# Symmetry of the Ground-State Wave Function of Many Particle System

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It is proved that, if the Hamiltonian of a system of spinless particles is symmetric with respect to interchange of the particles, the wave function with the lowest energy attainable without any restriction on its symmetry property, is symmetric with respect to interchange of the coordinates. It is also discussed what kind of conditions must be imposed upon the Hamiltonian for the theorem to be valid.

## §1. Introduction

Theorem: Let the Hamiltonian of a system of spinless particles be symmetric with respect to interchange of the particles. Then the wave function with the lowest energy attainable without any restriction on its symmetry property, is symmetric with respect to interchange of coordinates of the particles.

In real many-particle systems, if the Hamiltonian is symmetric with respect to interchange of the particles, they are identical and obey Bose or Fermi statistics. It might seem then that wave functions which are neither symmetric nor antisymmetric have no physical meaning. This is not true, however. For instance, if the Hamiltonian of a fermion system is spin-independent, the orbital part of the wave function can be separated from the spin part and has a complicated symmetry property with respect to interchange of the spatial coordinates. For the case of a mixture of He³ and He⁴, we can approximate the Hamiltonian by a symmetric one by neglecting the mass difference, but the wave function of the system is in general neither totally symmetric nor antisymmetric. When we study properties of a system, it is sometimes helpful to compare it with another system which has the same Hamiltonian but obey a different statistics. Thus the above theorem, if it is valid, may play roles in the study of many-particle systems.

The theorem means, for instance, that the ground-state energy of a fermion system is higher than that of a boson system if they both have an identical Hamiltonian. The statement is evidently true for the case of free particles. It also seems to be true for interacting particles, since a symmetrical wave function has no node and thus will give a smaller kinetic energy. Feynman<sup>1)</sup> once took advantage of this theorem in treating an impurity He<sup>3</sup> in liquid He<sup>4</sup>. He, neglecting the mass difference of the atoms, presumes

the ground-state wave function of the mixture to be identical with that of pure liquid with He³ replaced by He⁴.

So the question is: Is this theorem ever true generally? Is it valid with Hamiltonian of arbitrary structure? The present paper describes an analysis which we made in order to elucidate the range of validity of the theorem.

## §2. One-dimensional system of two particles

Let us begin the analysis with the case of a one-dimensional system of two particles, since the essence of the proof for a more general case will be shown in the following argument on this simple case.

The Hamiltonian of the system is given by

$$H = -\frac{1}{2m} \left( \frac{d^2}{dx_1^2} + \frac{d^2}{dx_2^2} \right) + V(x_1 - x_2), \tag{1}$$

with the interaction potential V satisfying

$$V(x) = V(-x)$$
,

in accordance with the symmetry with respect to interchange of the particles. As usual, we separate the motion of a center-of-mass coordinate  $X = (x_1 + x_2)/2$  from that of a relative one  $x = x_1 - x_2$ . As we are considering the ground state, we assume that the center of mass is at rest. Then the Hamiltonian reduces to

$$H = -\frac{1}{m} \frac{d^2}{dx^2} + V(x). \tag{2}$$

Let the wave function of the lowest energy and the energy of it be  $\psi_{\rm S}(x)$  and  $E_{\rm S}$ , when the wave function is chosen within symmetric ones, and those be  $\psi_{\rm A}(x)$  and  $E_{\rm A}$ , when it is within antisymmetric ones. We then construct a symmetric function  $\bar{\psi}_{\rm S}$  from  $\psi_{\rm A}$  through the procedure:

$$\bar{\psi}_{S}(x) = \begin{cases} \psi_{A}(x) & x > 0, \\ -\psi_{A}(x) & x < 0. \end{cases}$$
 (3)

This function  $\bar{\psi}_{\rm S}(x)$  has discontinuous derivatives at the origin x=0 generally. What is then the expectation value  $\bar{E}_{\rm S}$  of H in  $\bar{\psi}_{\rm S}$ ? Dividing the region of integration into three:  $x>\eta$ ,  $x<\eta$  and  $|x|<\eta$ ,  $\eta$  being a small positive quantity, we write

$$\begin{split} \overline{E}_{\mathrm{S}} &= \langle \bar{\psi}_{\mathrm{S}} | H | \bar{\psi}_{\mathrm{S}} \rangle \\ &= \int_{-\infty}^{-\eta} [-\psi_{\mathrm{A}}(x)] H [-\psi_{\mathrm{A}}(x)] dx + \int_{\eta}^{\infty} \psi_{\mathrm{A}}(x) H \psi_{\mathrm{A}}(x) dx \\ &+ \int_{-\eta}^{\eta} \bar{\psi}_{\mathrm{S}}(x) H \bar{\psi}_{\mathrm{S}}(x) dx \,. \end{split}$$

