Magnetic response for an ellipsoid of revolution in a magnetic field

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The quantum-mechanical spectrum and the magnetic response of noninteracting electrons confined to the surface of an ellipsoid of revolution are investigated. We have found the magnetic response both for the case of a fixed chemical potential and for the case of a fixed number of electrons. It is shown that the magnetic response of an ellipsoid of revolution depends on the thermodynamics of the system. In particular, for a fixed chemical potential, the magnetic response of an ellipsoid of revolution is a steplike function of a magnetic field. The dependence of the magnetic response of an ellipsoid of revolution on temperature and geometric parameters is found and investigated in detail.

I. INTRODUCTION

The analysis of the magnetic response of nanostructures with different geometry allows one to get important data concerning parameters of the electron energy spectrum and the potential of the geometric confinement in such systems.[1–10] This is because the magnetic response of a nanostructure is determined predominantly by the energy spectrum, which in turn depends on the geometric parameters of a nanostructure. Note that a magnetic field tilted to the symmetry axes of the system can lead to hybridization of the dimensional and magnetic confinement as a result of coupling of the motion of electrons parallel and perpendicular to the magnetic field.[3–5,11]

The recent progress in nanotechnology has promoted an experimental investigation of curved nanostructures. In particular, the so-called lift-off technology allows one to fabricate two-dimensional curved layers of GaAs heterostructures.[8,12–15] Moreover, a wide class of curved structures is formed by the carbon nanostructures such as nanotubes, fullerenes, and toroids. Theoretical and experimental studies of the magnetic and transport properties of these carbon structures are presented in Refs. 16–18. Thereby, the theoretical investigation of the spectral and magnetic properties of nanostructures with a nonzero curvature (in particular, quantum cylinders, spheres, and ellipsoids) is a subject of current interest. The investigation of the magnetic response for a nanostructure with cylindrical symmetry[1,8,12,13,19] shows that the curvature of surface of a system influences substantially the spectral and magnetic properties of this structure and leads to interesting physical effects.[1,7,13,15] Recent advances in technology[20] have made it possible to produce spherical nanostructures.[21–23] The energy spectrum, electronic correlations, and magnetic properties of a spherical two-dimensional electron gas have been considered in a number of theoretical works.[24–28] There is indirect evidence that the geometry of the above-mentioned systems plays a dominant role in the behavior of the electron energy spectrum: there is good agreement between the numerical results obtained in the framework of the tight-binding approximations and those obtained for the simplified model of noninteracting electrons.

In Ref. 24, a model of noninteracting electrons confined to the surface of a sphere has been used for a theoretical investigation of the quantum-mechanical spectrum and the magnetic response of electrons in the fullerene C_{60}. (Interacting electrons on various two-dimensional surfaces are considered in Refs. 29–33.) In this model, the energy spectrum of electrons on the sphere subjected to a uniform magnetic field has been calculated in the framework of perturbation theory. The radius of convergence of perturbation theory is defined by the condition $(R/l_B)^2 \ll 1$, where R is the radius of a sphere and l_B is the magnetic length. Since the effective radius of the C_{60} fullerene is of the order of 3.5×10^{-8} cm, we can estimate the magnitude of the magnetic field: $B \ll 100$ T. Obviously, this condition holds for all experimentally accessible magnetic fields.

If the magnetic field is absent, then the energy spectrum of electrons is $(2l+1)$-fold degenerate due to the spherical symmetry of the system (l is the orbital quantum number). An applied uniform magnetic field removes this degeneracy completely[25] and leads to the dependence of the energy spectrum on the magnetic quantum number m. Namely, the energy of the level with $m \geqslant 0$ increases with the field and with the quantum number m, whereas the energy of the level with $m<0$ decreases with the field. Since the distance between adjacent shells is large, it follows that there is no level crossing (i.e., there is no accidental degeneracy of the levels). However, for a very high field, the level crossing becomes essential and leads to a series of interesting effects (see discussion in Refs. 25 and 27).

In this paper we study the quantum-mechanical spectrum and the magnetic response of electrons moving on the surface of an ellipsoid of revolution. This system can be considered as a model for the electron system in the nanocluster C_{70}, the geometry of which is close to that of an ellipsoid of revolution. In this case, the semiaxes of the ellipsoid differ slightly from each other. Hence, the effect of the nonsphericity can be considered in the framework of perturbation theory. The magnetic response for an ellipsoid of revolution depends on the relationship between the two types of corrections to the energy spectrum: the corrections due to the magnetic field B and those due to the ellipsoidal geometry of the system. It is clear that the energy spectrum and the magnetic response of electrons confined to the surface of an ellipsoid of revolution depend on the angle ϑ_0 between the axis of

revolution and the magnetic field direction.

We consider below only the case of low magnetic fields, namely, the case $(R/l_B)^2 \ll 1$, because this inequality holds for all really accessible fields for C_{60} and C_{70}. Moreover, we consider not only the case of the ellipsoidal surface, but the case of the spherical surface as well. Note that the energy spectrum and the magnetic properties of the electron system on a sphere in presence of a uniform magnetic field have been studied in Refs. 24, 25, and 27, but in these articles an additional condition $(R/l_B)^2 \gtrsim 1$ has been supposed (the reason is that the authors of the cited articles are interested mainly in the effects related to the level crossing). For the simple model of noninteracting electrons, we obtain explicit perturbative expressions for the energy spectrum and the magnetic response. We shall show that in the case of low magnetic fields the magnetic moment of a sphere (C_{60}) and of an ellipsoid (C_{70}) is a steplike function of the field at a fixed chemical potential. By increasing the temperature the steps of this dependence are washed out.

II. ENERGY SPECTRUM OF AN ELLIPSOID OF REVOLUTION IN A MAGNETIC FIELD

We consider the case of noninteracting electrons confined to the surface of an ellipsoid of revolution in a uniform magnetic field **B**. The Hamiltonian of such a system reads

$$H=\frac{p^2}{2m_e}+\frac{|e|}{2m_e c}\mathbf{BL}+\frac{e^2}{8m_e c^2}[\mathbf{B},\mathbf{r}]^2, \tag{1}$$

where m_e is the mass of an electron and **L** is the angular momentum operator (for simplicity, we ignore the spin-dependent terms). For $B \ll 100$ T, the second and third terms are much less than the first one. Hence, they yield a weak perturbation of the energy spectrum of an ellipsoid by the magnetic field. The third term in Eq. (1) is proportional to B^2 and therefore it is much less than the second term.

