A QUANTUM OPERATOR OF FORCE AND ITS APPLICATIONS

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ABSTRACT

We propose a new force operator, $-i\hbar\partial^2/\partial t\partial x$, which is obtained from time-differentiating of momentum expectation of a quantum particle. If this operator is worked to plane-wavefunction, force expectation, $-i\hbar k\omega$, is obtained. We call this force expectation 'marion force'. Application of the marion force is proposed as a concept which is able to be understood easily and intuitively when mechanical property of mechanical materials is analyzed. The marion force is calculated as a function of electron density in free-electron solids. Average pressure from this marion force is proportional to five-thirds power of electron density. This pressure is in a good agreement to virial pressure which is obtained thermodynamically from average energy of free-electrons. In normal metals, there is out-direction pressure more than 100 gigapascal without any pressure from outside. This pressure is cancelled by Feynman force which is induced by Coulomb potential worked between a valence electron and a positive ion. In a stationary state we think this Feynman force and the marion force are balanced.

Introduction

Basic force which causes deformation, fracture, cohesion, friction, abrasion, crystalline phase transition, etc., of solid materials, is only the electromagnetic interaction. Binding force between atoms is created by a change of momentum state: energy of valence electrons which are outmost electrons of an atom. It is a well-known method to calculate crystalline energy as a function of lattice distortion, when we evaluate mechanical properties of solids. Especially, for metals and semiconductors there are many calculated results by the pseudopotential method [1-3]. Once we obtain the calculated results of energy, we can apply results these to questions of elastic deformation; phonon spectra; phase transition stress; ideal fractural strength, within the structure of thermodynamics and classical mechanics, and based on the dislocation theory, to plastic deformation; creep phenomena; mechanisms to toughen materials [4-7].

Furthermore, if it is able to calculate 'force' directly from the motive state of electrons, it is very intuitive on evaluating the mechanical property of solids and very useful to discuss the property of deformation and fracture strength, which is affected by shear stress. And to discuss the property of solids which has mechanical anisotropic strength. On this paper, We propose a new method and a 'force' operator which is led from the differential of momentum expectation value. We discuss force expectation which is obtained when this operator is worked to a wavefunction. And we apply this method to free-electron solids, calculate pressure and compare with pressure which is led from the normal virial theorem.

A new force operator

The time derivative of momentum p of a moving particle is force F, which is supplied for surrounding field.

$$F = \frac{dp}{dt} \tag{1}$$

If a quantum momentum operator $\hat{p}$ defined as $-i\hbar\frac{\partial\psi}{\partial x}$ ($\hbar$ is Planck's constant and i is imaginary unit.) is worked to a wavefunction ψ , expectation of momentum $\langle p \rangle$ is

$$\begin{aligned} \langle p \rangle &= \int\psi^*(-i\hbar\frac{\partial}{\partial x})\psi \, dx \\ &= \langle\psi|\hat{p}|\psi\rangle \; . \end{aligned} \tag{2}$$

A time-derived function of (2) is

$$\frac{d\langle p\rangle}{dt} = \langle\frac{\partial\psi}{\partial t}|\hat{p}|\psi\rangle + \langle\psi|\frac{\partial\hat{p}}{\partial t}|\psi\rangle + \langle\psi|\hat{p}|\frac{\partial\psi}{\partial t}\rangle \; . \tag{3}$$

Since $\hat{p}$ is an Hermite operator, the first and the third term are able to be rewritten to

$$\langle\frac{\partial\psi}{\partial t}|\hat{p}|\psi\rangle = \langle p\rangle\langle\frac{\partial\psi}{\partial t}|\psi\rangle \tag{4}$$

and

$$\langle\psi|\hat{p}|\frac{\partial\psi}{\partial t}\rangle = \langle p\rangle\langle\psi|\frac{\partial\psi}{\partial t}\rangle \; . \tag{5}$$

From normalized condition of the wavefunction,

$$\langle\psi|\psi\rangle = 1 \tag{6}$$

is given. Hence a time-derived term of the wavefunction is

$$\begin{aligned} \frac{\partial\langle\psi|\psi\rangle}{\partial t} &= \langle\frac{\partial\psi}{\partial t}|\psi\rangle + \langle\psi|\frac{\partial\psi}{\partial t}\rangle \\ &= 0 \; . \end{aligned} \tag{7}$$

