the coordinates as that between C–O,

$$V_{\text{bond}} = \frac{1}{2} k r_{\text{bond}}^2; \quad (12a)$$

and between CO and the Cu-surface we write

$$V_{\text{CO}=\text{Cu}} = \frac{1}{2} K R^2; \quad (12b)$$

where $\mathbf{R}$ is the center of mass coordinates of CO with respect to the surface. For brevity, we write it only in 1D along the z -axis without considering the bond-bending etc. with C at z from the Cu-surface, so that $\mathbf{R}$ is perpendicular to the Cu-surface and

$$R = z + z_{\text{CR}}; \quad z_{\text{CR}} = \frac{m_{\text{C}}(R - z) + m_{\text{O}}(z_{\text{O}} - R)}{m_{\text{C}} + m_{\text{O}}}; \quad (12c)$$

where z is the coordinate of C and z_{CR} the distance between C and the center of mass of CO; z_{O} is the coordinate of O. Therefore

$$V_{\text{CO}=\text{Cu}} = \frac{1}{2} K (z + z_{\text{CR}})^2; \quad (12d)$$

One of the vibration frequencies of C is nearly $\sqrt{\frac{k}{m_{\text{C}} + m_{\text{O}}}} = 2074 \text{ cm}^{-1} \gg 2169 \text{ (standard)}$ although the total potential affects on C is

$$V_{\text{bond}} + V_{\text{CO}=\text{Cu}} = \frac{1}{2} k (z_{\text{O}} - z)^2 + \frac{1}{2} K (z + z_{\text{CR}})^2; \quad \text{same mathematical } z \quad (12e)$$

as in the 1D expression. That means, in this (normal) mode of motion, C–O vibrates with V_{bond} independently from $V_{\text{CO}=\text{Cu}}$ no matter that it is the same z in the two potentials in (12e). If the potential energy in (12e) is summable for all z as a 1D-variable, we must have

$$\begin{aligned} V_{\text{bond}} + V_{\text{CO}=\text{Cu}} &= \frac{K_1}{2} (z - z_1)^2 + C; \quad \text{with} \\ K_1 &= k + K \frac{1}{(1 + 1)^2}; \quad m_{\text{C}} = m_{\text{O}}; \\ z_1 &= \frac{z_{\text{O}} k (1 + 1)^2 - [(1 - 1)R + z_{\text{O}}] K}{(1 + 1)^2 k + K}; \\ 2C &= - \frac{[z_{\text{O}} k (1 + 1) - (1 - 1)R + z_{\text{O}} K (1 + 1)]^2}{(1 + 1)^2 k + K} \\ &\quad + k z_{\text{O}}^2 + \frac{K}{(1 + 1)^2} [(1 - 1)R + z_{\text{O}}]^2; \end{aligned} \quad (12f)$$

with an entirely different but complicated combined vibrational frequency from K_1 , etc. This forces us to consider that r_{bond} is in a separated dimension from the CO–Cu-surface, viz., the $z + z_{\text{CR}}$ coordinate. While for the other potential $V_{\text{CO}=\text{Cu}}$ in (12e), because of the complications

of z_{CR} which itself depends on z in (12c), by simplification, we may consider this degree of freedom or the new dimensionality by way of a mean-free-path or mobility, etc. such as the one given in (29b). In the author's treatment, it provides a *new dimension*. For the kinetic energy term, similar to (12), we have a kinetic energy for the relative coordinates of C–O *and* another kinetic energy for the center of mass of CO/Cu.

The separation is particularly clear when the C–O makes a detachment from the surface to become a gas-phase particle. Since the mathematical surface is infinite in any direction, so to speak and measure, the ratio z_{CR} =surface dimension is always zero. It is a scale-free-measure, used in many different ways and academic branches. We must separate r_{bond} from z_{CR} as a new dimension since these quantities are not scale-free, particularly when a surface dimension, included as scale-free dimension, or surface quantities are involved. Furthermore, for $z_{CR} \text{ \AA } 10\text{ \AA}$, C–O is a gas-phase or free particle, and it must be determined by new dimensions or a new system of coordinates for this isolated system. Cf. Ref. [26].

Mathematics of linear independency: Dimensionality is determined mathematically by the judgment of the existence of the so-called “linear independency”. It is the mathematics of linear vector space theory: the linear independency of vectors in mathematics is restricted by the so-called “Gram determinant condition”. Rigorously in mathematics it must be an if-and-only-if or sufficient and necessary condition for linear independency. However the Gram determinant condition is only a condition, not a definition or a theorem. Linear dependency is determined by two ‘only if’ conditions, cf. Ch. 4 in Ref. [15]. We can say that linear independency is still an *open problem* in mathematics. For n -linearly-independent vectors, the non-vanishing of the Gram determinant is definitely not equivalent to the existence of n -mutually-perpendicular vectors, which constitute an orthogonal basis in the linear vector space. The mathematical linear independency is questioned by physical periodicity-split rule, (rule 2) below, cf. below (47a).

Many points referred in this paper can be compared with the review article of Ando, Fowler and Stern [23] for 2D electron systems. We quote some derivations from the text of the same author [15] which give a consistent results in deductions. The usual geometry of systems here is as follows: in parallel to the interface, we have the primitive translational vectors: **a** and **b**. For the third direction, it is usual to have a **C**-axis as shown in Fig. 3 instead of **c** which is an edge of the unit-cell for the standard fcc structure in Fig. 15 in Ch. 1 of Kittel's ISSP [7]. It is generally the case that

$$\mathbf{a} \cdot \mathbf{c} \neq 0 \quad (13)$$

and

$$\mathbf{b} \cdot \mathbf{c} \neq 0; \quad (14)$$

so that **c** is not used as the third direction to indicate the layer separations. However the original condition from the periodic system is to have the periodic potential

$$V_{\text{periodic}}(\mathbf{r}) = V_{\text{periodic}}(\mathbf{r} + n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}); \text{ for sets of integers } n_i; \quad (15)$$

From the usual theory, essentially applied to the subband theory in semiconductor physics, we

have the kinetic energy expressed in a general form as

$$K^{(1)} = i \frac{\hbar^2}{2} \sum_{ij} \mathbf{X} u_{ij} \frac{\partial^2}{\partial \mathbf{x}_i \partial \mathbf{x}_j} \quad (16)$$

for the system reciprocal effective-mass tensor $[u_{ij}]$ for consideration near the particular conduction-band minimum or valley. In (16), we propose to consider, in a general case, that the lattice system has $a \neq b \neq c$ in the unit cell. However the physical configuration becomes nearly impossible to treat mathematically from (45)–(46) below, when there is a plane-surface introduced for a crystal, such as a metal cap or gate on a semiconductor ‘crystal’. Further it is well-known that many times we cut the crystals at some small angles inclined to the routine (111)-plane, see e.g., [10, 11]. It is noted that this kind of set-up of crystals in papers of this kind is in fact a generalization of the high Miller’s indices discussed above, say for W(750), but sometimes mixed with the impurities such as was mentioned in Mullins’ defect model, cf. Fig. 1. On many occasions, we discuss strains of the surface and mismatch of the interface. We must try to understand solid physics applications to these systems: their relationship between a ‘cut-surface’ and the routine periodic configuration for periodic potentials. This is done in Sec. III below. We shall abandon the usual crystal classifications above, and in some fabrication processes of deposition, say from chemical solutions, etc. This argument, we shall illustrate, by a kind of reduced-fcc lattice as in our consideration in Sec. II below, is for the general cases. Further we change the unit cell to be a realistic one to fit the surface or interface plane, so as to treat Fig. 1(b) as being some structure as in Fig. 3 with a metal cap or gate on the top. Incidentally for high-Miller-indices- or stepped-surfaces without any contaminations or irregular depositions, we have other kinds of special treatments, such as in the stepped surface atoms movements, etc.