In the Cartesian coordinates x,y,z, the equation of an ellipsoid of revolution has the form $(x^2+y^2)/R^2+z^2/d^2=1$. Introducing new coordinates by the relations $\xi=x$, $\eta=y$, and $\zeta=Rz/d$, we rewrite the equation of an ellipsoid in the form $\xi^2+\eta^2+\zeta^2=R^2$. In these new coordinates, the Laplacian is given by the expression

$$\Delta=\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}+(1-\beta)^2\frac{\partial^2}{\partial\zeta^2}=\Delta^0+\beta(\beta-2)\frac{\partial^2}{\partial\zeta^2}, \tag{2}$$

where $\beta=1-R/d$ and $\Delta^0=\partial^2/\partial\xi^2+\partial^2/\partial\eta^2+\partial^2/\partial\zeta^2$.

It is clear that $\mathbf{BL}=B_x L_\xi+B_y L_\eta+B_z L_\zeta+o(B\beta)$, where L_ξ, L_η, and L_ζ are the corresponding components of the angular momentum operator. Let us denote R^2/a_j^2 by b_j, where $a_j^2=c\hbar/|e|B_j$ $(j=x,y,z)$ and $l_i=L_i/\hbar$ $(i=\xi,\eta,\zeta)$. Then we can rewrite the Hamiltonian (1) as follows:

$$H=\frac{\hbar^2}{2m_e R^2}(-\Delta^0_{\vartheta,\varphi}+V_1+V_2+V_3+V_4)+o(B\beta), \tag{3}$$

where

$$V_1=2\beta R^2\frac{\partial^2}{\partial\zeta^2},\quad V_2=-\beta^2 R^2\frac{\partial^2}{\partial\zeta^2},$$

$$V_3=b_x l_\xi+b_y l_\eta+b_z l_\zeta,\quad V_4=\frac{b^2}{4}\frac{1}{B^2R^2}[\mathbf{B},\mathbf{r}]^2,$$

and $\Delta^0_{\vartheta,\varphi}$ is the angular term of the Laplacian in the new coordinates. The representation of H in the form (3) will be used below in the two limiting cases $\beta=o(B^2)$ or $B=o(\beta^2)$. In both cases, the term $o(B\beta)$ is negligible compared to the remaining terms.

In what follows the terms V_1 and V_2 in Eq. (3) are called the deformation perturbations and the terms V_3 and V_4 are called the magnetic perturbations. The corrections to the energy spectrum due to these perturbations are called the deformation correction and the magnetic correction, respectively.

Let us consider the following three cases

(i) The deformation correction to the energy is of the order of the magnetic one, i.e., $\beta \approx \max|b_j|$.

(ii) The deformation correction to the energy is much larger than the magnetic one, i.e., $\beta \gg \max|b_j|$.

(iii) The deformation correction to the energy is much smaller than the magnetic one, i.e., $\beta \ll \sup|b_j|$.

First, we consider case (i). The eigenvalues and the eigenfunctions of $\Delta^0_{\vartheta,\varphi}$ are given by

$$\mathcal{E}^0_l=l(l+1);\quad |\psi^0_{l,m}\rangle=|Y_{l,m}(\vartheta,\varphi)\rangle\equiv|l,m\rangle, \tag{4}$$

where $Y_{l,m}(\vartheta,\varphi)$ is the spherical harmonic. We see that the spectrum of $\Delta^0_{\vartheta,\varphi}$ is $(2l+1)$-fold degenerate. The first-order correction ε_1 to the energy spectrum is determined by the secular equation: $\det[\langle l,m_1|V_1+V_3|l,m_2\rangle-\varepsilon_1\delta_{m_1,m_2}]=0$.

Because of the rotational symmetry of an ellipsoid of revolution, we can choose the direction of the magnetic field such that $B_y=0$ and therefore $b_y=0$. Using the properties of the spherical harmonics, after some algebra we obtain

$$\begin{aligned}\langle l,m_1|V_1+V_3|l,m_2\rangle &= \delta_{m_1,m_2}\left[b_z m_1-2\beta\frac{2(l+1)^2(l^2-m_1^2)+m_1^2(2l-1)}{(2l-1)(2l+3)}\right]\\ &+\delta_{m_1,m_2+1}\frac{1}{2}a_+(l,m_2)b_x+\delta_{m_1,m_2-1}\frac{1}{2}a_-(l,m_2)b_x,\end{aligned} \tag{5}$$

where $a_\pm(l,m)=\sqrt{l(l+1)-m(m\pm1)}$.

As can be seen from Eq. (5), the matrix $\langle l,m_1|V_1+V_3|l,m_2\rangle$ is a Hermitian three-diagonal matrix (i.e., a Jacobi matrix) of order $2l+1$. In the case of an arbitrary directed field, it is difficult to obtain an explicit expression for the first-order correction to the energy spectrum. At the same time, if the field is parallel to the symmetry axis of an ellipsoid ($\mathbf{B}\|Oz$), then the matrix $\langle l,m_1|V_1+V_3|l,m_2\rangle$ is diagonal. In this case,

$$\varepsilon_1=b_z m-2\beta\frac{2(l+1)^2(l^2-m^2)+m^2(2l-1)}{(2l-1)(2l+3)}. \tag{6}$$

If we neglect the higher-order contributions due to the perturbations V_2 and V_4, then

$$E_{l,m}=\frac{\hbar^2}{2m_eR^2}\left[l(l+1)+b_zm - 2\beta\frac{2(l+1)^2(l^2-m^2)+m^2(2l-1)}{(2l-1)(2l+3)}\right]. \quad (7)$$

Equation (7) allows us to understand how the deformation of a sphere into an ellipsoid of revolution decreases the level degeneracy. Let us consider the collection of all levels with the angular momentum l. The states of these levels form an electron shell. In the case of a sphere and a zero field, these levels merge into one $(2l+1)$-fold degenerate level. Putting $B=0$ in Eq. (7), we conclude that the deformation of a sphere into an ellipsoid of revolution splits the level of the lth shell into a set of $l+1$ levels. The level with $m=0$ is nondegenerate, whereas the levels with $m\neq 0$ are twofold degenerate. Consequently, the deformation removes partially the degeneracy with respect to the quantum number m. Note that the deformation correction of the first order is negative for all values of l and m. If $\mathbf{B}\neq 0$, then Eq. (7) shows that all the energy levels of the lth shell are nondegenerate; i.e., the magnetic field removes the degeneracy completely. Moreover, it is easy to see that the energy of the level with $m>0$ increases with the field, whereas the energy of the level with $m<0$ decreases; the level with $m=0$ does not change its position on the energy axis. The region of application for Eqs. (5) and (7) is determined by the conditions

$$\max(|b_x|,|b_y|,|b_z|,|\beta|)\ll 1,$$

$$\max(|b_x|,|b_y|,|b_z|)\approx|\beta|. \quad (8)$$

The second condition in Eqs. (8) is necessary, since otherwise the deformation and magnetic corrections are of different order, and we must take into account the perturbative terms of higher order.