Since  $\psi_A(x)$  is an eigenfunction of H, the first and second terms together will give  $E_A$  in the limit  $\eta \to 0$ . From the third term, a finite contribution may be expected in the limit  $\eta \to 0$  only when the integrand is singular at x=0. Hence the contribution from the potential vanishes in this limit and we are left with

$$\overline{E}_{S} = E_{A} - \frac{1}{m} \lim_{n \to 0} \int_{-n}^{n} \overline{\psi}_{S}(x) \frac{d^{2}}{dx^{2}} \overline{\psi}_{S}(x) dx. \tag{4}$$

Since  $d\bar{\psi}_{\rm S}(x)/dx$  is discontinuous at the origin,  $d^2\bar{\psi}_{\rm S}(x)/dx^2$  is a  $\delta$ -function:

$$\frac{d^2\bar{\psi}_{\rm S}(x)}{dx^2} = 2\left(\frac{d\psi_{\rm A}}{dx}\right)_{x=0}\delta(x).$$

Therefore the integral in (4) reduces to

$$2\left(\frac{d\psi_{A}}{dx}\right)_{x=0}\int_{-\eta}^{\eta}\bar{\psi}_{S}(x)\delta(x)dx=2\left(\frac{d\psi_{A}}{dx}\right)_{x=0}\bar{\psi}_{S}(0),$$

and is clearly seen to vanish because  $\bar{\psi}_{\rm S}(0) = 0$ . The final result is

$$\overline{E}_{\mathrm{S}} = E_{\mathrm{A}}$$
 (5)

On the other hand, since the lowest energy that is given by symmetric functions is  $E_s$ , we have from Schrödinger's variation principle

$$\overline{E}_{s} \geq E_{s}$$
.

From this and Eq. (5), one can conclude that

$$E_{\mathbf{A}} \geq E_{\mathbf{S}}$$
. (6)

It should be noticed that the conclusion depends on the structure of the Hamiltonian. The difference between  $\overline{E}_s$  and  $E_A$  vanishes since the Hamiltonian contains only a local potential and the kinetic energy given by a second-order differential operator. If it is a more general non-local Hamiltonian, a finite change in energy may be expected when the wave function  $\psi_A$  is modified to  $\overline{\psi}_s$ .

We can proceed a step further, if  $\psi_A$  has a non-vanishing first derivative at the origin. If  $(d\psi_A/dx)_{z=0} 
ightharpoonup 0$ ,  $\bar{\psi}_S$  has discontinuous derivatives there, and such a function with a kink can never be the ground-state wave function as far as the interaction potential is not singular. In fact we can construct a function  $\bar{\psi}_S$  with the energy expectation value lower than  $\bar{E}_S$  by modifying  $\bar{\psi}_S$  in the following way:

$$\tilde{\psi}_{S}(x) = \begin{cases} \bar{\psi}_{S}(x) & |x| > \varepsilon \\ \bar{\psi}_{S}(\varepsilon) & |x| < \varepsilon \end{cases},$$
(7)

where  $\varepsilon$  is a small positive quantity. As shown in Fig. 1,  $\tilde{\psi}_{\rm S}$  has discontinuous

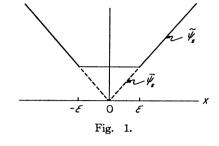
derivatives at  $x = \pm \varepsilon$ . Though  $\overline{\psi}_S$  is normalized if  $\psi_A$  is, this modified  $\widetilde{\psi}_S$  is not. We have

$$egin{aligned} raket \widetilde{\psi}_{\mathrm{S}} ig| \widetilde{\psi}_{\mathrm{S}} ig> &= 1 - \int_{-arepsilon}^{arepsilon} \overline{\psi}_{\mathrm{S}}(x)^2 dx \ &+ \int_{-arepsilon}^{arepsilon} \widetilde{\psi}_{\mathrm{S}}(x)^2 dx \,. \end{aligned}$$