But for this reduced-fcc lattice and for the purpose to have a surface parallel to x_1x_2 -plane, as shown in Fig. 3, we choose first a unit cell $\mathbf{a}, \mathbf{b}, \mathbf{c}$ to fulfill the requirement of (15)

$$\begin{aligned} \mathbf{a} &= a\mathbf{e}_1; \quad \mathbf{b} = b\mathbf{e}_2; \quad \text{with } C = ab: \\ \mathbf{c} &= \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{C}: \end{aligned} \quad (17)$$

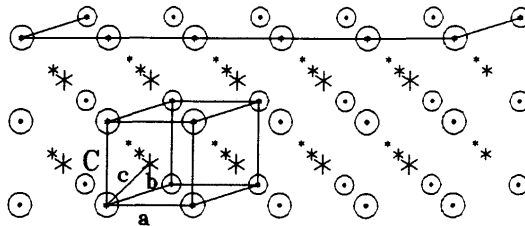


FIG. 3. Reduced-face-centered-cubic structure with substrate-plane on the top. Solid state primitive translation vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are shown together with surface physics translational vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$.

We consider the variables x_i ($i = 1,2$) in the directions of **a** and **b**. But z is in its usual direction of **C** not in the **c**-direction. This is to emphasize the active potential exhibited in the form of

$$V_{\text{act}} = V(z) \quad (18)$$

evaluated according to the variation in the *layer-change* direction (i.e. z -direction). This potential, according to the subband theory does have the periodicity

$$V(z) = V(z + d); \quad (19)$$

for layer separation d . Now we have to reformulate the kinetic energy to replace (16) by

$$K = i \sum_{i,j} \frac{\hbar^2}{2} \mathbf{X} w_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} \quad (20)$$

for system reciprocal effective-mass tensor $\mathbf{f} w_{i,j} \mathbf{g}$ for a coordinate system

$$x_1 = x; \quad x_2 = y; \quad x_3 = z; \quad i.e: \mathbf{f} \mathbf{a}; \mathbf{b}; \mathbf{C} \mathbf{g}\text{-system}; \quad (21)$$

where the x_i are perpendicular to each other.

In Sec. II, we formulate the subband theory from the kinetic energy tensor with a particular relation between tensor elements. In Sec. III, the *compatibility* of the surface equation, as the boundary condition $\mu(z)$ or by the validity of space-coordinate value $z > 0$, with the potential energy $V(z)$, is introduced. We find that for kinetic energy tensor elements: $w_{1,z} \neq 0$ and $w_{2,z} \neq 0$, this compatibility does not exist. The one-dimensional potential energy $V(z)$ is equal to a two-dimensional $V(ax_1^0 + bx_2^0)$ in (49) although $z = ax_1^0(t) + bx_2^0(t)$ for static z and lattice dynamical $x_i^0(t)$. Further investigation is left for future work.

II. Theory

We model a kind of structure for an easier and clearer formulation. It is not a model, as required in the theory and in experimental setups, which is perfectly general. This structural model is defined as a “reduced-fcc”. It is a face-centered-cubic but without the face-lattice-sites at all the parallel xy or **ab**-planes. It is shown in Fig. 3. For the interface or surface, it is shown on the top of Fig. 3. Then we have ordinary rectangular coordinates $x = x_1; y = x_2; z$, and (20) then provides the Schrödinger equation in the form

$$\begin{aligned} [K + V(z)] \psi(x_1; x_2; z) &= i \sum_{i,j=1;2;3} \frac{\hbar^2}{2} \mathbf{X} w_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} \psi + V(z) \psi(x_1; x_2; z) \\ &= E_{3D} \psi(x_1; x_2; z); \end{aligned} \quad (22)$$

to fit our model of a reduced-fcc in Fig. 3 with a square net on the **ab**-surface so that

$$\begin{aligned} w_{1,1} = w_{2,2} &= \frac{1}{m_a}; \quad w_{i,j} = w_{j,i} \neq 0; \quad \text{for } i \neq j = 1;2 \text{ and} \\ \text{otherwise } w_{1z} = w_{z1} &\neq 0; \quad w_{2z} = w_{z2} \neq 0; \quad w_{zz} = \frac{1}{m_z}. \end{aligned} \quad (23)$$

Sometimes we argue that we have small angle cut inclined from the **ab**-plane, etc. [10, 11] as described in the Introduction. Thus (22) becomes

$$\begin{aligned} & [K + V(z)]^a \psi_1(x_1; x_2; z) \\ & = \left[-\frac{\hbar^2}{2m^a} \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) - \frac{\hbar^2}{2} \sum_{i=1,2} w_{i;z} \frac{\partial^2}{\partial x_i \partial z} - \frac{\hbar^2}{2m_z} \frac{\partial^2}{\partial z^2} + V(z) \right] \psi_1(x_1; x_2; z) \end{aligned} \quad (24)$$

$$= E_{3D}^a \psi_1(x_1; x_2; z);$$

When we use a statistical model, we use E_{3D} as the one to be used in (3). We need to have a 3D Fermi energy $E_F^{(3D)}$ from E_{3D} . Sometimes the intuitive wave function is put as

$$\psi_1(x_1; x_2; z) = \psi^3(z) e^{ik_1 x_1 + ik_2 x_2} \quad (25)$$

by the ‘separable of variables’ method, conventionally called ‘separable’ instead of ‘separation’ for some reasons. A treatment of this kind is particularly suitable for all kinds of two dimensional electron gas systems (2DEG) [23]. We obtain an equation for $\psi^3(z)$,

$$\begin{aligned} & \left[-\frac{\hbar^2}{2m^a} (k_1^2 + k_2^2) - \hbar^2 (w_{x_1;z} k_1 + w_{x_2;z} k_2) \frac{\partial}{\partial z} - \frac{\hbar^2}{2m_z} \frac{\partial^2}{\partial z^2} + V(z) \right] \psi^3(z) \\ & = E_{3D} \psi^3(z) \end{aligned} \quad (25a)$$

for the function $\psi^3(z)$, which thus obeys a one-dimensional differential equation in a sense. The Fermi energy required in (25a) is still the 3D $E_F^{(3D)}$, the same one as in (3). This one-dimensional Schrödinger equation must be reconciled with its complete one-dimensional behaviour by the following processes: First

$$\begin{aligned} & \left[-\frac{\hbar^2}{2m_z} \frac{\partial^2}{\partial z^2} + \hbar^2 (w_{1;z} k_1 + w_{2;z} k_2) \frac{\partial}{\partial z} + V(z) \right] \psi^3(z) \\ & = E_{3D} - \frac{\hbar^2}{2m^a} (k_1^2 + k_2^2) \psi^3(z) \\ & \quad = E_{zn}^a \psi^3(z); \end{aligned} \quad (26)$$

after quantization to have 1D energy eigenvalues E_{zn}^a . For a statistical model we referred to (6) for the DOS. We need to define $E_{F1}^{(1D)}$ from this energy. Sometimes we refer to $\hbar^2(k_1^2 + k_2^2) = (2m^a)$ or even the whole term in the second line of (26) as the subband energy. It is possible to have the matrix coefficients $w_{i;z} = w_{i;z}(x; y)$ appearing somehow in (26) after reduction from (24). For (50)–(51) below, this possibility does exist. It *must be this case* for the cut-surface at a few degrees with respect to the conventional crystal basal plane, as given in Refs. [10, 11] introduced in the Introduction above. If we consider a way to indicate some pseudo-crystal-momentum-in-z-direction

$$k_z^{(2D)} \sim [w_{1;z} k_1 + w_{2;z} k_2] m_z \gg \hbar \frac{2/4}{L} (n_1 + n_2) m_z; \text{ for } w_{1;z} = w_{2;z} = \hbar \quad (27)$$