Second, we consider case (ii). In particular, in the case of the fullerene C_{70} we have $R\approx 3.5\times 10^{-8}$ cm, $\beta\approx 0.1$; therefore for the real field range 2 T$\leqslant B\leqslant$10 T, the perturbation V_3 due to the magnetic field is of lower order with respect to the perturbation V_1. In this connection, we consider the perturbative terms V_2 and V_3 in second-order perturbation theory only; the perturbation V_4, which is quadratic with respect to the field, can be neglected.

Using the standard perturbation theory, after some tedious calculations we get

$$E_{lm}=\frac{\hbar^2}{2m_eR^2}[l(l+1)+\varepsilon_1+\varepsilon_2], \quad (9)$$

where

$$\varepsilon_1=-2\beta\frac{2(l+1)^2(l^2-m^2)+m^2(2l-1)}{(2l-1)(2l+3)}$$

and ε_2 is given by

$$\varepsilon_2=b_zm+\beta^2\frac{2(l+1)^2(l^2-m^2)+m^2(2l-1)}{(2l-1)(2l+3)} + 2\beta^2\left[\frac{(l-2)^2(l+1)^2((l-1)^2-m^2)(l^2-m^2)}{(2l-3)(2l-1)^3(2l+1)} - \frac{l^2(l+3)^2((l+2)^2-m^2)((l+1)^2-m^2)}{(2l+1)(2l+3)^3(2l+5)}\right].$$

Note that the terms of the order of β^2 in Eq. (9) cannot be neglected. Indeed, if we neglect these terms, then we have to ignore the dependence of the energy spectrum on the magnetic field, since $|b_z|\approx\beta^2$. Therefore, in this approximation, the magnetic moment of the system is zero.

In this case, the energy spectrum depends on the z component of the field: $E_{lm}\propto|\mathbf{B}|\cos\vartheta$. The radius of convergence for perturbation theory is determined by the following conditions: $|\beta|\ll 1, |b_z|\approx\beta^2$. Therefore, if the field direction is almost perpendicular to the axis of revolution, then Eq. (9) is not applicable. In fact, in the considered case, the energy spectrum for a transversal magnetic field is independent of the field strength and coincides with the spectrum without the field. Note that the correction term of the third order with respect to the field ($|b_z|\approx|\beta|^3$) leads to the insignificant lowering of the energy levels.

Finally, we consider case (iii). Let the correction due to V_1 be of the second order with respect to the correction due to V_3. Then we can neglect the term V_2 in Eq. (3). We choose the Cartesian coordinates so that $b_y=0$. Neglecting V_1 and V_4, we find the first-order correction to the energy spectrum from the secular equation. It is convenient to rotate the coordinate system across the y axis about the angle $\vartheta_0=\arccos(B_z/B)$ so that in the new coordinates $B=B_z$. The new coordinate system ξ',η',ζ' is related to the initial one by the equations

$$\xi'=\xi\cos\vartheta_0-\zeta\sin\vartheta_0,$$

$$\eta'=\eta,$$

$$\zeta'=\xi\sin\vartheta_0+\zeta\cos\vartheta_0. \quad (10)$$

Hence, in this system $\tilde{V}_3=bl_{\zeta'}$. Therefore, $\varepsilon_1=bm$ and the corresponding eigenfunction is $|l,m\rangle$. Using the orthogonal projector method for the calculation of the perturbation matrix elements,[34] we get

$$\varepsilon_2=\langle l,m|\tilde{V}_1|l,m\rangle+\langle l,m|\tilde{V}_3Q\tilde{V}_3|l,m\rangle+\langle l,m|\tilde{V}_4|l,m\rangle, \quad (11)$$

where $\tilde{V}_1$, $\tilde{V}_3$, and $\tilde{V}_4=(b^2/4)\sin^2\vartheta$ are the perturbation operators in the new coordinates, and

$$Q=\sum_{l'\neq l}\frac{\sum_{m'}|l',m'\rangle\langle l',m'|}{\mathcal{E}_l^0-\mathcal{E}_{l'}^0}. \quad (12)$$

After some algebra, we obtain the following expression for the energy spectrum for an electron confined to the surface of an ellipsoid of revolution:

$$E_{l,m}=\mathcal{E}^{sph}-\frac{\hbar^2}{2m_eR^2}\beta\Bigg[3\sin^2\vartheta_0\frac{2l^2+2l+3}{(2l-1)(2l+3)}\times\left(m^2-\frac{1}{3}l(l+1)\right)+2\frac{2(l+1)^2(l^2-m^2)+m^2(2l-1)}{(2l-1)(2l+3)}\Bigg]. \tag{13}$$

Here $\mathcal{E}^{sph}$ is the energy spectrum of an electron confined to the surface of the corresponding sphere calculated up to second-order perturbation theory:

$$\mathcal{E}^{sph}=\frac{\hbar^2}{2m_eR^2}\left[l(l+1)+bm+\frac{b^2}{2}\frac{l^2+l-1+m^2}{(2l-1)(2l+3)}\right]. \tag{14}$$

The range of applications for this result is given by the conditions $|b|\ll 1, |\beta|\approx b^2$. Note that the deformation correction is always negative for all l and m. We consider the dependence of the energy spectrum on the angle of inclination ϑ_0. As can be seen from Eq. (13), the energy spectrum is symmetric with respect to $\vartheta_0=\pi/2$ because of the symmetry of the system about the xy plane. It should be noted that the lower is the magnetic field $|\mathbf{B}|$, the stronger is the dependence of the spectrum on the angle of inclination ϑ_0. The reason is that the ϑ_0-dependent term in Eq. (13) gives a greater contribution to the energy $E_{l,m}$ of an electron.

