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The Number of Levels of a Fermion System in a Parabolic Potential

Naoyo Matsushita (松 下 直 代) **and Giiti Iwata** (岩 田 義 一)

Department of Physics, Faculty of Science,
Ochanomizu University, Tokyo

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The grand partition function specified by the total particle number, the z-component of the total angular momentum and the total energy of a fermion system composed of particles moving independently in a central potential field is set up and evaluated approximately for a parabolic potential field. The distribution of the number of levels with respect to the z-component of the total angular momentum is found to be Gaussian with the dispersion roughly proportional to the four thirds power of the total number.

§1. Introduction

In his classical paper, Bethe[1] has initiated to calculate the energy level density of a heavy nucleus, starting from the statistical model of the nucleus. After him many authors[2][3][4] have treated the same problem. They have used in common the nucleus model consisting of independent particles in a central field, the partition function method of Sommerfeld, and the Gaussian distribution law for angular momenta, which law has been introduced, so to speak, ad hoc. The importance of angular momenta has been emphasized by all. Nevertheless the angular momenta seem to have so far received no legitimate treatment according to quantum mechanics. The difficulty springs from the composition rule of angular momenta. The representation theory of the rotation group informs us that the number of states with total angular momentum J is equal to the number of states with $M=J$, minus the number of states with $M=J+1$, M standing for the z-component of the total angular momentum.

To get the number of states with $M=J$, an ad hoc approach of the probabilistic view point has been taken so far instead of the consistent use of the partition function.

The energy of a particle moving in a central field, however, depends usually on its angular momentum and the agular momenta should be added according to quantum mechanics. The above remark, though theoretically obvious and evident, has so far completely been ignored to avoid the difficulty that might be aroused. Our aim in the present paper is the construction of the consistent partition function of a fermion system in a central field by the use of characters of the rotation group and an approximate evaluation of the ensuing partition function.

§ 2. The factorization of the partition function

Our system is assumed to be composed of fermion particles of spin 1/2 moving independently in a central field $V(r)$. A state of the system is marked by the total particle number N, the total energy E and the z-component M of the total angular momentum J.

We take the grand partition function Z defined by

$$Z = \text{trace } \exp[\alpha \boldsymbol{N} - \beta \boldsymbol{E} + \gamma \boldsymbol{M}] \tag{1}$$

instead of the partition function Ξ

$$\Xi = \text{trace } \exp[\alpha \boldsymbol{N} - \beta \boldsymbol{E} + \gamma \boldsymbol{J}] \tag{2}$$

since Z is more elemental than Ξ and gives Ξ by an integral transformation.

Eigenstates of the particle of spin 1/2 moving in the central field $V(r)$ may be marked by the angular momentum l, the z-component m of the angular momentum, the z-component s of the spin and the radial quantum number n.

The angular momentum l assumes discrete integers $0, 1, 2, \cdots$, the z-component m of the angular momentum l ranging over $-l, -l+1, \cdots, l$, and the radial quantum number ranging over $1, 2, 3, \cdots$.

If the energy of the eigenstate n, l, m, s is denoted by ϵ_{nlms}, the occupation number by ν_{nlms}, one sees that the total number N and the total energy E are obtained by adding up the contribution from each eigenstate, as follows

$$\boldsymbol{N} = \sum_{nlms} \nu_{nlms} \tag{3}$$

$$\boldsymbol{E} = \sum_{nlms} \epsilon_{nlms} \nu_{nlms} \tag{4}$$

the summation over n, l, m, s summarizing the summation over $n=1, 2, 3, \cdots$, $l=0, 1, 2, \cdots$, $m=-l, -l+1, \cdots, l$, and $s=-1/2, 1/2$.

It is to be noted that the occupation number ν_{nlms} takes 2 values 0 and 1 by virtue of the Pauli principle.

While the total angular momentum cannot be expressed with the occupation numbers ν_{nlms} so directly, the z-component M of the total angular momentum may be expressed as follows,

$$\boldsymbol{M}=\sum_{nlms}(m+s)\,\nu_{nlms} \tag{5}$$

since the z-component of the total angular momentum of any two eigenstates is the sum of the z-components of two eigenstates. So we have

$$\begin{aligned} Z &= \text{trace}\ \exp\Big[\sum_{nlms}\{(\alpha-\beta\epsilon_{nlms}+\gamma(m+s))\nu_{nlms}\}\Big] \\ &= \prod_{nlms}[1+\exp(\alpha-\beta\epsilon_{nlms}+\gamma(m+s))]\,. \end{aligned} \tag{6}$$

When the energy ϵ_{nlms} is independent of m and s, Z may be written

$$Z=\prod_{nlm}(1+z_{nl}\zeta^{m+1/2})(1+z_{nl}\zeta^{-m-1/2}) \tag{7}$$

where $z_{nl}=\exp(\alpha-\beta\epsilon_{nlms})$ and $\zeta=\exp(\gamma)$.