from (23), we have used this quantity for the second term in the first line in (26). This shows that E_{zn}^a measures the $k_1; k_2$ -coupling from other dimensions, viz., the x and y dimensions for a z -dependent equation (26). Thus it is not simply 1D. The role of $k_z^{(2D)}$ is to breakthrough from the subbands in 2D into the third dimension. Similar to $k \cdot p$ in current solid state physics, this $k_z^{(2D)}$ denotes some “structural effect” indicated by crystal momentum $\mathbf{k}$. This makes us completely confused whether the subband theory is 1D (in the final eigen-equation), or 2D (for its own energy value), or 3D (after the breakthrough in (26) with all 3D quantities included). This shows a failure-point in dimensionalities physically for the ‘separable of variables’ methods which are pure mathematics in $x; y; z$, while the system is different for physics, say $k_1; k_2$ in $k_z^{(2D)}$ in (27). A physical counterpart of this point, as given in pp. 234-235 in [2], is for the Fermi energy in transports. In semiconductors, the driving-force of movements is derived from Fermi energy. Dynamically, the transport-movement is directional and thus 1D. This induces that the used Fermi energy should be 1D. For (24) to apply to the complete picture of the ‘separable of variables’, we must have for (25)

$$\begin{aligned} E_{3D} + \frac{1}{3(z)} \frac{\partial^2}{2m_z \partial z^2} + \frac{i \partial^2}{m_z} k_z^{(2D)} \frac{\partial}{\partial z} + V(z) \psi^3(z) \\ = \frac{1}{e^{ik_1 x_1 + ik_2 x_2}} \frac{\partial^2}{2m^a} (k_1^2 + k_2^2) e^{ik_1 x_1 + ik_2 x_2} \\ = E_{3D} + E_{zn}^a: \end{aligned} \quad (24a)$$

We have separated the coordinate variable z positionally in contrast to $x_1; x_2$ in a certain way: in the first two lines of (24a), z appeared only on the first line while $x_1; x_2$ appeared only on the second line. Further, because of the equality, we have that they are independent of any $x_i; z$, variation from point to point, viz., constants. Thus we have a constant $E_{3D} + E_{zn}^a$ after the final equality which is exactly the subband energy. In physics, the physical properties indicated by constants, or constant dynamical variables, such as $k_z^{(2D)}$ including $k_1; k_2$, are still included on the first line of (24a). That is why we have (26) which is not simply one-dimensional because we fail in separation of the dimensions x_i $i = 1; 2$, in contrast to z . The connection between them is through *physical* reasons. It is obvious here that this way of treatment has generated some inclusion of interpretation in the new dimension.

For the quantum momentum in the z -direction $p_z = i \hbar \partial / \partial z$, we have (26) become

$$i \hbar \frac{\partial^2}{2m_z \partial z^2} + \frac{\hbar^2 k_z^{(2D)} p_z}{m_z} + V(z) \psi^3(z) = E_{zn}^a \psi^3(z): \quad (28)$$

The difference between (26) and (28) for E_{zn}^a , is that we consider in (28) the $\hbar^2 k_z^{(2D)} p_z / m_z$ -term to have the form of a $k \cdot p$ -perturbation in conventional solid state physics. This becomes general for perfect crystals of all kinds, when it is formulated from 3D reduced to 1D by (25). For instance, it is well-known that a $k \cdot p$ -perturbation changes the effective mass at the conduction band edge incorporated with the valence band states for 3D wave functions, (not the envelope $\psi^3(z)$), coupling two bands, as much current literature indicates. Here, there may be two subbands [21].

The peculiarity here is that $k_z^{(2D)}$ may not be purely one-dimensional or may not be the routine crystal momentum: $k_z = 2\pi n_z/L_z$ in the solution of $u_k(r)$ in the usual Bloch function (not the $k_z^{(2D)}$ above). It may couple properties from the z -direction into the xy -directions. In addition to this $k_z p_z$, we moreover have the simple $k_z^{(2D)} p_z$ -interaction in this subband theory. It is this term that makes the mobility of intrinsic semiconductors in Ref. [7] appear. However the difference of $k_z^{(2D)}$ in (27) from the k_z in 1D Bloch electron theory shown in eqn. (12), makes the equation here predict some peculiar mobilities. The effective mass of this case is supposed to be detectable by the cyclotron resonance frequency, and other experimental evidence.

Since our model is for a ‘reduced-fcc’, in parallel to the current theory [23], the wave function $\psi^3(z)$ in their consideration, is changed to an envelope function $\psi'(z)$ subjected to some simplified structural conditions by

$$\psi^3(z) = \psi'(z) \exp \left[i \frac{\hbar}{\hbar} k_z^{(2D)} \phi z \right] \gg \psi'(z) e^{i m_z \omega (2\pi/L)(n_1 + n_2)z}; \quad (29)$$

for $n_1 + n_2 \sim n_z = \text{integers}$. Here the effective thickness in the z -direction is equal to

$$L_z = \frac{L}{m_z \omega}; \quad (29a)$$

for L along the $x; y$ -directions! This is regardless of whether the structure is a delta-doped or semi-infinite material. This *reveals rather a new dimension* than the standard third direction. In the author’s intuition, the situation here is like an enveloping ‘surface charge $q_{\pm}(z \mid z_0)$ ’, represented by the wave function $\exp[i 2\pi n_z z/L_z]$, rather than a factor in new dimension, wrapping over a volume which is characterized by ψ' , described above in dimension theory ideas. Because the wave functions here indicate the behaviour of electrons, therefore the pictorial new idea here is exactly that described below (9) in the Introduction for 2D-surface charges in 3D-space. The whole entity is described by ψ^3 . Therefore $\psi'(z)$ should be the “*enveloped* wave function”. Whereas L_z is something like the value of $q_{\pm}(z \mid z_0)$ at $z = z_0$. This was emphasized in the Introduction regarding the dimensionality conception in (12)–(12e). It is not a property along the z -axis alone physically.

The probability distribution from (29) is

$$|\psi^3(z)|^2 = |\psi'(z)|^2 \exp \left[i \frac{\hbar}{\hbar} k_z^{(2D)} \phi z \right] \frac{\hbar}{\hbar}; \quad (29b)$$

The second factor with L_z actually may be controlled from sizes in the $(x; y)$ -directions and indicates the pseudo-thickness in the z -direction by Bloch theory for *finite* crystal influencing the (pseudo-surface) charge density contributed from the wave function probability, i.e. the $|\exp[i k_z^{(2D)} \phi z]|^2$ -part in its own (new) dimension. However from the electric potential calculation in electrodynamics, this new dimensional ‘surface charge’ does still contribute a potential electrically similar to the exact surface charges. The application is also applicable to semiconductor devices, such as the MOSFET. We replace the semiconductor oxide layer by polarizable materials, we are able to form a ‘new dimension’ charge layer described above with a certain prescribed thickness, to produce a (signal) “gate-charges” from some metal gate to replace the (signal) electric field in this field-effect transistor. Theoretically, the above interpretation of the wave function together with the 2D gate-charges, if the experiments show the existences correctly,

makes a judgment in favor of having a new dimension theory. A further development can be to investigate the ‘homogeneity-dimensions’ given on pp. 30, 49 in Ref. [2] for quantum physics.

Motivation for introducing a complex k : It is noted that we have the one-dimensional Bloch-type wave function form for $\psi(z)$ with $k_z^{(2D)}$ in (27) as our crystal momentum. This is the *second peculiar* crystal momentum which may breakthrough into other dimensionalities, apart from the *first one* where the complex nature in (11) indicates the mean free path. Since (28) has a k Φ -perturbation form, the mobility is related to

$$\frac{d}{dz} \frac{d}{dz} \psi(z) :$$

Here $V(z)$ is a periodic potential energy in the “z-direction” characterized in (19), with the separation between layers d , in the z-direction, not the c-direction as is usually provided by the Bloch theory.

