Probability distribution function in the gas of paramagnetic particles

E. V. Goldstein
Optical Sciences Center, University of Arizona, Tucson, Arizona 85721

Yu. Sadaui and V. M. Tsukernik
Physics Department, Kharkov State University, Kharkov 310077, Ukraine
(Received 7 August 1992)

In this paper we consider a system of noninteracting paramagnetic particles with a spin S in a dc magnetic field. The exact expression for the probability distribution function of a transverse spin component is obtained for the gas in thermodynamic equilibrium. Dependences of the probability on the thermofield parameter $\beta\mu H$ (β is the inverse temperature, μ is the Bohr magneton, H is a field strength) and S are investigated. It is shown that this distribution reflects the quantum nature of the spin and both the spin-wave and the classical approximation formulas are obtained.

PACS number(s): 05.70.Ce, 03.65.Ca, 05.30.−d, 32.60.+i

An electrically neutral quantum particle with spin S in an external magnetic field is described with the simplest Zeeman Hamiltonian [1]

$$\mathcal{H}=-2\mu\mathbf{H}\cdot\hat{\mathbf{S}} , \tag{1}$$

where $\mathbf{H}$ is a field strength, μ is the Bohr magneton, and $\hat{\mathbf{S}}$ is a spin operator. If the field $\mathbf{H}$ is constant its direction can always be chosen as z and the eigenvalues of the Hamiltonian will be

$$E_{\sigma_z}=-2\mu H\sigma_z . \tag{2}$$

Here $H\equiv H_z$, and $\sigma_z=-S,-S+1,\ldots,S$, where S is the value of the spin. In the case when the gas of the particles with the magnetic moment $2\mu S$ is in a stationary and homogeneous magnetic field in equilibrium with thermostat with temperature $T=1/\beta$ its state can be described with the Gibbs density matrix [2]

$$\hat{\rho}=\mathcal{Z}^{-1}\exp(-\beta\mathcal{H}) , \tag{3}$$

where $\mathcal{Z}=\mathrm{Sp}(e^{-\beta\mathcal{H}})$ is a partition function. From (3) it is easy to derive the probability distribution w_{σ_z} for the longitudinal spin component $\hat{S}_z$,

$$w_{\sigma_z}=\mathcal{Z}^{-1}e^{2\beta\mu H\sigma_z} . \tag{4}$$

Dependence of the probability (4) on the thermofield parameter $v=\beta\mu H$ is universal, i.e., its behavior does not depend on the spin value S. Particularly, for arbitrary S, w_{σ_z} decreases with v if $\sigma_z\le 0$, increases if $\sigma_z=S$, has a maximum for the finite values of v if $0<\sigma_z<S$, and goes to zero in the limit $v\to\infty$. Because of this property, v dependences of the quantum distribution function (Brillouin function) and its classical counterpart (Langevin function) are qualitatively indistinguishable [3].

The quantum nature of the spin can be seen explicitly from the probability distribution of the transverse component of the spin in a constant magnetic field. In this paper we demonstrate that the v dependence of the corresponding function is determined by the value of S. In particular, it is shown that v dependences of the quantum probability function and its classical counterpart, which corresponds to the limit $S\to\infty$, $\mu\to 0$, $2\mu S=m$, are different.

To obtain the probability distribution function the generalized coherent state representation [4] is used. This representation allows us to construct the generating function for the corresponding matrix elements from a partial differential equation of first order.

The probability for the spin component $\hat{S}_x$ to have the eigenvalue σ in the state described by the density matrix (3) is the diagonal matrix element

$$w_\sigma=\langle\sigma|\hat{\rho}|\sigma\rangle=\mathcal{Z}^{-1}\langle\sigma|e^{2v\hat{S}_z}|\sigma\rangle , \tag{5}$$

where $|\sigma\rangle$ is an eigenstate of the $\hat{S}_x$ operator

$$\hat{S}_x|\sigma\rangle=\sigma|\sigma\rangle,\quad \sigma=-S,-S+1,\ldots,S . \tag{6}$$