Thus, only the second term is remained on the right-hand side of the equation (3) .

$$\begin{aligned} \frac{d\langle p\rangle}{dt} &= \langle\psi| \; \frac{\partial\hat{p}}{\partial t} \; |\psi\rangle \\ &= \langle\psi| \; -i\hbar\frac{\partial^2}{\partial t\partial x} \; |\psi\rangle \end{aligned} \tag{8}$$

We define the equation (9) as a new force operator $\hat{F}$.

$$\hat{F} = -i\hbar \, \frac{\partial^2}{\partial t\partial x} \tag{9}$$

Force expectation is

$$\begin{aligned} \langle F\rangle &= \langle\psi|\hat{F}|\psi\rangle \\ &= \int\psi^*(-i\hbar \, \frac{\partial^2}{\partial t\partial x})\psi \, dx \; . \end{aligned} \tag{10}$$

We give a name 'marion force' to this force expectation.

Until now Feynman's method is known as a force operator to obtain force which interacts on quantum particles [8]. Feynman force operator is defined as follows. Hamiltonian $\hat{H}$ works to particle-system moving in a potential field V. As $\hat{H}$ equals $\hat{T} + \hat{V}$, where $\hat{T}$ is a kinetic energy operator and $\hat{V}$ is a potential energy operator, expectation of energy is

$$\langle U \rangle = \langle \psi | \hat{H} | \psi \rangle \ . \tag{11}$$

Force F defined by thermodynamics is

$$F = \frac{-\partial U}{\partial x} \ . \tag{12}$$

A space-derived function of <U> becomes

$$\begin{aligned} \frac{\partial \langle U \rangle}{\partial x} &= \langle \psi | \ \frac{\partial \hat{H}}{\partial x} \ | \psi \rangle \\ &= \langle \psi | \ \frac{\partial \hat{V}}{\partial x} \ | \psi \rangle \ . \end{aligned} \tag{13}$$

This operator, $-\frac{\partial \hat{V}}{\partial x}$ is defined as Feynman force operator. When this operator is worked to a wavefunction, force expectation <F> is obtained.

$$\langle F \rangle = \int \psi^* \left(- \frac{\partial \hat{V}}{\partial x}\right) \psi \ dx \tag{14}$$

This potential force <F> is called Feynman force. In a stationary state we think that this Feynman force F_F and marion force F_M, defined by the formula (10), are balanced.

Applications and discussions

1. Quantum free particles

Assume a wavefunction of a quantum particle is approximated to a planewave as

$$\psi = \exp\,[i(kx - \omega t)] \tag{15}$$

where k is a wavenumber and ω is an angular frequency. If it is operated by the marion force operator, the following equation is obtained as marion force F_M from the formula (10).

$$F_M = -i\hbar k\omega \tag{16}$$

Kinetic energy U of a particle of which mass is m, is

$$U = \frac{\hbar^2 k^2}{2m} \tag{17}$$

and

$$U = \hbar\omega \ . \tag{18}$$

The marion force F_M is represented by the following equation as a function of U.

$$F_M = \frac{-i(2m)^{1/2}U^{3/2}}{\hbar} \quad (19)$$

For a photon, c is the velocity of light and k is equal to $\frac{\omega}{c}$, the marion force is

$$F_M = \frac{-iU^2}{\hbar c} . \quad (20)$$

For example, we show results of a photon, electron, proton and carbon ion in Figure 1. These mean the force when a moving particle is stopped quickly (of which time is an order of $\frac{1}{\omega}$, and the force diverges to infinite in the classical theory.) or the force of the maximum when the moving particle transfers force to environmental field.