Let us define the angle ϑ_1 such that $\sin^2\vartheta_1=2/3$. It follows from Eq. (13) that at $\vartheta_0=\vartheta_1$ the deformation correction to the energy is independent of the magnetic quantum number m, and the spectrum of the ellipsoid differs from that of the sphere only on a slight shift of all the levels downwards:

$$E_{l,m}\big|_{\vartheta_0=\vartheta_1}=\mathcal{E}^{sphere}-\frac{\hbar^2}{2m_eR^2}\cdot\beta\frac{2}{3}l(l+1). \tag{15}$$

Equation (13) implies the following statement: If $m^2<l(l+1)/3$, then the energy of the level increases with the increase of the angle ϑ_0 from 0 to $\pi/2$; if $m^2>l(l+1)/3$, then this energy decreases. With the help of this statement, we can determine the levels of the shell having the maximum or the minimum at $\vartheta_0=\pi/2$. Namely, in the case of $m^2<l(l+1)/3$ [$m^2>l(l+1)/3$], the function $E_{l,m}(\vartheta_0)$ has the maximum (minimum) at $\vartheta_0=\pi/2$.

III. MAGNETIC MOMENT OF A SPHERE AND AN ELLIPSOID OF REVOLUTION

Let us consider the dependence of the magnetic moment **M** on **B** for an ellipsoid of revolution. As mentioned above, in case (i), it is difficult to obtain an explicit expression for $E_{l,m}(B)$ if the magnetic field is not parallel to the rotational symmetry axis. Thereby, in this case we have to restrict ourselves to the case of a longitudinal field. Then in all considered cases, only the z component of the field gives a nonvanishing contribution to the energy spectrum of an ellipsoid of revolution. Therefore, $M=M_z$ for all cases. We use the standard formula

$$M=-2\sum_{l,m}\frac{\partial E_{l,m}}{\partial B_z}f_0(E_{l,m}), \tag{16}$$

where $f_0(E_{l,m})$ is the Fermi distribution function. From here on we take into account the spin degeneracy with the help of the factor of 2 in front of the sum over all quantum states.

It is necessary to distinguish two cases corresponding to the two types of statistical ensembles. In the first case (grand canonical ensemble), there is an exchange of both energy and particles between the ellipsoid and the thermostat. In this case, the chemical potential μ depends weakly on the field B, and this dependence can be neglected. Indeed, let $\mu=\mu_0+\Delta\mu$, where μ_0 is the chemical potential in the absence of the field and $\Delta\mu$ is the term due to the field B. Since in the thermal equilibrium $(\partial F/\partial\mu)_{\mu=\mu_0}=0$, we have, for the difference of the free energy ΔF,

$$\Delta F=\frac{1}{2}\left(\frac{\partial^2F}{\partial\mu^2}\right)_{\mu=\mu_0}(\Delta\mu)^2. \tag{17}$$

Since $\Delta\mu$ is independent of the field direction, we have $\Delta\mu\propto B^2$, and therefore $\Delta F\propto B^4$.[35] On the other hand, the magnetic correction is calculated up to terms of the order of B^2. Hence, $\Delta\mu$ is negligible in this order of accuracy.

In the second case, there is an exchange only of the energy between the system and the thermostat (the number N of particles in the system is fixed). In this case, the dependence of μ on B is essential. This dependence is determined completely by the normalization condition

$$N=2\sum_{l,m}\frac{1}{1+\exp[(E_{l,m}-\mu)/T]}. \tag{18}$$

At zero temperature, the magnetic moment is given by

$$M(T=0)=-2\sum_{E_{l,m}\le\mu}\frac{\partial E_{l,m}}{\partial B_z}. \tag{19}$$

With the help of the results of the previous section, $\partial E_{l,m}/\partial B_z$ can be written as

$$\frac{\partial E_{l,m}}{\partial B_z}=\begin{cases} m\mu_B, & \text{for case (i) when } (B\|Oz),\\ m\mu_B, & \text{for case (ii)},\\ m\mu_B+b\mu_B\dfrac{l^2+l-1+m^2}{(2l-1)(2l+3)}, & \text{for case (iii)}.\end{cases} \tag{20}$$

In all considered cases, Eqs. (19) and (20) may be used to obtain explicit expressions for the magnetic moment at zero temperature. Namely, if μ_B is the Bohr magneton and l_0, m_0 are the quantum numbers of the highest occupied level, then we have, for case (i) (for $m_0>0$),

$$\frac{M(T=0)}{\mu_B}=(l_0-m_0)(l_0+m_0+1), \tag{21}$$

for case (ii),

$$\frac{M(T=0)}{\mu_B}=|m_0|-m_0, \tag{22}$$

and for case (iii),

$$\frac{M(T=0)}{\mu_B}=(l_0-m_0)(l_0+m_0+1)-\frac{2b}{3}(l_0+1)^2-\frac{b}{3}\frac{m_0(m_0+1)(2m_0+1)-l_0(l_0+1)(2l_0+1)-6(l_0-m_0)(l_0^2+l_0-1)}{(2l_0-1)(2l_0+3)} \tag{23}$$

[from here on we suppose that $\vartheta_0 \in (0,\pi/2)$]. Even though β does not explicitly appear in Eqs. (21)–(23), the magnetic moment depends on β. Indeed, the quantum numbers l_0 and m_0 are defined by $\mu=E_{l_0 m_0}$, where E_{lm} in turn is defined by Eqs. (7), (9), and (13) [case (i), case (ii), and case (iii), respectively]. Thus, the quantum numbers l_0 and m_0 depend on β for fixed μ, since $E_{lm}=E_{lm}(\beta)$. Therefore, M also depends on β.

It may be seen that Eq. (22) [case (ii)] does not match with Eqs. (21) and (23) [case (i) and case (iii), respectively]. Figure 1 explains this mismatch. In this figure, we display the energy levels of the fifth shell ($l=5$) of electrons as a function of a magnetic field. As can be seen from this figure, for case (ii), only the highest occupied level can give a contribution to the magnetic moment (contributions from other levels are exactly compensated). In cases (i) and (iii), the relative position of the energy levels changes with respect to that for case (ii). In these cases, the magnetic moment can contain contributions of several levels of the highest occupied shell. Thus, the behavior of the magnetic response for case (ii) differs from that for case (i) and case (iii), although the spectrum in cases (i), (ii), and (iii) differs only by the higher-order corrections.

In conclusion to this section, we present some results for the case of a sphere. Direct calculations show that the magnetic moment for a sphere is given by Eq. (21) if we restrict ourselves to linear terms with respect to the field in the spectrum (14). On the other hand, if the second-order terms are taken into account, then the magnetic moment is given by Eq. (23).