Here we modify the ordinary energy band theory for the purpose of terms applicable to apply to systems *with surfaces or interfaces* having a 2D nature, as in a (2+1)-dimensional system. The final Schrödinger equation is still one-dimensional in the form of (28) with eigenfunctions $\psi_n(z)$ and eigenvalues $E_n^{(sl)}$

$$\begin{aligned} i \frac{\hbar^2}{2m_z} \frac{d^2}{dz^2} \psi_n(z) + V(z) \psi_n(z) &= H_z(z; p_z) \psi_n(z) \\ &= E_{zn}^{(a)} i \frac{\hbar^2}{2m_z} k_z^{(2D)2} \psi_n(z) \\ &= E_n^{(sl)} \psi_n(z) \end{aligned} \quad (30)$$

For a statistical model, we introduce $E_{F3}^{(1D)}$ in (8) for $E_n^{(sl)}$ -statistics. From a study of (30) we have two points to discuss:

(I) for semi-infinite materials, $V(z) = V(z)\mu(z)$; and for delta doped materials, $V(z) \gg V(r) \pm (z \mp z_0)$, the conditions of the Bloch electron theory of periodic systems in the z-direction are not satisfied. From (30), if the solution ψ_n is localized, i.e., in (29), $\psi(z) \gg$ tight-binding or a linear combination in Gaussian distributions, or LCAO as usual in solid state physics, we have no Bloch crystal momentum (BCM). From the appearance of (29), the pseudo-BCM part in $\psi(z)$ is controlled by the x; y-direction behaviour in $k_z^{(2D)}$. It is a new kind of behaviour, contrary to the Bloch theory for periodic structures in 1D in solid state physics. For instance, we have an $\psi(z)$ to replace the $u_k(r)$ in the Bloch function with $u_k(r) = u_k(r + R)$ for a lattice point separation R . There will be no actual lattice point along the z-direction with layer-separation d , such as in Fig. 2, for the same x; y-coordinates, no lattice point at a distance $z = d$ from the lattice point at $z = 0$. There is no $k\Phi$ -term for a k totally determined by the z-direction property in (30). This is different from the pure 1D Bloch theory where we have Bloch function results for $\psi(z)$ since we have delta-doped layer or semi-infinite medium, although the periodicity $V(z) = V(z + d)$ still holds. Here we introduce a complex k . However the physical picture of ψ_n is the same one as given in the transformation of Stern and Howard [24]. Because of the real physical configuration

given above, we need to reconsider the mobility or there are no mobilities for $\psi_n(z)$ rigorously, with different dimensionalities instead. If we try to put in the mean free path, we need to choose

$$k_z = k_{zR} + ik_{zI} = \text{complex};$$

like the one described in (11) above. Here we have incorporated a surface or interface or 2D plane, but we do not have to be very clear about the physics behaviour. The physical picture is still the one given in (11). This implies (29)

$$\psi^3(z) = \psi'(z) e^{i(k_{zR} + ik_{zI})z} = \psi'(z) e^{i|z|z=2}, e^{i k_{zR}z} \quad (29b)$$

for the mean free path λ_z in the z-direction no matter what the structural form of the material and whether ψ' is localized or not. Here we have reconciled the sense of Kohn's Wannier function for a complex k discussion as mentioned below eqn. (9) in the Introduction. The last equation expresses a kind of effective thickness in the z-direction, with a similar restriction as derived from (29) disregarding the actual physical thickness in the z-direction. Here we have the second interpretation for λ_z , emphasized in a statistical sense.

(II) From (28), (24a) and (30), we can see that

$$E_n^{(sl)} = E_{zn}^a - \frac{\hbar^2}{2m_z} k_z^{(2D)2} = \text{subband ladder energy}; \quad (30a)$$

which is the realistic 1D energy of 1D energy quantum packet. The coupling of k_1, k_2 in $k_z^{(2D)}$ in another 1D energy E_{zn}^a is subtracted. Here E_{zn}^a is of 3D energy quantum packet. This also concludes our discussion of $E_{Fi}^{(nD)}$, $n = 1, 2, 3$ in (9) in the Introduction. There we have extended the fact for $E_{Fi}^{(nD)}$, etc. to be initiated (a) by a complex k in the Introduction; (b) to some special mobilities; or (c) by introducing new dimension(s) directly.

From (26) and (30), the 3D energy packet

$$\begin{aligned} E_{3D}(n; k_1; k_2) &= E_{zn}^a + \frac{\hbar^2}{2m^a} [k_1^2 + k_2^2] \\ &= E_n^{(sl)} + \frac{\hbar^2}{2} \left[\frac{1}{m^a} + w_{1,z}^2 m_z \right] k_1^2 \\ &\quad + 2(w_{1,z} w_{2,z} m_z) k_1 k_2 + \frac{\hbar^2}{2} \left[\frac{1}{m^a} + w_{2,z}^2 m_z \right] k_2^2 : \end{aligned} \quad (31)$$

It is noted that E_{zn}^a is the "z-direction" energy with the mobility calculated from the three-dimensional Bloch energy E_{3D} band theory. It includes $k_z^{(2D)}$ itself. When we apply it to semiconductors to consider the intrinsic semiconductors at 0 K, we have the electrons filled up to the top of the energies $E_n^{(sl)}$, i.e. $E_{F3}^{(1D)}$. This is the way we calculate the hole density in a heterostructure [15]. This $E_{F3}^{(1D)}$ is exactly the top energy E_v of the valence band from the definition of intrinsic semiconductor when the conduction and valence bands are considered along one particular direction in $\mathbf{k}$ -space, or in the perpendicular direction to a surface compatibly. When we assign the Fermi level $E_F^{(3D)}$ from the three-dimensional theory of solid state physics, from

E_{3D} , the components of the corresponding Fermi levels in the z -direction must be assigned from E_{zn}^a from (26), (i.e. $E_{F1}^{(1D)} \neq E_{F3}^{(1D)}$ above). However

$$\begin{aligned} E_F^{(3D)} &= E_{F3}^{(1D)} + \frac{\hbar^2}{2m^a}(k_1^2 + k_2^2) + \frac{\hbar^2}{2m_z}k_z^{(2D)2} = \frac{\hbar^2 k_1^2}{2m^a} + \frac{\hbar^2 k_2^2}{2m^a} + E_{zn}^a(\max); \\ E_{zn}^a(\max) &= E_{F3}^{(1D)} + \frac{\hbar^2}{2m_z}k_z^{(2D)2} = E_v + \frac{\hbar^2}{2m_z}k_z^{(2D)2}. \end{aligned} \quad (32)$$

This is why we have Fermi levels with values in the energy gap between the conduction and valence band top $E_v = E_{F3}^{(1D)}$ from (32), not down to $E_{F1}^{(1D)}$ or $E_n^{(sl)}$.

Following Stem *et al.*, since E_{zn}^a and $E_n^{(sl)}$ may be negative, in order to compare which one of E_{zn}^a and $E_n^{(sl)}$ has a lower value of energy according to the energy level assignment on a surface, we investigate and develop the usual calculated energy band diagrams:

(A) It is most common to assign the zeroes of the energy levels at the Fermi energy which is unique. The exceptions of this uniqueness are for the so-called “non-thermal equilibrium” in semiconductors [14] and pp. 73 in [16], such as (Ga,Al)As quantum wells. There we can have the so-called ‘quasi-Fermi levels’. We can even have two or more quasi-Fermi levels.