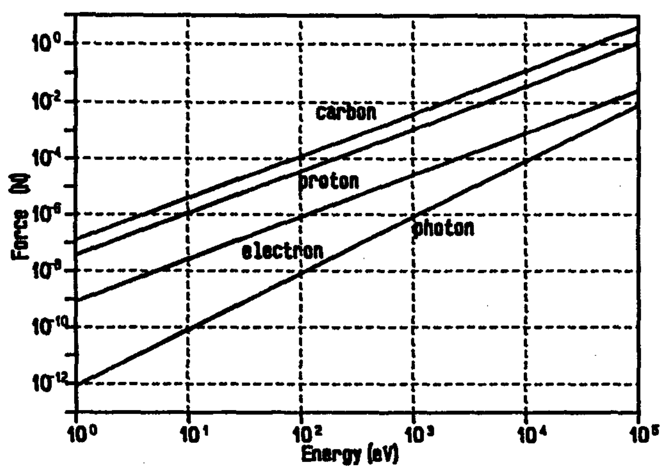

Figure 1. Marion force of free particles such as a photon, electron, proton and carbon ion.

We think that the marion force will become an interesting concept about mechanical analyses in rarefield gas and plasma gas motion; thin and multi-layered film production by sputtering; ion plating; particle milling.

In case of an electron of hydrogen, moving in periodic orbit with Coulomb attraction, a centrifugal force F_R is

$$F_R = mr\omega^2 = \hbar k\omega = iF_M \quad (21)$$

where r is a orbital radius in Bohr model. This F_R is consistent with the marion force F_M. Wavenumber k is

$$k = \frac{n}{2\pi r} \quad (22)$$

where n is an integer not equal zero. As the wavenumber is represented discrete value, the marion force is also discrete eigenvalue. On this condition, Feynman force F_F is able to be obtained from the equation (14) by using Coulomb potential V, and must be balanced with the marion force. There is the same discussion about valence electrons in free-electron model (which potential V is zero in one region, otherwise infinite.) of metals or semiconductor when the condition (22) with cyclic orbit is regarded as periodic condition for a wavefunction.

2. Free-electron solids

There are N valence electrons in a metal of which volume is Ω : a potential V is zero: we use free-electron approximation. Energy U of an electron with a wavevector $\mathbb{k}$ is from the equations (17) and (18)

$$U = \frac{\hbar^2 |\mathbb{k}|^2}{2m} = \hbar\omega \ . \qquad (23)$$

The marion force for X-direction F_{Mx} is from the equation (16)

$$F_{Mx} = \frac{-i\hbar^2}{2m} |\mathbb{k}|^2 k_x \qquad (24)$$

where k_x is wavenumber for X-direction. The total marion force $\bar{F}$ of electrons which has positive k_x for X-direction and less than the Fermi energy in a k space is

$$\begin{aligned}\bar{F} &= \Sigma_k F_{Mx}(k) \\ &= \frac{2\Omega}{(2\pi)^3} \int_0^{|\mathbb{k}|<k_F} \frac{-i\hbar^2}{2m} |\mathbb{k}|^2 k_x d\mathbb{k} \ . \end{aligned} \qquad (25)$$

It is rewritten to spherical coordinates.

$$\begin{aligned}\bar{F} &= \frac{\Omega}{4\pi^3} \frac{-i\hbar^2}{2m} |\mathbb{k}|^2 (|\mathbb{k}| \cos\theta)(|\mathbb{k}|^2 \sin\theta) \, d|\mathbb{k}| d\theta d\phi \\ &= \frac{\Omega}{24\pi^3} \frac{-i\hbar^2}{2m} k_F^6 \end{aligned} \qquad (26)$$

Using valence electron density $\frac{N}{\Omega}$, Fermi wavenumber k_F of free electron solids is

$$k_F = (3\pi^2)^{1/3} \left(\frac{N}{\Omega}\right)^{1/3} \ . \qquad (27)$$

It is obtained that all marion force $\bar{F}_M$ for one direction, substituting this in (26).

$$\bar{F}_M = \frac{3\pi^2}{8} \frac{-i\hbar^2}{2m} \frac{N^2}{\Omega} \qquad (28)$$