§ 3. The relation of Z and Ξ

If we regard ζ as a complex variable, Z can be expanded into a power series

$$Z=\sum_{M=-\infty}^{\infty}Z^M\zeta^M \tag{8}$$

$2M$ ranging over all integers. From (7) it is evident that $Z_{-M}=Z_M$.

If we expand Ξ into a power series

$$\Xi=\sum_{J=0,\,1/2,\,1,\,\cdots}\Xi_J\zeta^J \tag{9}$$

the representation theory of the rotation group shows that

$$\Xi_J=Z_J-Z_{J+1}\,. \tag{10}$$

If we denote the sum $\zeta^J+\zeta^{J-1}+\cdots+\zeta^{-J}$ by χ_J, we see then that

$$\begin{aligned} Z &= Z_0+Z_{1/2}(\zeta^{1/2}+\zeta^{-1/2})+Z_1(\zeta+\zeta^{-1})+Z_{3/2}(\zeta^{3/2}+\zeta^{-3/2})+\cdots \\ &= Z_0\chi_0+Z_{1/2}\chi_{1/2}+Z_1(\chi_1-\chi_0)+Z_{3/2}(\chi_{3/2}-\chi_{1/2})+\cdots \\ &= (Z_0-Z_1)\chi_0+(Z_{1/2}-Z_{3/2})\chi_{1/2}+(Z_1-Z_2)\chi_1+\cdots \\ &= \Xi_0\chi_0+\Xi_{1/2}\chi_{1/2}+\Xi_1\chi_1+\cdots\,. \end{aligned}$$

In brief, the Ξ_J is the coefficient of χ_J in the expansion of Z in a series in χ_J. If we put $\gamma=i\theta$, the χ_J is nothing but the character of the representation $\mathfrak{D}_J$, θ denoting the angle of the rotation around the z-axis. The orthogonality relation of the characters

$$\frac{1}{\pi}\int_0^{2\pi}\chi_J(\theta)\chi_{J'}(\theta)\sin^2\frac{\theta}{2}\,d\theta=\delta_{JJ'}$$

allows us to deduce that

$$\Xi_J = \frac{1}{\pi}\int_0^{2\pi} Z(\theta)\chi_J(\theta)\sin^2\frac{\theta}{2}\,d\theta \tag{12}$$

$$\Xi = \frac{1}{\pi}\int_0^{2\pi} Z(\theta')\sum_J \zeta^J \chi_J(\theta')\sin^2\frac{\theta'}{2}\,d\theta' . \tag{13}$$

§ 4. An approximate evaluation of $\log Z$

In the infinite product (7), the product of two terms

$$(1+z_{nl}\zeta^{m+\frac{1}{2}})(1+z_{nl}\zeta^{-m-\frac{1}{2}})$$

may be modified as follows

$$1+2z_{nl}\cosh\left(m+\frac{1}{2}\right)\gamma + z^2_{nl} = (1+z_{nl})^2 + 4z_{nl}\sinh^2\frac{2m+1}{4}\gamma$$

so that one may rewrite

$$Z = \prod_{nlm}\left\{(1+z_{nl})^2 + 4z_{nl}\sinh^2\frac{2m+1}{4}\gamma\right\} . \tag{14}$$

Therefore one gets, up to the second order in γ,

$$\begin{aligned} &\log Z = p + q\gamma^2 + 0(\gamma^4) \\ &\quad p = 2\sum_{nlm}\log(1+z_{nl}) \\ &\quad q = \frac{1}{16}\sum_{nlm}\frac{4z_{nl}}{(1+z_{nl})^2}(2m+1)^2 . \end{aligned} \tag{15}$$

To evaluate p and q, we use a parabolic potential field such that the energy of a particle there is given by $(2(n-1)+l)\epsilon$, ϵ being an appropriate unit of energy.

The first sum p may be evaluated by the method of Sommerfeld or by the use of the formula of Mellin transform

$$\log(1+x) = \frac{1}{2\pi i}\int\frac{\pi}{s\sin\pi s}x^s ds \qquad 0<\Re s\equiv\sigma<1 \tag{16}$$

the path of integration extending from $\sigma - i\infty$ to $\sigma + i\infty$, as follows,

$$\begin{aligned} p &= 2\sum_{nlm}\log(1+z_{nl}) = 2\sum_{nl}(2l+1)\log(1+e^{\alpha-\beta\epsilon(2n-2+l)}) \\ &= \frac{1}{2\pi i}\int\frac{\pi}{s\sin\pi s}e^{\alpha s}\frac{2}{(1-e^{-\beta\epsilon s})^3}ds \\ &= \delta\left(\frac{1}{12}\xi^4 + \frac{1}{2}\xi^3 + \xi^2 + \frac{3}{4}\xi\right) \\ &\quad + \frac{1}{\delta}\frac{\pi^2}{6}(\xi^2+3\xi) + \cdots \end{aligned} \tag{17}$$

where $\delta=\beta\epsilon$ and $\xi=\alpha/\delta$.