It is possible to use formula (5) directly to obtain w_σ for small values of the parameter v, expanding (5) in series in v. For arbitrary values of v an expression for w_σ can be derived with the generating function

$$\mathcal{F}(z,z^*,v)=\langle z|e^{2v\hat{S}_z}|\sigma\rangle , \tag{7}$$

where $|z\rangle$ is a normalized generalized coherent state vector [4] defined as

$$|z\rangle=(1+|z|^2)^{-S}e^{z\hat{S}^-}|S\rangle . \tag{8}$$

Here $\hat{S}^-\equiv\hat{S}_x-\iota\hat{S}_y$ is the annihilation spin operator, $|S\rangle$ is an eigenvector of the $\hat{S}_z$ operator with a maximum eigenvalue S, and z is a complex variable. Vectors (8) are not orthogonal, but they form a complete system where the expansion of the unitary operator is

$$\frac{2S+1}{\pi}\int\frac{d^2z}{(1+|z|^2)^2}|z\rangle\langle z|=\hat{I} \tag{9}$$

Here $d^2z=d(\mathrm{Re}z)d(\mathrm{Im}z)$ and integration is performed over the entire complex plane z. In this representation the wave function is $\langle z|\psi\rangle=(1+|z|^2)^{-S}\varphi(z^*)$, where

$\varphi(z^*)$ is a polynomial in z^* with a power not exceeding $2S$ and the operators $\hat{S}_z$ and $\hat{S}^{\pm}=\hat{S}_x \pm \iota \hat{S}_y$ have the form

$$\langle z|\hat{S}_z=\langle z|[S-z^*(\partial/\partial z^*)],\quad \langle z|\hat{S}^+=\langle z|(\partial/\partial z^*)\ ,$$
$$\langle z|\hat{S}^-=\langle z|[2Sz^*-z^{*2}(\partial/\partial z^*)]\ . \tag{10}$$

Considering the function $f(z^*,v)\equiv(1+|z|^2)^S\mathcal{F}(z,z^*,v)$ and differentiating it in v, one obtains the partial differential equation

$$(\partial f/\partial v)+2z^*(\partial f/\partial z^*)=2Sf\ , \tag{11}$$

the general solution of which has the form

$$f(z^*,v)=e^{2Sv}\chi(z^*e^{-2v})\ , \tag{12}$$

where χ is an arbitrary function. To determine χ one can use an "initial condition" $\mathcal{F}(z,z^*,0)=\langle z|\sigma\rangle$, which follows from (7). The function $\langle z|\sigma\rangle$ is an eigenvector of the operator $\hat{S}_x$ in a coherent state representation,

$$\langle z|\hat{S}_x|\sigma\rangle=\sigma\langle z|\sigma\rangle\ , \tag{13}$$

and using (10) we have

$$\langle z|\hat{S}_x|\sigma\rangle=\tfrac{1}{2}(1+|z|^2)^{-S}[2Sz^*+(1-z^{*2})(\partial/\partial z^*)]$$
$$\times(1+|z|^2)^S\langle z|\sigma\rangle\ . \tag{14}$$

Comparing (13) and (14) one obtains the equation for $\langle z|\sigma\rangle$,

$$\tfrac{1}{2}(1-z^{*2})(\partial\varphi/\partial z^*)+Sz^*\varphi=\sigma\varphi\ , \tag{15}$$

with $\varphi\equiv(1+|z|^2)^S\langle z|\sigma\rangle$, the normalized solution of which is

$$\varphi_\sigma(z^*)=(C_{2S}^{S-\sigma}/2^{2S})^{1/2}(1-z^*)^{S-\sigma}(1+z^*)^{S+\sigma}\ . \tag{16}$$

Here $C_{2S}^{S-\sigma}$ is a binomial coefficient.

Substitution of (16) in (12) gives an expression for the generating function:

$$\mathcal{F}(z,z^*,v)=e^{2Sv}(C_{2S}^{S-\sigma}/2^{2S})^{1/2}(1+|z|^2)^{-S}$$
$$\times(1-z^*e^{-2v})^{S-\sigma}(1+z^*e^{-2v})^{S+\sigma} \tag{17}$$

or

$$\mathcal{F}(z,z^*,v)=e^{2Sv}(C_{2S}^{S-\sigma}/2^{2S})^{1/2}(1+|z|^2)^{-S}(1+z^*)^{2S}$$
$$\times\{\cosh v+[(1-z^*)/(1+z^*)]\sinh v\}^{S+\sigma}$$
$$\times\{\sinh v+[(1-z^*)/(1+z^*)]\cosh v\}^{S-\sigma}\ . \tag{18}$$