Or putting

$$\bar{\Psi}_{\mathrm{S}}(x) = \left(\frac{d\psi_{\mathrm{A}}}{dx}\right)_{x=0} |x|,$$

$$\tilde{\Psi}_{\mathrm{S}}(x) = \left(\frac{d\psi_{\mathrm{A}}}{dx}\right)_{x=0} \varepsilon$$



for  $|x| < \varepsilon$ , we find

$$\langle \widetilde{\psi}_{\mathrm{S}} | \widetilde{\psi}_{\mathrm{S}} \rangle \cong 1 + \frac{4}{3} \left( \frac{d\psi_{\mathrm{A}}}{dx} \right)_{x=0}^{2} \varepsilon^{3}.$$

If the potential is not singular at the origin, the correction to its expectation value is calculated in a similar way, the result being

$$\langle \tilde{\psi}_{\mathbf{S}} | V | \tilde{\psi}_{\mathbf{S}} \rangle \cong \langle \bar{\psi}_{\mathbf{S}} | V | \bar{\psi}_{\mathbf{S}} \rangle + \frac{4}{3} V(0) \left( \frac{d\psi_{\mathbf{A}}}{dx} \right)_{z=0}^{2} \varepsilon^{3}.$$

On the other hand, due to the discontinuity of the first derivative of  $\tilde{\psi}_s$  at  $x = \pm \varepsilon$ , its second derivative becomes a  $\delta$ -function there. We get, therefore, the expectation value of the kinetic energy as

$$\begin{split} \left\langle \tilde{\psi}_{\mathrm{S}} \middle| -\frac{1}{m} \frac{d^{2}}{dx^{2}} \middle| \tilde{\psi}_{\mathrm{S}} \right\rangle \\ &= \left\langle \bar{\psi}_{\mathrm{S}} \middle| -\frac{1}{m} \frac{d^{2}}{dx^{2}} \middle| \bar{\psi}_{\mathrm{S}} \right\rangle - \frac{1}{m} \int \tilde{\psi}_{\mathrm{S}}(x) \left( \frac{d\psi_{\mathrm{A}}}{dx} \right)_{x=0} [\delta(x+\varepsilon) + \delta(x-\varepsilon)] dx \\ &\quad + \mathrm{O}(\varepsilon^{3}) \\ &= \left\langle \bar{\psi}_{\mathrm{S}} \middle| -\frac{1}{m} \frac{d^{2}}{dx^{2}} \middle| \bar{\psi}_{\mathrm{S}} \right\rangle - \frac{2}{m} \left( \frac{d\psi_{\mathrm{A}}}{dx} \right)_{x=0}^{2} \varepsilon + \mathrm{O}(\varepsilon^{3}). \end{split}$$

Thus finally  $\widetilde{E_{\mathrm{s}}}$  is given by

$$\widetilde{E}_{S} = \frac{\langle \widetilde{\psi}_{S} | H | \widetilde{\psi}_{S} \rangle}{\langle \widetilde{\psi}_{S} | \widetilde{\psi}_{S} \rangle} 
= \overline{E}_{S} - \frac{2}{m} \left( \frac{d\psi_{A}}{dx} \right)_{z=0}^{2} \varepsilon + O(\varepsilon^{3}).$$
(8)

From Eqs. (5) and (8), we get for a small  $\varepsilon$ ,

$$\widetilde{E}_{\mathrm{S}} - E_{\mathrm{A}} = -\frac{2}{m} \left( \frac{d\psi_{\mathrm{A}}}{dx} \right)_{x=0}^{2} \varepsilon < 0.$$

Since  $E_s \leq \widetilde{E}_s$ , one can conclude that

$$E_{\rm S} \!\! < \!\! E_{\rm A}$$
 . (9)

If  $(d\psi_A/dx)_{z=0}=0$ , however, we cannot lower the energy in this way. To examine this case in some detail, let us follow the inverse procedure starting from a symmetric wave function  $\psi_S$ . We define an antisymmetric function by

$$\bar{\psi}_{A}(x) = \begin{cases} \psi_{S}(x) & x > 0 \\ -\psi_{S}(x) & x < 0. \end{cases}$$

Then, in a similar way as before, we have

$$\langle \bar{\psi}_{A}|H|\bar{\psi}_{A}\rangle = E_{S} - \frac{1}{m} \lim_{n \to 0} \int_{-n}^{n} \bar{\psi}_{A}(x) \frac{d^{2}}{dx^{2}} \bar{\psi}_{A}(x) dx$$
.