The second sum may be approximated by collecting the terms in which $\alpha-\beta\epsilon_{nl}\approx 0$ since the term $4x/(1+x)^2$ has its maximum 1 at $x=1$ dropping sharply away from there. We have then

$$q=\frac{1}{16}\sum_{nl}\frac{4z_{nl}}{(1+z_{nl})^2}\,\frac{8l^3+12l^2+10l+3}{3}$$

$$\doteqdot\frac{1}{48}\sum_{l=0,2,\cdots}^{\alpha/\delta}(8l^3+12l^2+10l+3)$$

$$\doteqdot\frac{1}{48}\left\{\xi^4+6\xi^3+\frac{25}{2}\xi^2+\frac{21}{2}\xi\right\}. \tag{18}$$

§ 5. An approximate evaluation of the number of levels

The infinite product (7) of Z may be converted into an infinite series

$$Z=\sum_{N,M,E}L(N,M,E)\exp(\alpha N+\gamma M-\beta E)$$

the summations being taken over total particle number $N=0, 1, 2, \cdots$, the z-component M of the total angular momentum, $M=0, \pm 1/2, \cdots$, and the total energy $E=0, \epsilon, 2\epsilon, \cdots$. The $L(N, M, E)$ denotes the number of states or levels specified by N, M and E.

The number of levels L may be determined by the Fourier transform of the Z as

$$L(N,M,E)=\frac{1}{(2\pi i)^2}\int_{-\pi i}^{\pi i}d\alpha\int_{-\pi i}^{\pi i}d\beta\, Z_M\exp(-\alpha N+\beta E)$$

$$Z_M=\frac{1}{4\pi i}\int_{-2\pi i}^{2\pi i}Z\cdot\exp(-\gamma M)d\gamma\,.$$

An approximate value of Z_M is given by the substitution of $p+q\gamma^2$ for $\log Z$ and by extending the range of integration infinitely as

$$Z_M=\frac{1}{4\pi}\sqrt{\frac{\pi}{q}}\exp\left(p-\frac{M^2}{4q}\right).$$

The saddle point method may give an approximate value of L

$$L(N,M,E)=(\text{the value of }\exp F\text{ at the saddle})/2\pi D^{1/2}$$

$$F=\log Z_M-\alpha N+\beta E$$

where the parameters α, β are determined by the saddle condition $F=$stationary,

$$\frac{\partial F}{\partial\alpha}=0\qquad\frac{\partial F}{\partial\beta}=0$$

D standing for the determinant

$$D=\begin{vmatrix} \dfrac{\partial^2 F}{\partial \alpha^2} & \dfrac{\partial^2 F}{\partial \alpha \partial \beta} \\ \dfrac{\partial^2 F}{\partial \alpha \partial \beta} & \dfrac{\partial^2 F}{\partial \beta^2} \end{vmatrix}_{\text{at the saddle.}}$$

With the notations $\epsilon\beta=\delta$ and $\alpha/\delta=\xi$, the F will, up to the order δ^{-1}, be

$$F=\delta f(\xi)+g(\xi)+\frac{1}{\delta}h(\xi)+\delta\left(\frac{E}{\epsilon}-N\xi\right)$$

$$f(\xi)=\frac{1}{12}\xi^4+\frac{1}{2}\xi^3+\xi^2+\frac{3}{4}\xi$$

$$g(\xi)=-\frac{M^2}{4q(\xi)}-\frac{1}{2}\log q(\xi)-\log 4\sqrt{\pi}$$

$$h(\xi)=\frac{\pi^2}{6}(\xi^2+3\xi)\,.$$

If the values of ξ and E at $\delta=\infty$ are denoted by ξ_0 and E_0, the parameters at the saddle point and the value of F will be given by

$$\xi=\xi_0-\frac{g'_0}{\delta f''_0}$$

$$\delta=\sqrt{\left\{\frac{\epsilon}{E-E_0}\cdot\frac{2h_0f''_0-g'^2_0}{2f''_0}\right\}}$$

$$F_{\text{saddle}}=g_0+\sqrt{\frac{(E-E_0)(2h_0f_0''-g'^2_0)}{2f_0''\epsilon}}$$

the suffix 0 attached to f, g or h denoting the value at $\xi=\xi_0$. Since

$$f'(\xi_0)=N\,;\qquad E_0=\epsilon(N\xi_0-f(\xi_0))$$

ξ_0 is determined solely by the total particle number N.

In our approximation the distribution of L with respect to M is substantially Gaussian with the dispersion $\sigma^2=2q(\xi_0)$, which is roughly equal to $6^{1/3}N^{4/3}/8$ and is independent of the total energy E.

The above calculation shows that the number of levels with total angular momentum J, that is given by $L(N, J, E)-L(N, J+1, E)$, is roughly proportional to

$$(2J+1)\exp\left(-\frac{J(J+1)}{2\sigma^2}\right).$$

This is rather satisfactory in view of the numerical calculations of Critchfield and Oleksa.[5)2)]

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