From the definition (7) of the generating function and expression (16) it follows that

$$\mathcal{F}(z,z^*,v)=\sum_{\sigma'}\langle z|\sigma'\rangle\langle\sigma'|e^{2v\hat{S}_z}|\sigma\rangle$$
$$=(1+|z|^2)^{-S}\sum_{\sigma'}(C_{2S}^{S-\sigma'}/2^{2S})^{1/2}\langle\sigma'|e^{2v\hat{S}_z}|\sigma\rangle(1+z^*)^{S+\sigma'}(1-z^*)^{S-\sigma'}\ . \tag{19}$$

On the other hand, the product of the binomials in (18) is a generating function for Jacobi polynomials [5,6],

$$(\cosh v+x\sinh v)^{2S-n}(\sinh v+x\cosh v)^n=\cosh^{2S}v\sum_{m=0}^{2S}x^m[n!(2S-n)!/m!(2S-m)!]^{1/2}(q_2!p_1!/q_1!p_2!)^{1/2}$$
$$\times(\tanh v)^{\min(n,m)-q_2}(\tanh v)^{\min(2S-n,2S-m)-q_2}(1-\tanh^2 v)^{q_2}P_{q_2}^{(p_2-q_2,p_1-q_2)}(\cosh 2v)\ , \tag{20}$$

where $n=S-\sigma$ $(n=0,1,\dots,2S)$, $q_2=\min(m,n,2S-n,2S-m)$, $p_1=\max(m,n,2S-n,2S-m)$, and $q_1+q_2=p_1+p_2=2S$.

The probability distribution function is a diagonal matrix element ($\sigma=\sigma'$). From the symmetry of the system it follows that the probability of interest does not depend on the sign of σ. We shall demonstrate this explicitly below; now we shall assume that $\sigma\geq 0$ for definiteness. Comparing (19) and (20) one obtains

$$\langle\sigma|e^{2v\hat{S}_z}|\sigma\rangle=\cosh^{2\sigma}v\,P_{S-\sigma}^{(0,2\sigma)}(\cosh 2v)\ . \tag{21}$$

Taking into consideration that the partition function for the system (2) is $Z=\sinh(2S+1)v/\sinh v$, the expression for the probability distribution is

$$w_\sigma=[\sinh v/\sinh(2S+1)v]\cosh^{2\sigma}v\,P_{S-\sigma}^{(0,2\sigma)}(\cosh 2v)\ . \tag{22}$$

To investigate the dependence of the probability w_σ on the thermofield parameter v and to obtain asymptotic results for $S\to\infty$ it is more convenient to use the integral representation of (22). To obtain an integral form of (22) one can multiply (16) by $\langle\sigma|z\rangle$ and integrate over z. Using expansion (19) and the orthonormalization of $\langle\sigma|z\rangle$ one has

$$w_\sigma=Z^{-1}(c_{2S}^{S-\sigma}e^{2vS}/2^{2S})[(2S+1)/\pi]$$
$$\times\int\frac{d^2z}{(1+|z|^2)^{2S+2}}(1+z)^{S+\sigma}(1-z)^{S-\sigma}$$
$$\times(1+z^*e^{-2v})^{S+\sigma}(1-z^*e^{-2v})^{S-\sigma}\ . \tag{23}$$

One can notice here that after switching to polar coordinates in the complex z plane ($z=|z|e^{\iota\phi}$) and carrying out the integration over phase ϕ the integrand depends only on $|z|^2$. Hence e^{-v} can be distributed arbitrarily between z and z^* and the following expression for w_σ can be obtained:

$$w_\sigma=Z^{-1}(c_{2S}^{S-\sigma}e^{2vS}/2^{2S})[(2S+1)/\pi]$$
$$\times\int\frac{d^2z}{(1+|z|^2)^{2S+2}}|(1+ze^{-v})^{S+\sigma}(1-ze^{-v})^{S-\sigma}|^2\ , \tag{24}$$

which is symmetric in $\pm\sigma$.

As pointed out above, the dependence of the probability w_σ on v as $v\ll 1$ can be obtained directly from (5).

The expansion in powers of v is

$$w_\sigma=[1/(2S+1)]\{1+[\tfrac{1}{3}S(S+1)-\sigma^2]v^2\} . \tag{25}$$

For $v=0$ formula (25) gives equal probabilities $w_\sigma=(2S+1)^{-1}$, which are independent of σ. This means that there is not any chosen direction in zero external field. If $v\neq 0$ the additional term in (25) is positive for $\sigma^2<\frac{1}{3}S(S+1)$, and negative for $\sigma>\frac{1}{3}S(S+1)$. In the case $\sigma^2=\frac{1}{3}S(S+1)$ one has to consider the v^4 term in (25), which is negative for such σ. Thus in this region of v the probability increases if $\sigma^2<\frac{1}{3}S(S+1)$ and decreases if $\sigma^2\geq\frac{1}{3}S(S+1)$.