Note that Eqs. (21), (22), and (23) are valid both for the case of a fixed chemical potential μ and for the case of a fixed number of particles, N. At the same time, there is a fundamental difference between these cases. Namely, for fixed μ, the field dependence of the magnetic moment is a steplike one. These steplike features in $M(B)$ arise from the chemical potential crossing by either the highest occupied levels or the lowest unoccupied levels. This crossing leads to a change of the quantum numbers l_0 and m_0, and, consequently, to a jump in the magnetic moment. It should be mentioned that the number of jumps or steps is strictly limited. The finiteness of the number of steps is caused by the following reasons. First, only the levels of one shell (the highest occupied shell) can cross the Fermi level. Second, this crossing is possible only for the levels with the energy that either increases or decreases with the field. Strictly speaking, for the case of a sphere (the energy spectrum is calculated in second-order perturbation theory) and for case (iii) (the magnetic correction is much greater than the deformation one), the dependence of the magnetic moment on the field is not strictly steplike [see Eq. (23)], because the magnetic moment depends linearly on the field in the plateau of a step. However, when the geometric confinement is much stronger than the magnetic one (this is the case for the experimentally accessible field range and for $R<5\times10^{-8}$ cm), this linear dependence $M(B)$ is negligibly small, and we can consider this dependence as a nearly steplike one. On the other hand, when the magnetic confinement becomes essential with respect to the geometric one (for the real field range and for $R\geqslant10^{-7}$ cm), the dependence of the magnetic moment on the field is rather a sawtoothlike one. For fixed N, the quantum numbers l_0 and m_0 are not changed, since there is no accidental level degeneracy for the considered field range. Hence, the magnetic moment is a monotone continuous function of the magnetic field. Namely, for cases (i) and (ii), the magnetic moment is independent of the field, and for case (iii), the magnetic moment is a linear function of a magnetic field.

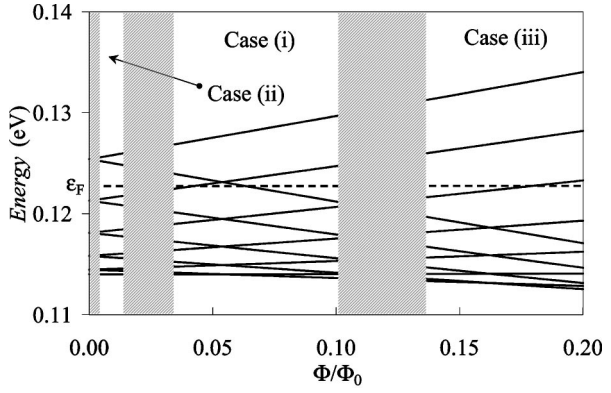

FIG. 1. Energy levels of the fifth shell ($l=5$) of electrons on an ellipsoid of revolution with $R=10^{-7}$ cm and $\beta=0.1$ as a function of a dimensionless magnetic field at $\vartheta_0=0$. Shaded areas indicate regions which are out of the scope of perturbation theory.

IV. ANALYTICAL STUDY AND NUMERICAL ANALYSIS OF THE MAGNETIC RESPONSE

First, we consider the case of a fixed chemical potential. As can be seen from Eq. (14) for the case of a sphere, the energy of the level $E_{l,m}$ with $m\geqslant0$ (with $m<0$) increases (decreases) with the field. Hence, for $\mu>E_{l_0,0}$ (for $\mu<E_{l_0,0}$), only the levels $E_{l,m}$ with $m\geqslant0$ (with $m<0$) can cross the chemical potential. Note that for $(R/l_B)^2\ll1$, there is no level crossing because b_z is very small. The steplike dependence $M(B)$ is associated with the crossing of the Fermi energy by the levels of the highest occupied shell with $l=l_0$. It is clear that the number of these steps in the case of the closed highest occupied shell is equal to the number of increasing or decreasing levels of this shell with the field; i.e., the maximum number of the steps is equal to $l_0|_{B=0}+1$.

For the sphere, the dependence $M(B)$ is depicted in Fig. 2. In this figure we can see sharp steps of the magnetic moment at $T=0.1$ K. The steplike behavior of the magnetic moment is caused by crossing the chemical potential with the

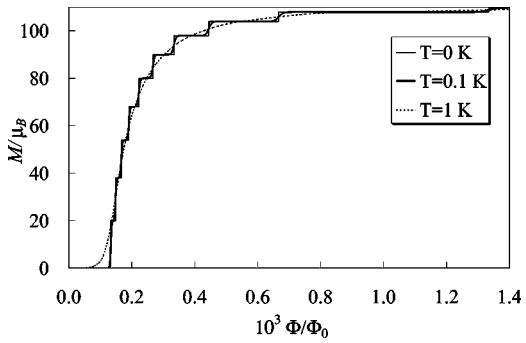

FIG. 2. Magnetic moment of electrons on a sphere of radius $R=3.5\times10^{-8}$ cm as a function of a dimensionless magnetic field for the fixed chemical potential $\mu=34.22$ eV.

highest occupied levels $E_{l_0,m}$ of electrons on a sphere. These steps are washed away by the temperature $T=1$ K.

Now we consider the field dependence of the magnetic moment for a sphere at a fixed number of electrons, N. Let $T=0$. Then the Fermi energy is equal to the energy of the highest occupied level E_{l_0,m_0}, where the quantum numbers l_0 and m_0 depend on the total number of electrons N. As can be seen from Eq. (21) or Eq. (23), the magnetic moment of a sphere is negative if the highest occupied shell is closed and positive if this shell is partially filled. In both these cases, the magnetic moment is a linear function of a magnetic field. In the limit $B=0$, the magnetic moment is equal to the Bohr magneton times an integer (for the case of C_{60} we have $M|_{B,T=0}=20\mu_B$).

If $T\neq0$, then at the beginning it is necessary to find the dependence $\mu(B)$ using the normalization condition (18). For some partial values of temperature, this dependence is shown in Fig. 3. As shown in this figure, the chemical potential depends monotonically on the magnetic field. Let us discuss this behavior of $\mu(B)$. Kim, Vagner, Sundaram, Jauregui, and Marchenko showed that a variation of the level degeneracy with the magnetic field[36] and the level crossings (the case of high magnetic fields[25]) leads to oscillatory features in μ as a function of B. However, in this paper we consider only the case of low magnetic fields. In this case, there is no level crossing; besides that the degeneracy of the levels is not changed with the field B. Therefore, the chemical potential is a monotone function of B for the considered region of fields.