(B) The second way is to assign the zero level at the free-particle-zeroes to determine the space charge layer by the same author [1]. This is particularly useful for the Fermi-Dirac statistics cases. The introduction of negative values of energies in the statistics of this kind has resolved into ‘for energy domain $j = 1$ to $+1$ ’ for finite temperatures, e.g. in (Ga,Al)AS. This is evident for the paramagnetic cases. However we move on to discuss systems of “free-particles” [25]. Many cases give the bottom of the parabolic band of energy as zero. This includes the ‘conduction band zeroes’ at some Fermi energy $= 1$, for Fermi-Dirac statistics for electrons,

$$f^{FD}(E) = \frac{1}{1 + e^{-(E-1)}};$$

where unavoidably $1 = E_F^{(3D)}$ in many current textbooks; or the ‘valence band zeroes’ for holes statistics in semiconductors,

$$f_h(E) = 1 - f^{FD}(E);$$

cf. Ch. 4, pp. 195–207 in [14]. Here the zeroes are all three-dimensional Fermi energies for quantum well layers! However these zeroes are in the energy band gap with no electrons occupied when the interfaces are concerned, say at the j -point. Further this assignment is not good for electron density calculations in Thomas-Fermi model. Incidentally, if there are materials or heterostructures in which the Fermi energy is not in the gap for the statistics, e.g., we may apply the $E_{F3}^{(1D)}$ as our Fermi energy for the Fermi-Dirac statistics, then we can have much more carrier density for such a kind of “1D statistical heterostructures”, say holes, that we are looking for. The electron, or other carrier densities will be drastically changed.

(C) We assign the zero at the potential-energy-zero. For instance, in (30), the energy-zero of $E_n^{(sl)}$ coincides with the zero of $V(z)$. Actually it is the kinetic energy zero in **(B)** above. However there are dimensionality problems [15]: e.g. in (22), E_{3D} -zero is at $V(z)$ -zero for 3D.

But E_{zn}^a in (26), and $E_n^{(sl)}$ in (30), respectively, have zeroes different from that of $V(z)$ for 1D when any of $k_1, k_2 \neq 0$ in the other two dimensions, as shown in (31) for E_{3D} , E_{zn}^a , and $E_n^{(sl)}$, if the kinetic part is not zero. Further, if the kinetic part is not zero, according to Ref. [26] for energy-levelling-matching, we may have energy-non-conservation problems. This is shown explicitly in (34) below. Another trouble is that for the coulombic potential $\propto 1/r$ with zero at $r = \infty$. For solid calculations there is no such zero-at-infinity points.

(D) Other kinds of rather arbitrary assignments: e.g., in heterostructures we may have the zeroes at the middle or at some point inside the band-gap between the conduction band and the valence band.

Here is a criticism for judging the property of these choices. In (35) and (36) below, we have to decide which one of E_{3D} , E_{zn}^a , and $E_n^{(sl)}$ has the largest magnitude when they have the same zero reference level. These energies are determined by (26) and (30). On the contrary, from (31), if we choose the origin of E_{3D} at $E_F^{(3D)}$, and of $E_n^{(sl)}$ at $E_{F3}^{(1D)}$

$$E_{3D} - E_F^{(3D)} = E_n^{(sl)} - E_F^{(3D)} + \frac{\hbar^2}{2m_z} k_z^{(2D)2} + \frac{\hbar^2}{2m} (k_1^2 + k_2^2) \quad (33)$$

$$\neq E_n^{(sl)} - E_{F3}^{(1D)} + \frac{\hbar^2}{2m_z} k_z^{(2D)2} + \frac{\hbar^2}{2m} (k_1^2 + k_2^2):$$

Here

$$E_{3D} - E_F^{(3D)} \neq E_n^{(sl)} - E_{F3}^{(1D)}; \quad (34)$$

because of the different reference levels on both sides. An energy-non-conservation result is given in Ref. [26]. An application of the change of energy absolute values of this kind also appeared in Ref. [26]. This is also correct for both positive or negative E_{zn}^a . However for the cases: (a) $E_{zn}^a < 0$ or (b) both of $E_{3D} < 0$ and $E_{zn}^a < 0$, we may have the opposite inequality as in (36) in comparison with (35). These are entirely dependent on the proper zero of the Schrödinger equations. Similar comparison can be made for $E_n^{(sl)}$. When we treat the subband problem similar to the parabolic band cases, i.e. all energies are positive in (31), we can have

$$E_{3D} > E_{zn}^a > E_n^{(sl)}: \quad (35)$$

On the other hand, when we consider (24), (26), and (30) in practical calculation cases: i.e. from the tight-binding or LCAO cases. All the energies are negative in (31), as

$$|E_{3D}| < |E_{zn}^a| < |E_n^{(sl)}|: \quad (36)$$

A structural consideration with surface or interfaces is given in next section.

III. Why subband theory is not the 2D Bloch theory of electrons

From purely mathematical methods, we wonder if we can diagonalize (20) to the so-called “principal values”, i.e. for the kinetic energy in our set-up for the surface-cut described between

(18) and (22), i.e. in addition to (23) and (27) for our reduced-fcc in Fig. 3,

$$\begin{aligned}
 w_{1z} &= w_{z1} = w_{2z} = w_{z2} = \dot{w}; \\
 K &= i \frac{\hbar^2}{2} (\mathcal{Q})^T (K) (\mathcal{Q}); \\
 (\mathcal{Q}) &= \begin{pmatrix} 0 & 1 \\ \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_2} \\ \frac{\partial}{\partial z} & 0 \end{pmatrix}; \quad (\mathcal{Q})^T = \text{transpose of } (\mathcal{Q}); \\
 (K) &= \begin{pmatrix} 0 & 1 \\ \frac{1}{m^a} & 0 \\ 0 & \frac{1}{m^a} \end{pmatrix} \begin{pmatrix} 1 \\ \dot{w} & \dot{w} & \frac{1}{m_z} \end{pmatrix}; \\
 K &= i \frac{\hbar^2}{2} (\mathcal{Q})^T S S^{-1} (K) S S^{-1} (\mathcal{Q}); \\
 S^{-1} (K) S &= \begin{pmatrix} 0 & 1 \\ a_1 & 0 \\ 0 & a_2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ a_3 \end{pmatrix}; \quad A = \text{diagonal};
 \end{aligned} \tag{37}$$

by standard mathematical methods. The similarity transformation matrix S is to be found by the secular equation of (K) , viz.,

$$j(K) = a \det j = 0; \quad S = (S_1 \ S_2 \ S_3); \tag{38}$$

We find the three eigenvalues of a ,

$$\begin{aligned}
 a_1 &= a_+; \quad a_2 = a_i; \quad a_3 = \frac{1}{m^a}; \\
 a_s &= \frac{1}{2} \left(\frac{1}{m_z} + \frac{1}{m^a} \right) \pm \frac{1}{2} \sqrt{\left(\frac{1}{m_z} - \frac{1}{m^a} \right)^2 + 8\dot{w}^2};
 \end{aligned} \tag{39}$$

and their eigenvectors

$$\begin{aligned}
 S_1 &= C_+ \begin{pmatrix} 0 & 1 \\ \frac{1}{A_+} & 1 \end{pmatrix}; \quad S_2 = C_i \begin{pmatrix} 0 & 1 \\ \frac{1}{A_i} & 1 \end{pmatrix}; \quad S_3 = \begin{pmatrix} 0 & 1 \\ \frac{1}{2} & \frac{1}{2} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ \dot{w} \\ \dot{w} \end{pmatrix}; \\
 A_s &= 2\dot{w} \frac{1}{m_z} \pm a_s; \\
 C_s &= \frac{1}{2 + A_s^2};
 \end{aligned} \tag{40}$$

We can have orthonormality of the vectors S_1, S_2, S_3 , since (K) is symmetric,

$$\begin{aligned} S_i^T S_i &= 1; \quad i = 1; 2; 3; \quad \text{or} \quad C_{\xi}^2 (2 + A_{\xi}^2) = 1; \\ S_i^T S_{j \neq i} &= 0; \quad \text{or} \quad 2 + A_+ A_i = 0; \quad \text{etc:} \end{aligned} \quad (41)$$

From the mathematics of symmetric matrices, we have that

$$S^{i-1} = S^T = \begin{pmatrix} 0 & 1 & 0 \\ S_1^T & S_2^T & S_3^T \end{pmatrix} \mathbf{A} = \begin{pmatrix} 0 & 1 & 0 \\ C_+ & C_+ & C_+ A_+ \\ C_i & C_i & C_i A_i \end{pmatrix} \begin{pmatrix} 1 \\ A_+ \\ A_i \end{pmatrix} \quad (42)$$