In the inverse limit case $v\gg 1$ one can obtain dependence on v from (24), expanding it in powers of e^{-2v}. With accuracy up to e^{-4v} one has

$$w_\sigma\approx\frac{C_{2S}^{S-\sigma}}{2^{2S}}\left\{1+\left[1-\frac{2\sigma^2}{S}\right]e^{-2v}-\left[\frac{2\sigma^2}{S}-\frac{(2\sigma^2-S)^2}{2(2S-1)}\right]e^{-4v}\right\} . \tag{26}$$

It follows from (26) that w_σ increases with v for $2\sigma^2\leq S$ and decreases for $2\sigma^2>S$. The limit value w_σ when $v\to\infty$ (extremely strong magnetic field or low temperatures) is $C_{2S}^{S-\sigma}/2^{2S}$.

From (25) and (26) it follows that for $S>\frac{1}{2}$ (in the case $S=\frac{1}{2}$ the probability does not depend on v and equals $\frac{1}{2}$) the probability increases with v for $\sigma^2\leq S/2$, decreases with v for $\sigma^2\geq S(S+1)/3$, and has a maximum at some finite value of v for $(S/2)<\sigma^2<S(S+1)/3$. All these features are shown explicitly in Figs. 1(a)–1(d), where $\omega_\sigma(v)$ is plotted for $S=\frac{7}{2}$. An asymptotic behavior for the probability w_σ when $S\gg 1$ depends on the relation between S and σ.

Consider first the case when $\sigma\ll S$. Using Sterling's formula for factorials [5] and the stationary phase approximation for the integration in (24), one has

$$w_\sigma=(\tanh v/\pi S)^{1/2}\exp(-x^2\tanh v) , \tag{27}$$

where $x=\sigma/\sqrt{S}$. Then

$$dw_x=(\tanh v/\pi)^{1/2}\exp(-x^2\tanh v)dx . \tag{28}$$

This result coincides with the distribution function of the coordinate of an oscillator [2]. One can derive (28) directly from the Hamiltonian (1), changing the spin operators to Bose operators and the generalized coherent-state representation to Glauber coherent-state representation (i.e., the space of the polynomials with the space of the analytical functions). Such a substitution corresponds to a Holstein-Primakoff representation for spin operators [7].

Another limit case is a transition to the classical angular momentum of a fixed magnitude. This transition corresponds to the limit $S\to\infty$, $\sigma\to\infty$, $\mu\to 0$ when $2\mu S=m$ and $2\mu\sigma=m_x$. Switching to the new variable $z'=ze^{-v}$ in (24) and introducing the parametrization $z'=\tan(\theta/2)e^{i\phi}$, $0\leq\theta\leq\pi$, $0\leq\phi\leq 2\pi$, one has

$$w_\sigma=(e^{2v(S+1)}/Z)(C_{2S}^{S-\sigma}/2^{2S})[(2S+1)/\pi]\times\int[1+(e^{2v}-1)\sin^2\theta/2]^{-2S}\times(1+\sin\theta\cos\phi)^{S+\sigma}(1-\sin\theta\cos\phi)^{S-\sigma}dO , \tag{29}$$