This time the derived function  $\bar{\psi}_{\rm A}$  is discontinuous in its value at the origin. Therefore  $d\bar{\psi}_{\rm A}(x)/dx \approx \delta(x)$  and  $d^2\bar{\psi}_{\rm A}(x)/dx^2 \approx \delta'(x)$ , and hence the integral above, except the factor -1/m, reduces to

$$2\psi_{\mathrm{S}}(0)\int_{-\eta}^{\eta}\bar{\psi}_{\mathrm{A}}(x)\delta'(x)dx = -2\psi_{\mathrm{S}}(0)\left(\frac{d\bar{\psi}_{\mathrm{A}}}{dx}\right)_{s=0}.$$

This clearly diverges with negative sign if  $\psi_8(0) \neq 0$ . Thus in this case the counterpart to Eq. (5) cannot be obtained and, therefore, the inverse relation to (6) does not apply. However, if  $\psi_8(0) = 0$ , the value of the function  $\bar{\psi}_A(x)$  is continuous and we obtain the inverse inequality  $E_8 \geq E_A$ . The final conclusion is that  $E_A = E_S$  if  $\psi_S(0) = 0$ . This means  $\bar{\psi}_S = \psi_S$  and  $\bar{\psi}_A = \psi_A$ , and so we have  $(d\psi_A/dx)_{z=0} = 0$ . This conclusion is consistent with the previous result that the energy could not be lowered if  $(d\psi_A/dx)_{z=0} = 0$ . The situation corresponds to a potential barrier of infinite height. In this particular case it is natural that the symmetric and antisymmetric states should be degenerate. It should be noticed, however, that this is possible only in a one-dimensional system.

### §3. Many particle system

The proof given in the last section can be generalized to the case of a three-dimensional system of N particles whose Hamiltonian is given by

$$H = -\frac{1}{2m} \sum_{i} \mathbf{r}_{i}^{2} + V(\mathbf{r}_{1}, \mathbf{r}_{2}, \cdots, \mathbf{r}_{N}). \tag{10}$$

Here the potential V is a symmetric function of the coordinates  $r_1, r_2, \dots, r_N$ . An external potential, if any, may also be included in V, and the interaction is not restricted to the usual two-body central force.

Suppose that an eigenfunction  $\phi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$  with the energy eigenvalue E is found which is not totally symmetric with respect to interchange of the coordinates. It can be taken as a real function with an appropriate choice of the phase factor. Now suppose that it is not symmetric with respect to interchange of, say,  $\mathbf{r}_1$  and  $\mathbf{r}_2$ . We can easily antisymmetrize it by taking a linear combination

$$\phi(r_1, r_2, r_3, \dots, r_N) - \phi(r_2, r_1, r_3, \dots, r_N),$$

which still is an eigenfunction with the same energy. Thus we can assume, without loss of generality, that the eigenfunction is antisymmetric with respect to interchange of these coordinates:

$$\phi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_N) = -\phi(\mathbf{r}_2, \mathbf{r}_1, \mathbf{r}_3, \dots, \mathbf{r}_N). \tag{11}$$

Introducing a center-of-mass coordinate and a relative one of  $r_1$  and  $r_2$  by

$$R=\frac{1}{2}(r_1+r_2), \quad r=r_1-r_2,$$

we define a function  $\psi$  of r, R,  $r_3$ ,  $\cdots$ ,  $r_N$ :

$$\psi(\mathbf{r},\mathbf{R};\mathbf{r}_3,\cdots,\mathbf{r}_N) \equiv \phi\left(\mathbf{R} + \frac{\mathbf{r}}{2},\mathbf{R} - \frac{\mathbf{r}}{2},\mathbf{r}_3,\cdots,\mathbf{r}_N\right). \tag{12}$$

According to Eq. (11), it satisfies

$$\psi(\mathbf{r}, \mathbf{R}; \mathbf{r}_3, \cdots, \mathbf{r}_N) = -\psi(-\mathbf{r}, \mathbf{R}; \mathbf{r}_3, \cdots, \mathbf{r}_N). \tag{13}$$

Therefore  $\psi$ , as a function of  $\mathbf{r}$ , has a nodal plane P on which it vanishes:

$$\psi(\mathbf{r}, \mathbf{R}; \mathbf{r}_3, \dots, \mathbf{r}_N) = 0$$
 for  $\mathbf{r} \in \mathbf{P}$ .