In (37), the matrix K includes

$$S^{i-1}(\mathbf{A}) = \begin{pmatrix} 0 & 1 & 0 \\ \frac{\partial}{\partial x_1^0} & \frac{\partial}{\partial x_2^0} & \frac{\partial}{\partial x_3^0} \end{pmatrix} \mathbf{A} = \begin{pmatrix} 0 & 1 & 0 \\ C_+ \frac{\partial}{\partial x_1} + C_+ \frac{\partial}{\partial x_2} + C_+ A_+ \frac{\partial}{\partial z} \\ C_i \frac{\partial}{\partial x_1} + C_i \frac{\partial}{\partial x_2} + C_i A_i \frac{\partial}{\partial z} \end{pmatrix} \begin{pmatrix} 1 \\ A_+ \\ A_i \end{pmatrix} \quad \text{etc:} \quad (43)$$

If we want (K) to be diagonalized, we must have the transformation

$$\begin{pmatrix} 0 & 1 & 0 \\ x_1^0 & x_2^0 & x_3^0 \end{pmatrix} \mathbf{A} = S^{i-1} \begin{pmatrix} 0 & 1 & 0 \\ x_1 & x_2 & z \end{pmatrix} \mathbf{A} = \begin{pmatrix} 0 & 1 & 0 \\ C_+ x_1 + C_+ x_2 + C_+ A_+ z \\ C_i x_1 + C_i x_2 + C_i A_i z \end{pmatrix} \begin{pmatrix} 1 \\ A_+ \\ A_i \end{pmatrix} \quad (44)$$

This transformation makes the kinetic energy in (37), in ‘principal values’, to become

$$K = \sum_{i=1}^3 \frac{1}{2} \mathbf{X} \mathbf{a}_i \frac{\partial^2}{\partial x_i^2} \quad (45)$$

It is our conception that the form of the kinetic energy in (35) is the ideal one for our ‘3D perfect crystal’ in which we can have the periodic condition on the potential energy

$$\psi(x_1^0; x_2^0; x_3^0) = \psi(x_1^0 + d_1; x_2^0 + d_2; x_3^0 + d_3) \quad (45a)$$

for periodicities d_i . But it also makes the equation of the surface or interface plane,

$$z = 0; \quad (46)$$

to become

$$z = \begin{pmatrix} 0 & 0 & 1 \\ S & S & S \end{pmatrix} \begin{pmatrix} x_1^0 \\ x_2^0 \\ x_3^0 \end{pmatrix} \mathbf{A} \mathbf{A} = C_+ A_+ x_1^0 + C_i A_i x_2^0 = 0; \quad (47)$$

which is no longer the plane

$$x_3^0 = 0; \quad (48)$$

For (46), $z = 0$ is one equation in 3D-space together with one compatible periodicity condition (19); it represents a 2D-surface. Furthermore for most physics cases, we have considered that the first equality $z = 0$ of (47) is static, without any time-dependence. Whereas the second equality

$$C + A + x_1^0(t) + C_i A_i x_2^0(t) = 0; \quad (47a)$$

should be “stationary”, i.e. it is time-dependent just like the $x; p$ in the Hamiltonian $H(x; p)$. Either Newton’s equation or Schrödinger equation shows that $x = x(t) \gg x_0 + v_0 t + at^2/2$ say, or $\langle x \rangle =$ time-varying in Heisenberg picture, etc. Therefore the $x_i^0(t)$ here are dynamical variables, this is particularly clear from Fig. 3, $x_i^0(t)$ are the coordinate (sites) of lattice points! It is a necessary consideration that $x_i^0(t)$ is needed to consider the degrees of freedom in motions, particularly in kinetics or lattice dynamics.

As usual, one equation in a 3D space represents a 2-dimensional surface. However from the physics and the mathematics for dynamical variables in (47a), this 2D surface is not necessarily 2D. For example, (46) $z = 0$, a constant always, so that we can have $x; y$ varying arbitrary on the $z = 0$ plane. We have left two degrees of freedom as free variables. After transforming to (47a), for x_1^0, x_2^0 , we can have two choices: (a) 2D, because there is only one equation, always like static, i.e. (46) in 3D space; or

(b) two variables or degrees of freedom ‘used’ so that we can have only one degree of freedom “totally free”. Nevertheless, for the two degrees of freedom used in (b) here, we must judge whether it is:

(b-1) $x_1^0; x_2^0$ determined only by one linear independency in total. However there is no direct relationship to determine the dimensionality from the linear independency. There may be other non-linear independencies in some other theories (such as our periodicity-split rule in (Rule 2) below), which may lead to making another decision as to the dimensionalities of the spaces.

(b-2) $x_1^0; x_2^0$ used to determine *two* linearly independent degrees of freedom. From (49)–(49c), if our judgement is to choose the ‘periodicity-split’ rule as a decision for linear independency, so that $x_1^0; x_2^0$ are two linearly independent variables in two directions. This leads us to have two degrees of freedom for the determination of one equation (47a). Totally we have that $x_1^0; x_2^0$ are two independent degrees of freedom plus a two-dimensional plane $z=0$ in (46). By an intuitive judgement, we can have four dimensions in total. At the least, we can judge the correctness of a discrete primitive translational space for the four degrees of freedom.

The linear independency is described in the Introduction as being determined by the Gram determinant and is not a necessary condition; we can have non-linear independencies! In fact in Fig. 3, we have x_1^0 and x_2^0 , two independent directions provided for a periodicity condition. This configuration is different from current mathematical thoughts: 3D-space is ‘spanned’ by three perpendicular axes, or a 2D-plane plus a z -direction perpendicular to the plane. The investigations cease usually at the point that the x_1^0 and x_2^0 directions are not (both) perpendicular to the 2D surface (cut-surface). In a discrete lattice primitive translation space, do they form a 4D space? They are related to the homogeneity-dimensions somehow.

As to the dimensionality investigation, in a Bravais lattice, we can pick the line of the periodic condition along the coordinate axis, explicitly, if there is a condition

$$V(x_i^0) = V(x_i^0 + a_i); \text{ for various } i$$

then we can assign x_i^0 as an axis. From the existence of axes in this way, by the definition above, we can have one set of basis-vectors corresponding to the above assigned axes. This is what we

call the “basis-choice” in periodic crystals. This way of description of crystals, as it usually is, does not fulfill the above restriction when there is a cut-surface incorporated. That is, because the cut-surface is not always the coordinate plane by the above definition, x_i^0 ; $i = 1; 2$ do not have the condition: “perpendicular to the cut-surface”.

Perfect 3D crystal description: Here we consider that the framework is a 3D perfect crystal defined by (45) and (45a) as *the 3D crystal space*. To imagine (46) we have a metal cap or gate expressed by $z=0$ in $fx_1; x_2; zg$ -coordinates. To have a periodic potential energy we have

$$V(z) = V(z + d): \quad (46a)$$

This is equivalent to a plane surface together with an ‘inward normal’ being defined, similar to the case of surface area of Gauss’s divergence theorem. Now transformed to fx_i^0g -coordinates, for (47) we imagine a 2D metal cap, but we can *not* have the periodicity for 1D potential energy as general as

$$V(x_1^0; x_2^0) = V(x_1^0 + d_1; x_2^0 + d_2) \quad (47b)$$

as a static potential, over all directions, included the x_1^0 and x_2^0 directions. On the other hand we can have this potential as a 2D one as described above by

$$V(z) \rightarrow V(x_1^0; x_2^0) \stackrel{(47b)}{=} V^{(2D)}(C + A + x_1^0 + C_i A_i x_2^0) \quad (47c)$$

which is the same one as $V(z)$ in (46a) with z replaced by the dynamical x_i^0 from (47). For both the static (46) and dynamical (47c) simultaneously in a theory with properties of all kinds, such as periodicity, etc., they all satisfy (46a). On the other hand, the periodicity conditions indicated in (47b) for the potential energy are, after an intensive study, equivalent to ‘two (normal) directions’ being defined. Or two specific directions, x_1^0 - and x_2^0 -directions, with the indicated periodicities given in (47b). As these are ‘two normals’, they are not parallel to each other. It is usually impossible to have such ‘two directions’ being along two periodicity-directions, for one single surface-plane. They are only ‘two peculiar directions’ not-perpendicular-for-normal-definition and they *reveal some new dimensions for a picture of 3D of the xy-plane plus z-direction*. For ‘such simultaneously two directions’, the impossibility for a single dimension is seen. Intuitively, by equation-demonstration, we have for z on the one hand and $C + A + x_1^0(t) + C_i A_i x_2^0(t)$ on the other in (47), as follows

$$z + Nd = C + A + (x_1^0 + n_1 d_1) + C_i A_i (x_2^0 + n_2 d_2) \quad (47d)$$

for the set of three ‘least’ integers $N; n_1; n_2$ discussed below. The appearance of (47d) is required for the periodicity in (46a) to become (47c) after the transformation, i.e.