where the integration is performed over the unit sphere

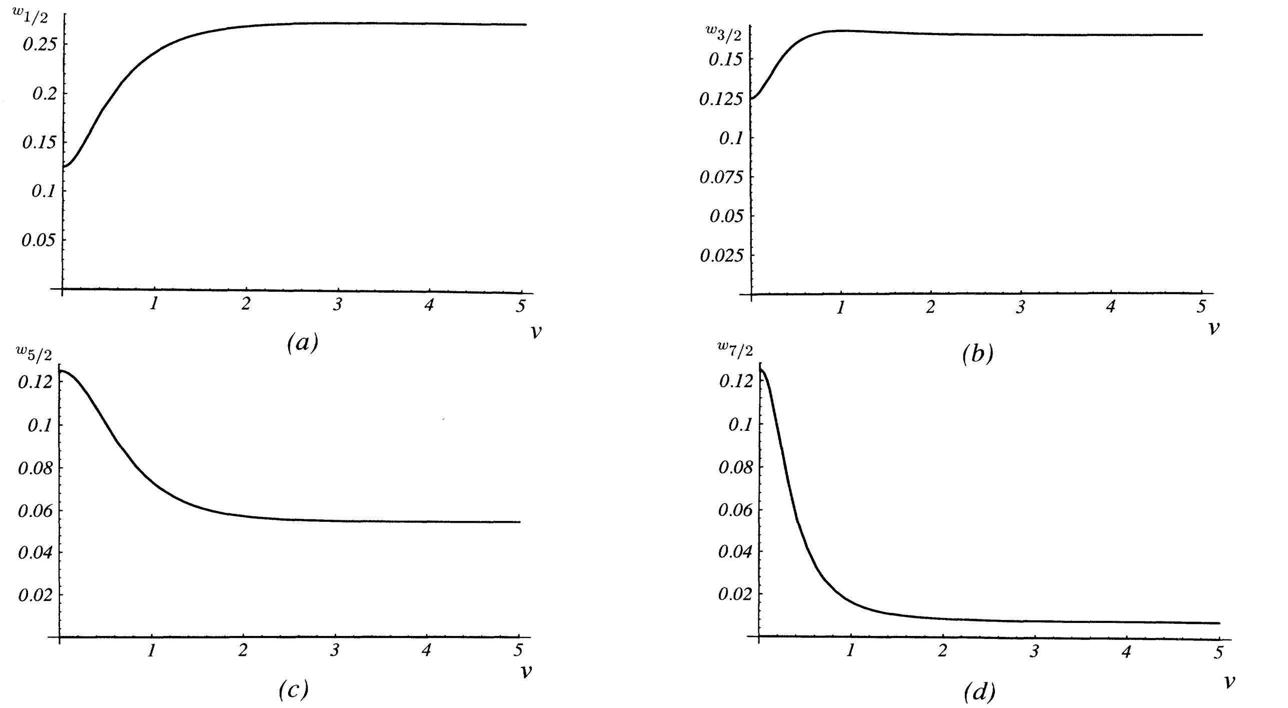

FIG. 1. Dependence on the thermofield parameter of the quantum probability distribution function for $S=\frac{7}{2}$ for (a) $\sigma=\frac{1}{2}$ $\sigma^2<S/2$; (b) $\sigma=\frac{3}{2}$, $S/2<\sigma^2<S(S+1)/3$; (c) $\sigma=\frac{5}{2}$; and (d) $\sigma=\frac{7}{2}$, $\sigma^2>S(S+1)/3$.

$dO = \sin\theta\, d\theta\, d\phi$. The limit expression for the first factor in the integrand is

$$\lim_{2vS \to \beta mH, S \to \infty} e^{2v(S+1)}[1+(e^{2v}-1)\sin^2(\theta/2)]^{-2S} = e^{\beta mH \cos\theta} . \tag{30}$$

To determine the asymptotes in the rest of the factors in (29) one should notice that the product

$$P_{2S}^{S-\sigma} = C_{2S}^{S-\sigma} \left[\frac{1+\sin\theta\cos\phi}{2} \right]^{S+\sigma} \left[\frac{1-\sin\theta\cos\phi}{2} \right]^{S-\sigma} \tag{31}$$

is the binomial probability distribution for the realization of an event $(S-\sigma)$ times in $2S$ trials, if the probability of an event realization in each trial is $p=(1-\sin\theta\cos\phi)/2$. The asymptote of such a distribution when $S\to\infty$ and $S-\sigma\to\infty$ is the limit Muavre-Laplace formula [8]

$$P_{2S}(S-\sigma) \approx \frac{1}{\sqrt{2\pi npq}} \exp\left[-\frac{1}{2}\left(\frac{m-np}{\sqrt{npq}}\right)^2 \right] . \tag{32}$$

Here $n=2S$, $m=S-\sigma$, and $q=1-p$. Performing the transition to the limit one has

$$\lim_{S-\sigma\to\infty\, S\to\infty} SP_{2S}(S-\sigma) = \delta[\sin\theta\cos\phi-(m_x/m)] \tag{33}$$

and

$$w_\sigma = (Z^{-1}/\pi)\int dO\, e^{\beta mH\cos\theta}\delta[\sin\theta\cos\phi-(m_x/m)] . \tag{34}$$