The average marion force f_M for each electron is

$$f_M = \frac{3\pi^2}{8} \frac{-i\hbar^2}{2m} \frac{N}{\Omega} . \tag{29}$$

It is proportional to valence electron density $\frac{N}{\Omega}$. Thus, pressure P_M for out direction which is given by the marion force is

$$P_M = \frac{f_M}{(\frac{\Omega}{N})^{2/3}} = f_M(\frac{N}{\Omega})^{2/3}$$

$$= \frac{3\pi^2}{8} \frac{-i\hbar^2}{2m} (\frac{N}{\Omega})^{5/3} \tag{30}$$

We also call this pressure 'marion pressure'. Otherwise, the average energy u for each electron of free-electron solids with Fermi energy u_F is

$$u = \frac{3}{5} u_F$$

$$= \frac{3}{5} (3\pi^2)^{2/3} \frac{\hbar^2}{2m} (\frac{N}{\Omega})^{2/3} . \tag{31}$$

This pressure P_v called virial pressure, which is obtained thermodynamically is represented

$$P_v = - \frac{du}{d(\Omega/N)}$$

$$= \frac{2}{5} (3\pi^2)^{2/3} \frac{\hbar^2}{2m} (\frac{N}{\Omega})^{5/3} . \tag{32}$$

We show both pressure as marion pressure and virial pressure in Figure 2. There is a few difference between both data. We think that it comes from a difference between average of force and average of energy. Anyway, in normal metals in which electron Fermi energy is about 10 eV, there is out-direction pressure more than 100 gigapascal without any pressure from outside. This pressure is cancelled by Feynman force which is induced by Coulomb potential worked between a valence electron and positive ion: the valence electron is trapped inside the metal.

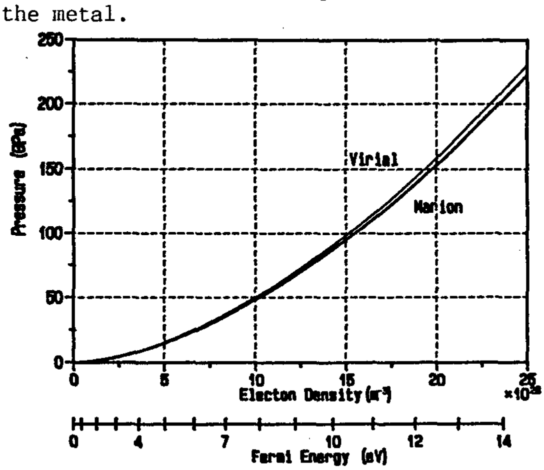

Figure 2. Marion pressure and virial pressure as a function of electron density of free-electron solids.

Introducing periodic potential-field by arrange of positive ions, the marion force of the valence electron has a band gap at Brillouin zone boundary like energy band structure of a solid-state electron. Thus, we can think force band structure with the formula (16). We think this force band structure will be a most important in electronic solid-state property like an idea of energy band. For example, from the idea of the force band gap, it is obtained an knowledge about stress in crystalline zone boundary; stress of contact between different materials; surface tension; fracture of brittle-ductility. This directive method is useful and fruitful when problems approached by an idea of energy are too confused, such as the property of fracture of metal; semiconductor; ceramics, brittle-ductility transition with pressure or temperature, hydrogen brittle, etc.

Conclusions

We proposed a new force operator, $-i\hbar\frac{\partial^2}{\partial t\partial x}$, which is obtained by time-deriving the expectation <p> of momentum of quantum particles, operates as the force operator. When this operates to a plane-wavefunction, expectation of force $\langle F\rangle = -i\hbar k\omega$ is obtained, and we call this force 'marion force'.

We also calculated the marion force as a function of electron density in free-electron solids, and obtained average force f_M for one-direction for each electron.

$$f_M = \frac{3\pi^2}{8}\frac{-i\hbar^2}{2m}\frac{N}{\Omega}$$

From this force, average pressure P_M is

$$P_M = \frac{3\pi^2}{8}\frac{-i\hbar^2}{2m}\left(\frac{N}{\omega}\right)^{5/3} .$$

It is proportional to five-thirds power of electron density. It almost agrees quantitatively with virial pressure which is obtained from thermodynamical average of energy of free electron.

We propose application of force band structure by the marion force which is understood easily and directly when we analyze solid property of mechanical materials. Especially, we indicate that an force band gap is an interesting idea.

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