$$\begin{aligned} V(z) &= V(z + Nd) \\ &\stackrel{(47c)}{=} V^{(2D)}(C + A + (x_1^0 + n_1 d_1) + C_i A_i (x_2^0 + n_2 d_2)) \stackrel{\text{transf}}{=} \\ &V^{(2D)}(x_1^0; x_2^0) \stackrel{(47c)}{=} V^{(2D)}(C + A + (x_1^0 + n_1 d_1) + C_i A_i (x_2^0 + n_2 d_2)) \end{aligned} \quad (49)$$

for a set of integers $fN; n_1; n_2$ which have no common-factor and are 'least'. These equations are satisfied as set-up formulas for Laue spots in electron diffraction theory. This is shown in the second layer passing through the empty lattice point $(\mathbf{a}/2, \mathbf{b}/2, \mathbf{C}/2)$ in Fig. 3. For an electron diffraction interpretation we need to consider the electron matter waves reflected (or diffracted) from this empty lattice point. (49) is to express that the active potential energy $V_{\text{act}} = V(z)$ is to be an active one in a changeable way: Since the kinetic energy (20) with elements given in (23) is transformed to (45), while the above active potential energy changes its functional behaviour together with the dimensionality to $V_{\text{act}} = V^{(2D)}(x_1^0; x_2^0)$. Here we can have several rules to be obeyed:

(1) Sum rule of the increments: (47) implies

$$\Phi z = C_+ A_+ \Phi x_1^0(t) + C_- A_- \Phi x_2^0(t); \quad (\text{Rule 1})$$

It is obvious that there are only two cases: (1-1) *Mathematical surfaces*, as shown in Fig. 2, are those which have one of $\Phi x_i^0 = 0$ so that $\Phi z \neq \Phi x_{i0}^0$; and (1-2) we do not have (1-1) so that Φz must be sum of two Φx_i^0 . They are coupled. We have a variation along the *cut-surface*. For the case (1-2), we have the following: The right hand side is 2D (two variants from $(\Phi x_1^0$ and $\Phi x_2^0)$ while the left hand side is 1D (one variant or one degree of freedom (Φz)).

(2) In the above, (1), we have discussed the equation and the boundary condition of the surface where z is a static variable. In this, (2), we discuss the changes of behaviour of the potential energy V_{act} due to the transformation (37). The periodicity-split rule of $V^{(2D)}$ must fit $V(z)$, i.e. all the periodic points must on the same static $z = \text{constant}$ line, as illustrated in (49a) below. Consequences of this change are entirely different in behaviour from the changes of the surface equation. One of the reasons is because there is a physical surface or interface at $z = 0$ in (46) and we need to have the condition $V(z) = V(z + d)$. Inside $V(z)$, z is a dynamical variable.

For instance, as pictured in Fig. 2, the lattice constant of this 2D square-net is assumed to be a . In this example, (47) states

$$\begin{aligned} z &= \frac{1}{2}(x_1^0(t) + x_2^0(t)) = 0; \\ \Phi z &= \frac{1}{2}(\Phi x_1^0(t) + \Phi x_2^0(t)); \end{aligned} \quad (47e)$$

which shows that there are two coupled variations in $x_{ip}^0(t)$. Then for (49), we have $Nd = a = \frac{a}{2}$, and $n_1 d_1 = a$, $n_2 d_2 = a$. Therefore we choose $d = \frac{a}{2}$; $d_1 = d_2 = \frac{a}{2}$; and $N = n_1 = n_2 = 1$. The periodicity rule corresponds to

$$\begin{aligned} V(z) &= V(z + d) \\ &= V(z + 2d) \text{ etc.} \quad \text{transf:} \\ &= V^{(2D)}(x_1^0; x_2^0 + a) = V^{(2D)}(x_1^0 + a; x_2^0) \quad , \quad \text{on } z = d = \frac{a}{2}; \\ V^{(2D)}(x_1^0; x_2^0) &= V^{(2D)}(x_1^0 + a; x_2^0 + a) = V^{(2D)}(x_1^0 + 2a; x_2^0); \\ &= V^{(2D)}(x_1^0; x_2^0 + 2a) \quad , \quad \text{on } z = 2d; \text{ etc.:} \end{aligned} \quad (\text{Rule 2})$$

The second equation in (Rule 2) shows clearly that the general periodicity conditions are split to distribute over $z = \text{constant}$ lines to relate to $V(z)$, like the one given in the first equation in (Rule 2). Nevertheless we can not have an integer $\hat{N}$ with the correspondence which does not satisfy the above periodicity-split rule (2) such as

$$\begin{aligned} V^{(2D)}(x_1^0; x_2^0) &= V^{(2D)}(x_1^0 + 2a; x_2^0) = V^{(2D)}(x_1^0; x_2^0 + a) \quad (\text{transf:} \\ V(z) &= V(z + \hat{N}d); \quad \hat{N} = \textcircled{0}; \end{aligned} \quad (49a)$$

where $\textcircled{0}$ does not exist, because the lattice points $fx_1^0 = 2a; x_2^0 = 0g$ and $fx_1^0 = 0; x_2^0 = ag$ are not on the same straight-line $z = \text{any constant}$, or $x_1^0; x_2^0$, 2 variables or 2D while z , 1 variable or 1D.

A similar but more general demonstration is given below as: For (47c) or (47b) for dynamical $x_i^0(t)$, we have the rule (1)

$$\textcircled{C} z, \quad C + A + \textcircled{C} x_1^0(t) + C_i A_i \textcircled{C} x_2^0(t);$$

a correspondence for 1 degree of freedom z to 2 degrees of freedom $x_1^0; x_2^0$. For rule (2) the periodicity-split rule given in (Rule 2) also appears as

$$\begin{aligned} V^{(2D)}(x_1^0; x_2^0) &= V^{(2D)}(x_1^0; x_2^0 + d_1) = V^{(2D)}(x_1^0 + d_1; x_2^0), \quad \text{on } z = d; \\ V^{(2D)}(x_1^0; x_2^0) &= V^{(2D)}(x_1^0 + d_1; x_2^0 + d_2) = V^{(2D)}(x_1^0 + 2d_1; x_2^0); \\ &= V^{(2D)}(x_1^0; x_2^0 + 2d_2), \quad \text{on } z = 2d; \text{ etc.} \end{aligned} \quad (49b)$$

The demonstration of the periodicity-split due to the surface in (49a) also appears as

$$V^{(2D)}(x_1^0; x_2^0) = V^{(2D)}(x_1^0 + 2d_1; x_2^0) = V^{(2D)}(x_1^0; x_2^0 + d_2); \text{ etc.} \quad (49c)$$