The plane includes the origin r=0, and divides the space of r into two regions, which we denote by  $\Omega_{+}$ .

Following the procedure we took in the last section, let us introduce a new function  $\bar{\Psi}$  by

$$\bar{\psi}(\mathbf{r},\mathbf{R};\mathbf{r}_3,\cdots,\mathbf{r}_N) = \begin{cases} \psi(\mathbf{r},\mathbf{R};\mathbf{r}_3,\cdots,\mathbf{r}_N) & \mathbf{r} \in \Omega_+ \\ -\psi(\mathbf{r},\mathbf{R};\mathbf{r}_3,\cdots,\mathbf{r}_N) & \mathbf{r} \in \Omega_- \end{cases}$$
(14)

which is an even function of  $\mathbf{r}$ . Clearly

$$\bar{\phi}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_N) \equiv \bar{\psi}\left(\mathbf{r}_1 - \mathbf{r}_2, \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}; \mathbf{r}_3, \dots, \mathbf{r}_N\right)$$
 (15)

is a symmetric function with respect to interchange of  $r_1$  and  $r_2$ . The function  $\bar{\psi}$  is not singular as a function of R,  $r_3$ , ...,  $r_N$ , but it has generally discontinuous derivatives perpendicular to the plane P.

In calculating the energy expectation value  $\overline{E}$  in  $\overline{\psi}$ ,

we divide the region of integration of r into three:  $\Omega_0^n$  and  $\Omega_{\pm}^n$ , as illustrated in Fig. 2. Here  $\Omega_0^n$  is a thin region of thickness  $2\eta$  which includes P, and  $\Omega_{\pm}^n$  are the remaining regions of  $\Omega_{\pm}$ :  $\lim_{\eta \to 0} \Omega_{\pm}^{\eta} = \Omega_{\pm}$ .

Then we have

$$\overline{E} = \int \cdots \int \left[ \int_{a_{1}^{n}} \psi H \psi d\mathbf{r} \right] \\
+ \int_{a_{2}^{n}} (-\psi) H (-\psi) d\mathbf{r} \\
+ \int_{a_{3}^{n}} \overline{\psi} H \overline{\psi} d\mathbf{r} d\mathbf{r} d\mathbf{r}_{3} \cdots d\mathbf{r}_{N}, \quad (16)$$

where  $\bar{\psi}$  has been replaced by  $\pm \psi$  in the first two integrals. In the limit  $\eta \rightarrow 0$ , the first two terms give  $E = \langle \phi | H | \phi \rangle$ , while the

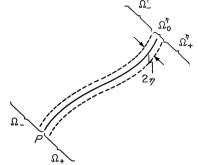


Fig. 2.

last term may have a nonvanishing contribution only when the integrand is singular. We are thus left with

$$\overline{E} = E + \int \cdots \int \left[ \lim_{\eta \to 0} \int_{2\eta} \overline{\psi} \left( -\frac{1}{m} \nabla_r^2 \right) \overline{\psi} d\mathbf{r} \right] d\mathbf{R} d\mathbf{r}_3 \cdots d\mathbf{r}_N.$$

If we take the cartesian coordinates (x, y, z) at each point on P in such a way that the x-axis is perpendicular to P, the singularity of the integrand comes from the  $d^2/dx^2$  term in  $\mathcal{F}_r^2$ , and the integral becomes

$$\int_{\mathbb{P}} \left[ \lim_{n \to 0} \int_{-n}^{n} \bar{\psi} \left( -\frac{1}{m} \frac{d^{2}}{dx^{2}} \right) \bar{\psi} dx \right] dS$$

with

$$dS = dydz$$
.