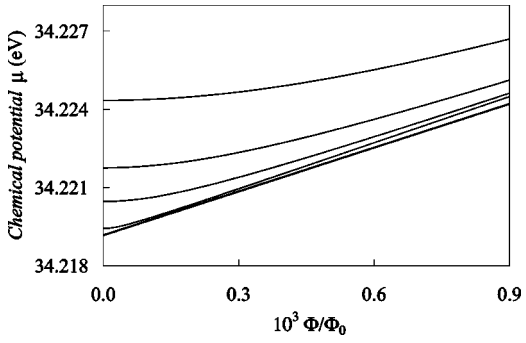

FIG. 3. Dependence of the chemical potential of an electron gas for a sphere of radius $R=3.5\times10^{-8}$ cm on a dimensionless magnetic field at $T=1,5,10,20$ K for fixed $N=240$. The heavy curve corresponds to the highest occupied level $E(l_0,m_0)$.

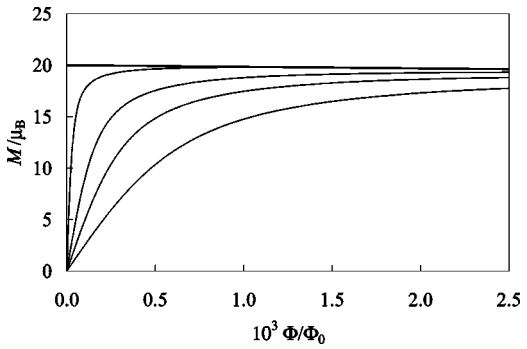

FIG. 4. Magnetic moment of electrons on a sphere of radius $R=3.5\times10^{-8}$ cm as a function of a dimensionless magnetic field at $T=1,5,10,20$ K for fixed $N=240$. The heavy curve corresponds to $T=0$.

As can be seen from Fig. 3, at low B, there is a region on the curve $\mu(B)$ where the chemical potential depends weakly on the magnetic field. The magnitude of this region increases with temperature. The region of the weak dependence $\mu(B)$ is changed by the region of the nearly linear dependence $\mu(B)$ with increasing B. As can be seen from Eqs. (14) and (16) and from a numerical analysis, the magnetic response increases with the field in the region where the chemical potential depends weakly on B. The magnetic response is almost constant in the region where μ is nearly a linear function of B. As shown in Fig. 4, at low T ($T\approx1$ K), the dependence $M(B)$ is determined by the field dependence of the chemical potential. The dependence of the magnetic moment is like a smeared step. The greater is the temperature, then the greater is the smearing of the steps. In addition, in the considered region of the fields, the value of the magnetic moment at finite temperature is always less than that at $T=0$. Since the levels $E_{l,m}$ as well as the chemical potential increase with B, there are no steps in the dependence $M(B)$ that are related to crossing μ by $E_{l_0,m}$. The dependence of the energy of the highest occupied level E_{l_0,m_0} on the magnetic field is clearly shown in Fig. 3.

The behavior of the magnetic response at a fixed chemical potential for the case of an ellipsoid of revolution differs from that for the case of a sphere. First, we consider case (ii); this case corresponds to the fullerene C_{70}. The energy spectrum depends on the z component of the field B. Therefore, the x and y components of the magnetic response are zero, and only the z component is nonzero. As mentioned before, only one energy level can cross the Fermi level. It follows that there is at most one step (Fig. 5).

It is clear that case (iii) for an ellipsoid is similar to the case of a sphere. For fixed μ, the dependence $M(B)$ is a steplike one. For the field range where perturbation theory is applicable, the number of steps on the plot of the magnetic moment is less than the maximum number of the steps $(l_0|_{B=0}+1)$ for the case of a sphere (Fig. 6).

Finally, for case (i), the behavior of the magnetic moment as a function of B is similar to that for case (iii) except that the term in Eq. (21) proportional to B is negligible (Fig. 7).

If N is fixed, then the behavior of the magnetic moment for an ellipsoid of revolution is qualitatively similar to that for a sphere. For case (ii), in the limit $T=0$, the magnetic moment depends on the multiplicity of the number of elec-

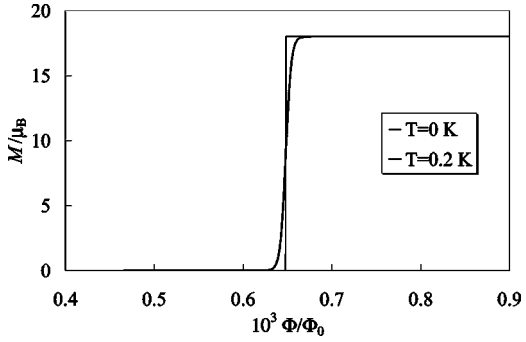

FIG. 5. Magnetic moment of electrons on an ellipsoid of revolution with $R=3.5\times10^{-8}$ cm and $\beta=0.1$ [case (ii)] as a function of a dimensionless magnetic field at $\vartheta_0=0$ for the fixed chemical potential $\mu=39.507$ eV.

trons in the highest occupied shell. Namely, if this number is divisible by 4, then $M(B)|_{T=0}=2|m_0|\mu_B$; otherwise $M(B)|_{T=0}=0$. This behavior of the magnetic moment is determined by the dependence of the quantum numbers l_0 and m_0 on the total number of electrons, N. For the considered limiting case, for $\beta>0$,

$$N=2[l_0^2+2|m_0|+\Theta(m_0)], \tag{24}$$

and, for $\beta<0$,

$$N=2[l_0^2+2l_0-2|m_0|+2-\Theta(-m_0)], \tag{25}$$

where

$$\Theta(x)=\begin{cases}1, & \text{for} \quad x\geqslant 0,\\ 0, & \text{for} \quad x<0.\end{cases}$$

We consider below only the case of a prolate spheroid ($\beta>0$) [the case of an oblate spheroid ($\beta<0$) is considered analogously]. In Eq. (24), $2l_0^2$ is the number of electrons in the filled shells, and $2[2|m_0|+\Theta(m_0)]$ is the number of electrons in the first open shell. It is easy to see that the case of $N=2(l_0+1)^2$ corresponds to the case of the closed highest occupied shell and therefore $2l_0^2<N\leqslant 2(l_0+1)^2$. The quantum number l_0 is determined completely by this condition. If the number $N-2l_0^2$ is divisible by 4, then $m_0<0$, and this leads to $m_0=-(N-2l_0^2)/4$. Using Eq. (22), we obtain

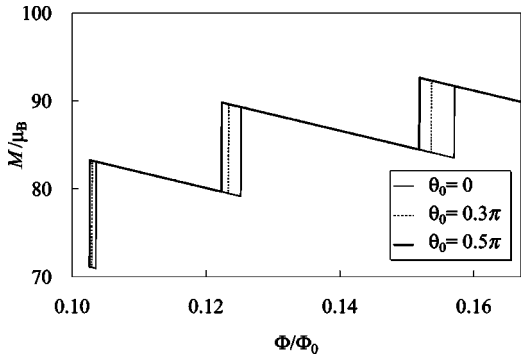

FIG. 6. Magnetic moment of electrons on an ellipsoid of revolution with $R=3\times10^{-7}$ cm and $\beta=0.001$ [case (iii)] as a function of a dimensionless magnetic field at $T=0$ K for the fixed chemical potential $\mu=0.5638$ eV.