This series of lattice points is not on a lattice (dynamic) plane of $z = \text{any constant}$. We do not consider that it confirms (45a) to be a part of a '3D perfect crystal' including lattice dynamics. Therefore we should view $V_{\text{periodic}}(\mathbf{r} + n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c})$ in (15) near any site $n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}$ to be labelled by the z -value of

$$(n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c})_z = n_1a_z + n_2b_z + n_3c_z$$

as

$$V_{\text{periodic}}(\mathbf{r}) = V_{\text{periodic}}(n_1a_z + n_2b_z + n_3c_z)(\mathbf{r} + n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}); \quad \text{for sets of integers } n_i:$$

We consider that the periodic potential energy with label

$$V_{\text{periodic}}(\mathbf{r}) = V_{\text{periodic}}[n_1a_z + n_2b_z + n_3c_z]_1(\mathbf{r} + n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c})$$

is *identically-equal* to

$$\begin{aligned} &= V_{\text{periodic}}[n_1^0a_z + n_2^0b_z + n_3^0c_z]_2(\mathbf{r} + n_1^0\mathbf{a} + n_2^0\mathbf{b} + n_3^0\mathbf{c}); \quad \text{provided} \\ &\text{by } [n_1a_z + n_2b_z + n_3c_z]_1 = [n_1^0a_z + n_2^0b_z + n_3^0c_z]_2; \end{aligned}$$

on the same lattice dynamic plane $z=\text{constant}$, while

$$\begin{aligned} V_{\text{periodic}}(\mathbf{r}) &= V_{\text{periodic}} [n_1 a_z + n_2 b_z + n_3 c_z]_1 (\mathbf{r} + n_1 \mathbf{a} + n_2 \mathbf{b} + n_3 \mathbf{c}) \\ &\stackrel{\text{generally}}{=} V_{\text{periodic}} [n_1^0 a_z + n_2^0 b_z + n_3^0 c_z]_2 (\mathbf{r} + n_1^0 \mathbf{a} + n_2^0 \mathbf{b} + n_3^0 \mathbf{c}); \quad \text{for} \\ &[n_1 a_z + n_2 b_z + n_3 c_z]_1 \notin [n_1^0 a_z + n_2^0 b_z + n_3^0 c_z]_2 \end{aligned}$$

are on different planes of $z = [n_1 a_z + n_2 b_z + n_3 c_z]_i$, $i = 1; 2$. Therefore the equalities in (15) are split by the above statement in the last two sets of equations: i.e. the first one is “identically-equal” while the second one is “generally equal”. This is the so-called “periodicity-split”. This is an assignment to fit the requirement of a 1D potential energy $V(z) = V(z + d)$, etc. from the 3D V_{periodic} .

Here we have shown that the proposed 1D potential energy, $V(z)$, in (18) or (46a) has *changed its dimensionality to 2D* in (47a), $V(x_1^0; x_2^0)$, because of the periodicity in (47a) and the transformation given in (47) or (49). This has *changed our dimensionality of the theory from 1D to 2D*. This is clearly shown in Fig. 2 for a ‘3D perfect crystal’: we need to have a physical cut with a surface as a “mathematical surface” in the figure to fit (49) for $V(x_1^0; x_2^0)$ with proper periodicities. The surface of this kind is a part of the perfect crystal with (45a). Nevertheless the potential energy is changed to two-variables x_1^0, x_2^0 as in 2D, due to the periodic requirement. For the actual ‘cut-surface’ we have some surface as the one of $z = 0$, as in (47), which is not mathematically a part of the 3D perfect crystal. But this cut-surface is of one variable z , i.e. 1D.

This leads (47) to be a surface *not* belonging as a part of the ‘3D perfect crystal’ defined by (45) and (45a). Nevertheless, (47) is still to provide us a *surface* in potential energy, not a line in Fig. 2 physically, and a boundary condition for subbands. Here we have a dimensionality theory in quantum mechanics [15], not included in mathematics. Therefore the diagonalization of (K) makes the surface not a simple plane (48) in the x_i^0 -coordinate system. We are not able to simplify our problems as we did for the complete 3D-whole-volume cases, e.g. in (30) the potential energy and the differential equation itself are no more one-dimensional than the subband theory itself.

A manifest example is given on p. 60 in Ref. [2] or in Ref. [27]. The Heaviside step function

$$\mu(z) = \left(\frac{1}{2} + z\right) \int_0^{\frac{1}{2} + z} dq J_1[q(\frac{1}{2} + z)] J_0(q\frac{1}{2}) \quad (50)$$

for Bessel function J_i of order i . This expansion is in the cylindrical coordinates r, z . It implies that a function of z has expansion coefficients dependent on $\frac{1}{2}$. This also shows that a flat plane surface has a mathematical description required to be at least of two variables, such as the cylindrical coordinates or according to the 3D cylindrical symmetry above. One of important consequences of the equality in (50) is that our intuitive action in the Schrödinger equation (51) below, say in the region $z < 0$ we just put zero in the potential energy term. We are not sure in this region $z < 0$ what will be happened if we use (50), e.g. $\frac{1}{2} \neq 1$, etc. Another point is that for $z > 0$ region, we have simply the term $V(z)$ in (51). However by the right hand side of (50), we could have another expression which contains two variables or two degrees of freedom or two dimensions so that we have two dimensions for the Schrödinger equation formally. That is different.

When we write rigorously in a generalized function form of the Schrödinger equation (30) for $z > 0$ inside the medium only, i.e. from (50)

$$\begin{aligned} & i \frac{\hbar^2}{2m_z} \frac{d^2}{dz^2} \psi_n + V(z) \mu(z) \psi_n \\ &= i \frac{\hbar^2}{2m_z} \frac{d^2}{dz^2} \psi_n + V(z) \left(\frac{1}{2} + z\right) \int_0^1 dq J_1[q(\frac{1}{2} + z)] J_0(q\frac{1}{2}) \psi_n \\ &= E_n^{(sl)} \psi_n \end{aligned} \quad (51)$$

This integral representation of the potential energy must be incorporated with the boundary conditions. Nevertheless we have the implication that the subband ladder energy $E_n^{(sl)}$ is not a simple one-dimensional entity.

In the author's opinion, this impossibility indicates the peculiarity of the (2+1)-dimensional mathematical space when there is a two-dimensional surface present inside the three-dimensional space. The dimensionality for the validity of physics is really important at this point of investigations [2].

Incidentally, for (37) for simple cubic (sc) lattice, we have

$$w_{i,z} = w = 0; \quad \text{for } i = 1, 2: \quad (\text{sc}) \quad (52)$$

This leads to

$$E_n^{(sl)} = E_{zn}^a: \quad (\text{sc}) \quad (53)$$

Conclusively we obtain the 'Schrödinger equation' for the envelope function (30), i.e.,

$$i \frac{\hbar^2}{2m_z} \frac{d^2}{dz^2} \psi_n(z) + V(z) \psi_n(z) = E_n^{(sl)} \psi_n(z); \quad (54)$$

with ψ_n having the position of the periodic function $u_k(z)$ in the Bloch function, if we consider the similarity between $\psi_n(z)$ and the usual 1D Bloch function. For tight-binding approximations, or the linear combinations of atomic orbitals (LCAO), we can solve (54) for $\psi_n(z) \gg u_k(z)$, as an atomic Schrödinger equation with discrete quantized energy eigenvalues $E_n^{(sl)}$. Applications to computations and extensions to other methods, such as statistical methods, are left for future investigations.

As a consequence of the two papers in this series, we find *physically*, that a two-dimensional classical surface, expressed by $\mu(z)$ in (51) e.g., is measurable in the three-dimensional Schrödinger equation (51) and in (47). The three-dimensional space is of lattice-like structure with a possible three-dimensional periodic potential energy. This should be compared with current mathematical thought: i.e. a two-dimensional space is not measurable in a three-dimensional space, this is clear in Riemann integral theory: a 2D area integral is a quantity of measure zero in the 3D volume integrals. Nevertheless physical *constants* included inside the 2D area are 3D.

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