In a similar way as in §2, this integral is found to vanish. Thus we obtain

$$\overline{E} = E$$
. (17)

Again we can construct a function  $\widetilde{\psi}$  with an energy expectation value  $\widetilde{E}$  lower than E by modifying  $\overline{\psi}$ . In a similar way as before, we introduce  $\widetilde{\psi}$  by

$$\widetilde{\psi}(\mathbf{r}, \mathbf{R}; \mathbf{r}_3, \dots, \mathbf{r}_N) = \begin{cases} \overline{\psi}(\mathbf{r}, \mathbf{R}; \mathbf{r}_3, \dots, \mathbf{r}_N) & |x| > \varepsilon \\ \overline{\psi}(\varepsilon, y, z, \mathbf{R}; \mathbf{r}_3, \dots, \mathbf{r}_N) & |x| < \varepsilon. \end{cases}$$
(18)

where x=0 corresponds to P. Then, using Eq. (8), we obtain to the first order in  $\varepsilon$ 

$$\widetilde{E} = \frac{\langle \widetilde{\psi} | H | \widetilde{\psi} \rangle}{\langle \widetilde{\psi} | \widetilde{\psi} \rangle} \cong \widetilde{E} - \frac{2\varepsilon}{m} \int \cdots \int \left\{ \int_{\mathbf{P}} \left( \frac{\partial \psi}{\partial x} \right)_{\mathbf{P}}^{2} dS \right\} d\mathbf{R} d\mathbf{r}_{3} \cdots d\mathbf{r}_{N}.$$

In contrast to the one-dimensional case, this is always smaller than  $\overline{E}$ , since such a peculiar situation is never expected that  $\partial \psi/\partial x=0$  everywhere on P for any value of  $\mathbf{R}$ ,  $\mathbf{r}_{3}$ ,  $\cdots$ ,  $\mathbf{r}_{N}$ . Thus we finally arrive at the relation

$$\widetilde{E} < \overline{E} = E$$
. (19)

This means that, if there is an eigenfunction with energy E which is not totally symmetric with respect to interchange of the coordinates, there is always another eigenfunction with energy lower than E. Therefore, if  $\phi$  is the eigenfunction with the lowest energy, it should be totally symmetric.

## §4. Example and discussion

4.1. In order to illustrate how we apply the theorem to actual problems, and how we must be careful in the application, we first give two examples.

Example 1. Let the Hamiltonian of a system of two fermions with stin

Example 1. Let the Hamiltonian of a system of two fermions with spin 1/2 be independent of the spins. Then the ground state of the system is a singlet.

The wave functions of a singlet state is antisymmetric in the spin variables and therefore is symmetric in the spatial variables, while the wave functions of a triplet state is symmetric in the spin variables and antisymmetric in the spatial variables. Since the Hamiltonian of the system is independent of the spins, a singlet state, which is symmetric in the spatial variables, should be the ground state according to the theorem. The statement is valid even when the particles are subject to any external potential field and the inter-particle interaction may take any form provided that it be symmetric with respect to interchange of particles.

Example 2. "The ground state of any atom with two electrons in the outer-most shell is a singlet."

If it be possible to represent the effect of the inner closed shells by a pure potential field, the problem reduces to Example 1 above, and the conclusion will be this statement. However, according to Hund's rule, it is a triplet when the outer-most shell is, for instance, p orbitals, in contradiction to the statement above.

This erroneous conclusion has been derived from the assumption that the effect of the inner shell electrons were represented solely by a potential field. If it were a simple potential, the one-electronic state with the lowest energy would be an s orbital. The reason that the electrons in hand occupy p orbitals instead of the s orbital is that the latter has already been occupied by the inner shell electrons. Thus we have a certain restriction on the wave functions which we can allot to the electrons in hand, and as a result the wave functions available do not make up a complete set. Then the variation principle which we used in the proof is no more valid. It can no more be justified that a singlular function such as  $\bar{\psi}_s$  or  $\tilde{\psi}_s$  appearing in the proof be expanded in terms of the functions now available. Hence Eq. (19) will in general be invalid.

A similar situation exists in the case of band electrons in solids. The theorem is evidently valid when we consider the entire system of electrons as moving in the field of nuclei, stipped of all electrons. This way of looking is too impracticable, however, to give any role to the theorem. On the other hand, when we discuss the electrons in one band, for instance, we are restricting the functional space and the proof given in the last section is no more valid.

4.2. We sometimes encounter systems with Hamiltonian of a more complicated structure than we discussed in the preceding sections. Therefore it is important to examine the applicability of the theorem to such cases.