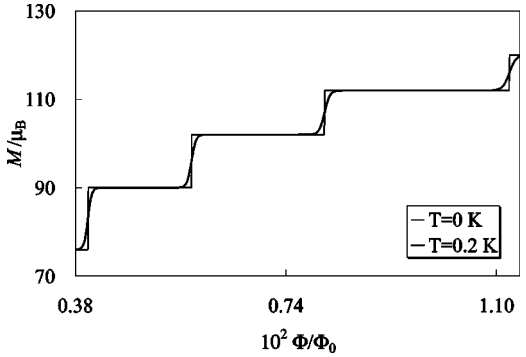

FIG. 7. Magnetic moment of electrons on an ellipsoid of revolution with $R=10^{-7}$ cm and $\beta=0.001$ [case (i)] as a function of a dimensionless magnetic field at $\vartheta_0=0$ for the fixed chemical potential $\mu=5.0292$ eV.

$M(B)|_{T=0}=2|m_0|\mu_B$. If the number $N-2l_0^2$ is not divisible by 4, then $m_0\geqslant 0$, and this leads to $m_0=(N-2l_0^2-2)/4$. Using Eq. (22), we obtain $M(B)|_{T=0}=0$. Note that for the case of the fullerene C_{70}, the magnetic moment is zero. Indeed, for C_{70} we have $N=280$. Therefore, for $\vartheta_0<\pi/2$, the quantum numbers l_0 and m_0 are equal to 11 and 9, respectively.

In cases (i) ($B_z\|Oz$) and (iii), the dependence of the magnetic moment for an ellipsoid of revolution on the magnetic field is similar to the respective dependence for the case of a sphere. For case (i), the energy spectrum depends linearly on the field. Therefore, in the limit $T=0$, the magnetic moment is independent of the field. And we see from Eq. (21) that the magnetic moment is equal to the Bohr magneton times an integer.

In both cases (a sphere and an ellipsoid of revolution), the dependence of the quantum numbers l_0 and m_0 on N can be written as

$$N=2(l_0^2+l_0+m_0+1). \tag{26}$$

Using the above-mentioned technique, the quantum numbers l_0 and m_0 are determined completely.

The magnetic moment for an ellipsoid of revolution depends on the angle ϑ_0 between the axis of revolution and the magnetic field direction. This dependence is caused by the dependence of the energy spectrum $E_{l,m}$ on ϑ_0. Thereby, at a fixed number of electrons, the chemical potential depends on ϑ_0. On the other hand, at a fixed chemical potential, the number of electrons can be changed with ϑ_0.

First, we consider the dependence of the magnetic moment M on the angle of inclination ϑ_0 at a fixed chemical potential. If the deformation perturbation is much larger than the magnetic one (this case corresponds to C_{70}), then the magnetic moment is positive ($M>0$) at $0<\vartheta_0<\pi/3$ and negative ($M<0$) at $2\pi/3<\vartheta_0<\pi$ (recall that the case of nearly perpendicular field direction to the axis of revolution is out of the scope of perturbation theory). Since the susceptibility is defined by $\chi=M/B$, the ellipsoid of revolution is paramagnetic ($\chi>0$) at $\vartheta\in(0,\pi)$. If the magnetic perturbation is much larger than the deformation one, then at $T=0$, the dependence of the magnetic moment on ϑ_0 is a jumplike one. Moreover, the dependence $M(\vartheta_0)$ is symmetric with respect to $\vartheta_0=\pi/2$. As mentioned in Sec. II, the levels with

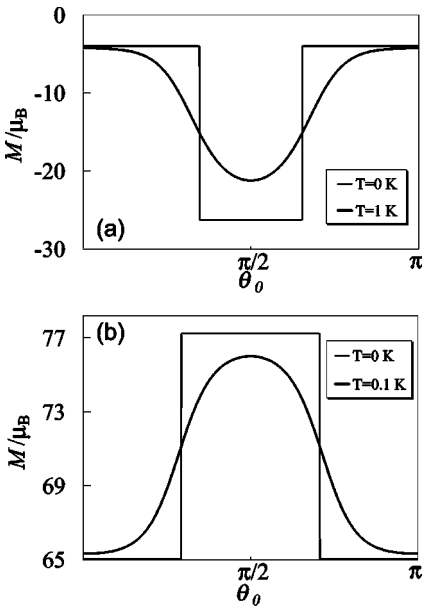

FIG. 8. Magnetic moment of electrons on an ellipsoid of revolution with $R=3\times10^{-7}$ cm and $\beta=0.001$ [case (iii)] as a function of increasing ϑ_0 at $B=20$ T for a fixed chemical potential. (a) The energy level with $l=11$, $m=11$ crosses the chemical potential $\mu=0.5713$ eV. (b) The energy level with $l=11$, $m=6$ crosses the chemical potential $\mu=0.56554$ eV.

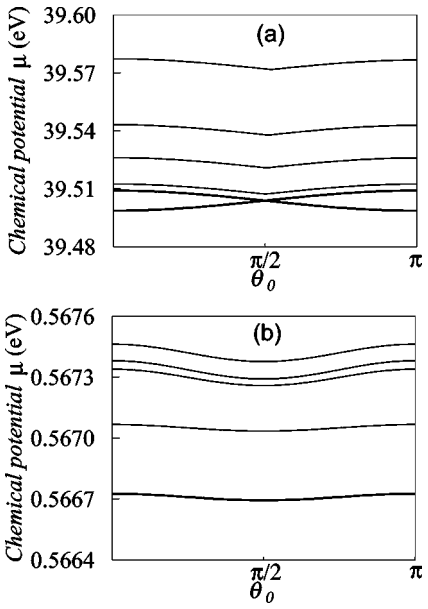

FIG. 9. (a) Chemical potential of an electron gas on an ellipsoid of revolution with $R=3.5\times10^{-8}$ cm and $\beta=0.1$ [case (ii)] as a function of increasing ϑ_0 at $T=1,5,10,20$ K and $B=10$ T for fixed $N=280$. (b) Chemical potential of an electron gas on an ellipsoid of revolution with $R=3\times10^{-7}$ cm and $\beta=0.001$ [case (iii)] as a function of increasing ϑ_0 at $T=0.1,1,15,20$ K and $B=20$ T for fixed $N=280$. The heavy curves correspond to the highest occupied levels.

