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TRANSFORMATION RULES FOR THE FIELD AND PARTICLE OPERATORS UNDER THE TIME REVERSAL (NONRELATIVISTIC CASE)

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1. INTRODUCTION

One of the most important aims of the statistical mechanics is to calculate mean values of various variables. For systems of interacting particles it is not trivial task to compute these mean values. In order to diminish the computation work one uses some sum rules and selection rules. The selection rules couple different components of tensors, real and imaginary parts of Fourier transforms, etc. They follow from symmetries of considered systems (cf. for example the paper by Bogolubov /1/). It is well known that one of the most restrictive symmetry property in this respect is an invariance under the time reversal (cf. for example Götze and Michel /2/ or Paszkiewicz /3/). Since usually the variables of quantum statistical mechanics are expressed in terms of field operators or even more frequently in terms of particle operators, the knowledge of the transformation properties of these basic operators is very useful. It seems that this problem has not been discussed in the frame of nonrelativistic quantum mechanics. The discussion given in quantum field theory (cf. for example Källén /4/) is not very well suited for the purposes of nonrelativistic quantum statistical mechanics. So, we shall give a simple and complete discussion of this topic.

2. TRANSFORMATION PROPERTIES OF THE FIELD AND PARTICLE OPERATORS

As usually in nonrelativistic quantum statistical mechanics we shall limit ourselves to the case of spinless bosons and spin-1/2 fermions. Our discussion can be generalized to more complicated cases.

Let us begin from a simpler case of spinless bosons. Denote an arbitrary n -particle state vector Φ_n and an arbitrary case vector in the position basis by $\Psi_{r_1 \dots r_n}$. For a matrix element of the time reversal operator θ we have (Wigner /5/)

$$(\Psi_{\vec{r}_1 \dots \vec{r}_n}, \theta\, \Phi_n) = (\Psi_{\vec{r}_1 \dots \vec{r}_n}, \Phi_n)^* = \Phi_n^* (\vec{r}_1, \dots, \vec{r}_n), \tag{1}$$

$\Phi_n(\vec{r}_1,...,\vec{r}_n)$ being the n-particle wave function. In order to establish the transformation properties of the field operators $\psi(\vec{r})$ we shall use the formula connecting the wave function $\Phi_n(\vec{r}_1,...,\vec{r}_n)$ with the mean value of the product of field operators (cf. for example Robertson /6/)

$$\Phi_n(\vec{r}_1,...,\vec{r}_n) = \frac{1}{\sqrt{n!}}(\Omega_0, \psi(\vec{r}_1)...\psi(\vec{r}_n)\Phi_n),$$

where Ω_0 is the nondegenerate vacuum of particles. Consider the time reversed state $\theta\Phi_n$. Since the vacuum state is invariant under the time reversal we have

$$(\Omega_0, \psi(\vec{r}_1)...\psi(\vec{r}_n)\theta\Phi_n) = (\theta\Omega_0, \psi(\vec{r}_1)...\psi(\vec{r}_n)\theta\Phi_n) = \tag{2}$$

$$= (\Omega_0, \theta^{-1}\psi(\vec{r}_1)\theta ... \theta^{-1}\psi(\vec{r}_n)\theta\Phi_n)^*.$$

Comparing this formula with Eq.(1) we see that it is consistent to set

$$\theta\psi(\vec{r})\theta^{-1} = \psi(\vec{r}), \qquad \theta\psi^+(\vec{r})\theta^{-1} = \psi^+(\vec{r}). \tag{3}$$

This means that for the time dependent operators we get

$$\theta\psi(\vec{r},t)\theta^{-1} = \psi(\vec{r},-t), \qquad \theta\psi^+(\vec{r},t)\theta^{-1} = \psi^+(\vec{r},-t),$$

where for example

$$\psi(\vec{r},t) = e^{\frac{iHt}{\hbar}}\psi(\vec{r})e^{-\frac{iHt}{\hbar}}.$$

Analogously, using the transformation rules for Pauli-spinors in the position basis (Wigner /5/), we obtain for the spin -1/2 particles

$$\theta\psi_{\frac{1}{2}s}(\vec{r},t)\theta^{-1} = (-1)^{\frac{1}{2}(s+1)}\psi_{-\frac{1}{2}s}(\vec{r},-t),$$

$$\theta\psi^+_{\frac{1}{2}s}(\vec{r},t)\theta^{-1} = (-1)^{\frac{1}{2}(s+1)}\psi^+_{-\frac{1}{2}s}(\vec{r},-t), \tag{4}$$

where $s = \pm 1$.

Since the field operators are not measurable, the transformation rules (3), (4) are not unique. This is a quite general property. For example, in the quantum field theory two different rules are used. One of them was proposed by Wigner and another one by Schwinger (cf. Källen /4/).