In the classical limit the partition function in (34) can be expressed in terms of the classical partition function $Z=SZ_{\rm cl}/2\pi$. Taking into account that dm_x/m in the classical case corresponds to $1/S$ in quantum considerations, one obtains the probability distribution function for the component m_x of the classical spin,

$$dw_{m_x} = dm_x \frac{Z_{\rm cl}^{-1}}{m}\int dO\, e^{\beta mH\cos\theta}\delta\left[\sin\theta\cos\phi-\frac{m_x}{m}\right] . \tag{35}$$

Performing the integration in (35) one has

$$dw_{m_x} = \frac{\beta H}{2\sinh\beta mH} I_0[\beta H(m^2-m_x^2)^{1/2}]dm_x , \tag{36}$$

where $I_0(u)$ is the modified Bessel function. In the region $\beta mH \ll 1$ the dependence of the probability distribution function (36) on the thermofield parameter is similar to that of the quantum function (25) (with the corresponding substitution $S+1\to S$). However, in the region $\beta mH \gg 1$ the classical formula (36) essentially differs from its quantum counterpart. In particular, there is no region of m_x (except $m_x=0$) where the probability distribution increases with βmH.

Thus, comparing results obtained for the probability distribution function of the transverse spin component $\hat{S}_x$ in the dc magnetic field with the probability distribution function (4) for the longitudinal spin component $\hat{S}_z$, one can see that the quantum nature of the spin is displayed explicitly in the distribution function for the transverse spin component. In the spin-wave approximation, quantization of the transverse spin component (i.e., discrete spectra) becomes unobservable.

We have derived an exact expression (22) for the quantum probability distribution function for the transverse spin component $\hat{S}_x$ for an equilibrium system of noninteracting paramagnetic particles in an external magnetic field. The probability dependence on the thermofield parameter depends on the relation between S and σ. Both the spin-wave ($S\to\infty$, $\sigma \ll S$) (28) and the classical ($S\to\infty$, $\sigma\to\infty$, $\mu\to 0$, $2\mu S=m$, $2\mu S_x=m_x$) (36) approximation formulas for the quantum probability distribution function are obtained. In both of these limit formulas the discreteness of the transverse spin component is unobservable.

The dependences on the thermofield parameter v of the quantum and the classical probability distribution functions can be understood from the following physical explanation:

(1) For $v=0$ all space directions are equivalent, so that $\langle \hat{S}_x^2\rangle = \langle \hat{S}_y^2\rangle = \langle \hat{S}_z^2\rangle = S(S+1)/3$. For $0<v\ll 1$, the z direction becomes slightly preferable (a spin chooses the field direction). This means that $\langle \hat{S}_z^2\rangle$ increases with v and hence because of the conservation of the spin magnitude and the symmetry in the xy plane, $\langle \hat{S}_x^2\rangle$ decreases with v. So the probability for the particle to have the transverse spin component σ increases with v for $\sigma^2 < S(S+1)/3$ and decreases for $\sigma^2 > S(S+1)/3$. It is evident that for this v region there is no difference in the quantum and the classical cases since the distribution of spin values is determined by thermal fluctuations.

(2) In strong magnetic fields or under low temperatures ($v \gg 1$) the spin tends to have the field direction. Classically, this means that up to an exponential accuracy the transverse spin components $m_x=m_y=0$, and the classical probability distribution increases with v only for $m_x=0$.

On the other hand, in the quantum case, because of the uncertainty principle the fluctuation of the transverse spin component in the eigenstate $|S\rangle$ of the longitudinal spin component $\hat{S}_z$ is $S/2$ and the probability for the particle to have the transverse spin value σ increases with v when $\sigma^2 \le S/2$ and decreases with v when $\sigma^2 > S/2$.

[1] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon, New York, 1977).

[2] L. D. Landau and E. M. Lifshits, *Statistical Physics* (Pergamon, New York, 1980).

[3] C. Kittel, *Introduction to Solid State Physics* (Wiley, New York, 1986).

[4] A. M. Perelomov, Usp. Fiz. Nauk. **123**, 23 (1977) [Sov. Phys. Usp. **20**, 703 (1977)].

[5] H. Bateman and A. Erdelyi, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. 2.

[6] E. V. Goldstein and V. M. Tsukernik, Fiz. Nizk. Temp. **12**, 279 (1986) [Sov. J. Low Temp. Phys. **12**, 158 (1986)].

[7] D. Mattis, *The Theory of Magnetism* (Springer, New York, 1987).

[8] W. Feller, *An Introduction to Probability Theory and Its Applications* (Wiley, New York, 1967).