$m^2<l(l+1)/3$ have the maximum at $\vartheta_0=\pi/2$, and the levels with $m^2>l(l+1)/3$ have the minimum at $\vartheta_0=\pi/2$. This mode of dependence of the energy spectrum on the angle of inclination affects the dependence $M(\vartheta_0)$ as follows. If the energy of a level increases as ϑ_0 runs through $(0,\pi/2)$, then the value of the magnetic moment increases stepwise as the considered level crosses the Fermi level. Conversely, if the energy of a level decreases with ϑ_0, then the value of the magnetic moment decreases stepwise. Both these cases are shown in Fig. 8.

In the case of a fixed number of particles, N, the chemical potential depends on the angle of inclination ϑ_0. At low T, this dependence is caused predominantly by the ϑ_0 dependence of the highest occupied level $E_{l_0,m_0}(\vartheta_0)$. These dependences are plotted in Fig. 9.

Now we consider case (ii) and study the dependence of the magnetic moment for an ellipsoid of revolution on the angle of inclination ϑ_0. Here we are interested only in the case when the number of electrons in the highest occupied shell is divisible by 4 (otherwise $M=0$). As can be seen from Eq. (22), the magnetic moment is positive at $\vartheta_0<\pi/3$ and negative at $\vartheta_0>2\pi/3$. Hence, in case (ii), if the number of electrons in the highest occupied shell is divisible by 4, then the dependence $M(\vartheta_0)$ is the same both for the case of fixed μ and for the case of fixed N (Fig. 10).

As can be seen from Eq. (23), for case (iii), for fixed N, the magnetic moment for an ellipsoid of revolution at $T=0$ is independent of the angle ϑ_0 (unlike the previous case), since the quantum numbers l_0 and m_0 are not changed. At nonzero temperature, the magnetic moment has a weak monotone dependence on ϑ_0 at $\vartheta_0\in(0,\pi/2)$. This dependence is caused by dependences of the energy levels and the chemical potential on ϑ_0 (Fig. 11).

V. RESULTS AND DISCUSSION

We have considered the energy spectrum of noninteracting electrons confined to the surface of an ellipsoid of revolution and found the magnetic response of this system both in the case of a fixed chemical potential and in the case of a fixed number of electrons. The case when the geometric confinement is much stronger than the magnetic confinement has been studied. In this connection, the perturbative corrections to the energy spectrum due to a deformation of a sphere into an ellipsoid (so-called deformation corrections) are supposed to be small. It is shown in Secs. III and IV that the relations between these corrections drastically affect the magnetic response as a function of the magnitude and the direction of a magnetic field.

It is shown that for a fixed chemical potential, the mag-

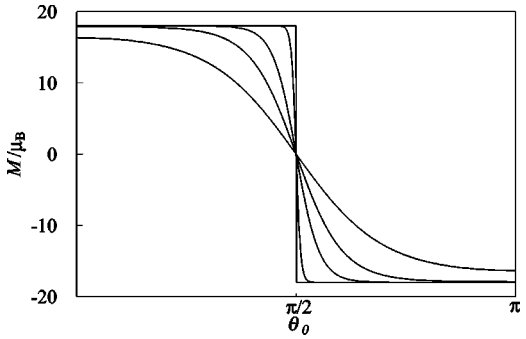

FIG. 10. Magnetic moment of electrons on an ellipsoid of revolution with $R=3.5\times10^{-8}$ cm and $\beta=0.1$ [case (ii)] as a function of increasing ϑ_0 at $T=0,1,5,10,20$ K and $B=10$ T for fixed $N=278$.

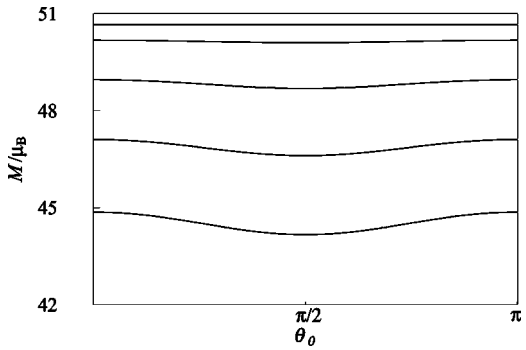

FIG. 11. Magnetic moment of electrons on an ellipsoid of revolution with $R=3\times10^{-7}$ cm and $\beta=0.001$ [case (iii)] as a function of increasing ϑ_0 at $T=0,5,10,15,20$ K and $B=20$ T for fixed $N=280$.

netic response for an ellipsoid of revolution is a steplike function of a magnetic field. The steps of this function are washed away by the temperature. For case (iii) (this case is similar to the case of a sphere), the plot of $M(B)$ has some steps (Fig. 6). For case (ii), only the z component of the magnetic moment does not vanish. In this case, the plot of $M(B)$ has only one step (see Fig. 5). Case (i) is similar to case (ii) if the field is parallel to the axis of revolution. The dependence of the magnetic response on the angle of inclination is investigated. In particular, for the case of a large magnetic correction, it is shown that the magnetic response is a steplike function of the angle ϑ_0 (Fig. 8).

In case (ii), for a fixed number of electrons, the chemical potential increases monotonically with the magnetic field. If the number of electrons in the highest occupied shell is divisible by 4, then the magnetic moment is positive for $\vartheta_0<\pi/3$ and negative for $\vartheta_0>2\pi/3$. If the number of electrons in the highest occupied shell is not divisible by 4 (this occurs for the case of C_{70}), then the magnetic response vanishes. As can be seen from Fig. 9(a), the chemical potential depends monotonically on ϑ_0 at $\vartheta_0\in(0,\pi/2)$.

If the magnetic correction is much larger than the deformation one, then the chemical potential is a slowly varying monotone function of the angle ϑ_0 [Fig. 9(b)]. In this case, the magnetic moment is positive and also depends on ϑ_0 weakly and monotonically [at $\vartheta_0\in(0,\pi/2)$].

It follows from the above discussion that the magnetic response for an ellipsoid of revolution depends on the thermodynamics of the system, unlike the bulk case (Landau diamagnetism) when the dependence of the magnetic response on the field is essentially the same both for the case of fixed μ and for the case of fixed N.[35]

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