In the single-band approximation for electrons in solids, we approximate the Hamiltonian by ignoring interband matrix elements. For spinless particles, the approximate Hamiltonian is in general of the form

$$H = \sum_{ij} \varepsilon_{ij} c_i^{\dagger} c_j + \sum_{ijkl} V_{ijkl} c_i^{\dagger} c_j^{\dagger} c_k c_l , \qquad (20)$$

in the Wannier-function representation. Here  $c_i^{\dagger}$  and  $c_i$  denote respectively the creation and annihilation operator for the Wannier state at the lattice site i which belongs to the band we are considering. This is a non-local Hamiltonian in the discrete space formed by lattice points. Thus, avoiding the difficulty of an incomplete functional space, we are forced to deal with this complicated Hamiltonian.

If we want to apply the theorem to a system with such a non-local Hamiltonian, we should be very careful, since it was proved only for a system with Hamiltonian of the form (2) or (10), but not for a system with a non-local one. The theorem does not hold generally for such a system. As a matter of fact, it is easy to find an example which contradicts it.

In Hamiltonian (20), the Fourier transform  $\varepsilon(p)$  of  $\varepsilon_{ij}$  gives the single-particle energy, and in general it is not a simple quadratic function of momentum. Sometimes it has two or more minima in the momentum space. Suppose  $\varepsilon(p)$  has two minima at  $p=p_1$  and  $p_2$ . Let us consider two particles. If there is no interaction, the energy of the symmetric (or boson) ground state is degenerate with that of the antisymmetric (or fermion) ground state. Suppose there acts interaction between particles of the form

 $V_{ijhl} = V\delta_{il}\delta_{jk}\delta_{ij}$  with V>0, i.e. a repulsive potential acts only when two particles are at the same lattice site. The energy of fermions is not affected by this interaction, for two fermions never come together on the same site. On the other hand the energy of bosons always increases by introduction of a repulsive interaction. Thus we see in this particular case that the ground-state energy of fermions is lower than that of bosons. It will be an interesting but difficult problem to examine what conditions should be imposed upon Hamiltonian for the theorem to hold.

4.3. Another interesting generalization of the theorem is to consider a system of charged particles in an external magnetic field. In this case wave functions cannot be taken as real functions and a straightforward generalization of the proof is impossible. If  $\psi$  is complex, the existence of the nodal plane on which  $\psi(r)=0$  does not result from the antisymmetric property of the function. We can find for example a plane P on which  $\text{Re }\psi=0$ . However, if we introduce  $\bar{\psi}$  by

$$ar{\psi}(r)\!=\!egin{cases} \psi(r) & r\!\in\!\Omega_+ \ -\psi(r) & r\!\in\!\Omega_- \,, \end{cases}$$

with a similar definition of  $\Omega_{\pm}$  as before,  $\bar{\Psi}$  is discontinuous in its value on P. Therefore, the last integral in Eq. (16) gives a finite contribution even in the limit  $\eta \rightarrow 0$ , and we cannot obtain Eq. (17). One way to construct a modified function which is continuous on P is to define  $\bar{\Psi}$  by

$$ar{\psi}(r) = egin{cases} \psi(r) & r \in \Omega_+ \ -\psi^*(r) & r \in \Omega_- \end{cases}$$

In this case, however,  $\psi^*$  is an eigenfunction with a different energy from that of  $\psi$ , and the first two integrals of Eq. (16) does not give E.

These considerations seem to suggest that the theorem does not hold generally in this case. At least it is not valid in its original form, since we can easily find an example in which the ground-state energy of fermions is the same as that of bosons. It is a simple case of non-interacting particles in a uniform magnetic field. The lowest Landau level in a uniform field is degenerate, and its degeneracy increases with increasing strength of the field. Therefore, if the field is sufficiently strong, or the number of particles is sufficiently small, the energy of the ground state, in which all particles occupy the lowest level, is clearly the same for fermions and bosons. It is very plausible that it becomes lower for fermions than for bosons by introduction of an appropriate repulsive interaction.

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It is our great pleasure to dedicate this paper to Professor M. Kobayasi in celebration of his sixtieth birthday.

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1) R. P. Feynman, Phys. Rev. 94 (1954), 262.