The occupation number representation requires the introduction of the complete orthonormal set of one-particle wave functions $\{u_n(\vec{r})\}$. The field operators are expanded in terms of this set. e.g.,

$$\psi(\vec{r}) = \sum_n u_n(\vec{r})a_n .$$

With the use of the transformation rules (3) and the orthonormality condition for the set $\{u_n(\vec{r})\}$, the transformation properties of the annihilation and creation operators can be easily established. For example

$$\theta a_n \theta^{-1} = \sum_{n'} \int d^3\vec{r}\, u_n(\vec{r})u_{n'}(\vec{r})a_{n'}, \tag{5}$$

$$\theta a_{n,\frac{1}{2}s}\theta^{-1} = \sum_{n'}(-1)^{\frac{1}{2}(s+1)}\int d^3r\, u_n(\vec{r})u_{n'}(\vec{r})a_{n',-\frac{1}{2}s}. \tag{6}$$

For the complete set of plane waves in a box of the volume V we have

$$u_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}}e^{i\vec{k}\vec{r}},$$

where $\vec{k}$ is a wave vector. From Eqs. (5) and (6) one can deduce that

$$\theta a_{\vec{k}}\theta^{-1} = a_{-\vec{k}}, \quad \theta a_{\vec{k},\frac{1}{2}s}\theta^{-1} = (-1)^{\frac{1}{2}(1+s)}a_{-\vec{k},-\frac{1}{2}s}. \tag{7}$$

Note that the first rule differs from those proposed by Enz for the phonon operators/7/.

Let us consider two simple examples of the derivation of the transformation rules for physical variables. Using the relation (3) one can easily check that the current density operator $\vec{j}(\vec{r})$

$$\vec{j}(\vec{r}) = \frac{\hbar}{2mi}[\psi^+(\vec{r})\nabla\psi(\vec{r}) - (\nabla\psi^+(\vec{r}))\psi(\vec{r})]$$

is odd under time reversal

$$\theta\vec{j}(\vec{r})\theta^{-1} = -\vec{j}(\vec{r}).$$

The second example is the Fourier transform of the spin density operator $\vec{s}_{\vec{k}}$

$$\vec{s}_{\vec{k}} = \frac{1}{2}\sum_{\vec{q},s,s'}(\vec{\sigma})_{ss'}\, a^+_{\vec{q}-\vec{k},\frac{1}{2}s}\, a_{\vec{q},\frac{1}{2}s'},$$

where $\vec{\sigma}$ is the vector which components are the Pauli matrices. The second of the relations (7) and the corresponding relation for the creation operator imply that

$$\theta \vec{s}_{\vec{k}}\, \theta^{-1} = -\vec{s}_{-\vec{k}} \ .$$

3. THE EXAMPLE

Now we can present a simple example of the selection rule which follows from the established transformation rules. For this purpose we shall consider the mean value of an operator A in the time reversed basis which we shall denote using the index $(-\vec{h})$, where $\vec{h}$ is a vector of the strength of a magnetic field or the angular velocity. We shall use the formula (Zubarev /8/)

$$<\theta A \theta^{-1}>_{-\vec{h}} = <A>^{*}_{\vec{h}} = <A^{+}>_{\vec{h}} \ , \qquad (8)$$

where $<A>$ means the expectation value of the variable A for the system in the thermodynamic equilibrium. As a simple example we take the density of electrons

$$A = \psi^{+}_{\frac{1}{2}s}(\vec{r})\, \psi_{\frac{1}{2}s}(\vec{r}).$$

Relations (4) and (8) yield

$$<\theta\ \psi^{+}_{\frac{1}{2}s}(\vec{r})\, \psi_{\frac{1}{2}s}(\vec{r})\theta^{-1}>_{-\vec{h}} = <\psi^{+}_{-\frac{1}{2}s}(\vec{r})\, \psi_{-\frac{1}{2}s}(\vec{r})>_{-\vec{h}} \ ,$$

$$<\theta\, \psi^{+}_{\frac{1}{2}s}(\vec{r})\ \psi_{\frac{1}{2}s}(\vec{r})\theta^{-1}>_{-\vec{h}} = <\psi^{+}_{\frac{1}{2}s}(\vec{r})\, \psi_{\frac{1}{2}s}(\vec{r})>^{*}_{\vec{h}} = <\psi^{+}_{\frac{1}{2}s}(\vec{r})\, \psi_{\frac{1}{2}s}(\vec{r})>_{\vec{h}}$$

Therefore the above formulas imply that

$$<\psi^{+}_{\frac{1}{2}s}(\vec{r})\, \psi_{\frac{1}{2}s}(\vec{r})>_{\vec{h}} = <\psi^{+}_{-\frac{1}{2}s}(\vec{r})\, \psi_{-\frac{1}{2}s}(\vec{r})>_{-\vec{h}} .$$

For a vanishing external field we obtain the obvious relation

$$<\psi^{+}_{\frac{1}{2}s}(\vec{r})\, \psi_{\frac{1}{2}s}(\vec{r})> = <\psi^{+}_{-\frac{1}{2}s}(\vec{r})\, \psi_{-\frac{1}{2}s}(\vec{r})> .$$

Less trivial relations can be derived for the time dependent correlation functions or for Green functions.

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