Anomalous muonium in diamond-structure crystals

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(Submitted 5 July 1978)
Zh. Eksp. Teor. Fiz. **75**, 1999–2009 (December 1978)

A complete theory is developed for describing the experimental data on diamond-type crystals without allowance for relaxation processes. It is shown that our hypothesis of localization of muonium in tetrahedral and octahedral voids [Sov. Phys. JETP **47**, 331 (1978)] explains fully the results of recent experiments on Si. A complete theoretical analysis is made of the spin Hamiltonian. The analytic solutions obtained are used to suggest a series of experiments for investigating crystal structures with the aid of positive muons.

PACS numbers: 61.70.Ey, 36.10.Dr

1. We recently put forward[1] a theory of the behavior of positive muons in crystals with the diamond structure. This theory is based on a fundamentally new (for the muon method) assumption that a muonium atom (Mu) formed in a semiconductor or an insulator may have several equilibrium positions corresponding to different crystallographic voids. If the potential wells corresponding to these voids are separated by a potential barrier, several types of muonium atom should be observed in crystals. In the case of diamond-type crystals we may expect a Mu atom to have just two potential wells corresponding to tetrahedral and octahedral voids (also called tegragonal and hexagonal voids).

Since the potential relief for an Mu atom cannot be at present calculated reliably from the first principles, only experimental results can be used to determine whether a Mu atom occupies several equilibrium positions. Brewer *et al.*[2] investigated Si single crystals and discovered two types of Mu atom: normal and anomalous. The theory developed by us earlier[1] has made it possible to explain all the observed effects, and to identify the normal and anomalous muonium with the location of Mu in the tetrahedral and octahedral voids, respectively.

It has been shown that purely group-theoretic considerations indicate that the spin Hamiltonian of the hyperfine interaction for the tetrahedral voids in crystals with the diamond structure is of the same form as the corresponding Hamiltonian for vacuum (the influence of the crystal field reduces to renormalization of the hyperfine interaction frequency ω_0); in the case of octahedral voids the invariant form of the spin Hamiltonian is

$$H=\hbar\Omega_\perp\sigma_e\sigma_\mu+\hbar(\Omega_\parallel-\Omega_\perp)(\sigma_e\mathbf{n})(\sigma_\mu\mathbf{n})-\mu_e\mathbf{B}\sigma_e-\mu_\mu\mathbf{B}\sigma_\mu, \qquad (1)$$

where $\Omega_\parallel$ and $\Omega_\perp$ are the hyperfine interaction constants; **B** is an external magnetic field; **n** is a unit vector directed along the c_3 symmetry axis; μ_e and μ_μ are the magnetic moments of a muonium electron and of a positive muon, respectively.

We made various predictions in Ref. 1 and analyzed a series of interesting experimental possibilities which follow from the theory. However, the analysis has been limited to the case when an external field is either parallel to the c_3 ([111]) symmetry axis or perpendicular to this axis. Recent series of striking precision experiments[3-5] have shown that two types of Mu atom are observed in Si at low temperatures in p- and n-type samples with different impurity concentrations. Obviously, the authors of Refs. 3–5 were unaware of our theory[1] but in their theoretical interpretation they reached independently the conclusion that anomalous muonium is described by the Hamiltonian (1) and that the two types of Mu atom in Si correspond to the capture by tetrahedral and octahedral voids. Thus, the theoretical parts of the investigations reported in Refs. 3–5 are in basic agreement with our theory.[1] The results of Ref. 1 are partly reproduced: the spin Hamiltonian is diagonalized numerically but analytic solutions are not obtained. We shall show that the experimental results of Refs. 3–5 show unambiguously that, at least at temperatures below 80°K, muonium atoms in silicon can exist simultaneously in octahedral and tetrahedral voids. Therefore, all the subsequent interpretations of the behavior of the muon polarization in silicon should be carried out bearing this fact in mind.

Finally, we must stress that the experimental results of Refs. 2–5 and the theory developed by us[1] provide new extensive opportunities for using the muon method in investigations of fine details of the structure of the internal crystal field and of the potential relief in solid lattices. There is every reason to expect that very soon the existence of two (or maybe even several) types of Mu atom will be discovered in many crystals.

We shall carry out a complete analysis of the behavior of the polarization of positive muons in single crystals with the diamond structure for an arbitrary mutual orientation of the field **B** and the symmetry axis c_3. We shall give the formulas for the total polarization of anomalous muonium (following Ref. 1, we shall call it O muonium) for three simple cases most convenient for experimental analysis. We shall not consider here the processes of polarization relaxation so that we restrict ourselves to the case when the relaxation rate is $\nu \ll \omega_0$.

2. We must stress that consideration of arbitrary orientation of **B** and c_3 is necessary for complete analysis of the experimental data on silicon. In fact, an octahedral void in Si is located in the middle of the [111] axis joining two tetragonal voids. Consequently, four octahedral voids have four different directions of the symmetry axis. If a crystal is subjected to a magnetic field, the four octahedral voids for the O muonium are generally under different conditions because of the dif-

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ferent angles between the direction of the field and the symmetry axis of a given void. If, for example, the field is directed along the [111] axis, two varieties of the O muonium may be observed: one of them is located in an octahedral void whose symmetry axis is parallel to the field and the other in the remaining three types of octahedral void. In general, we can observe up to four "different" types of O muonium.

It is pointed out in Ref. 1 that in the $\mathbf{B} \| c_3$ configuration the energy levels cross in weak and strong fields, whereas in the $\mathbf{B} \perp c_3$ case this occurs only in strong fields. Consequently, if the field is parallel to the symmetry axis, the projection of the total spin onto the quantization axis, parallel to the field B, is conserved. If the field is perpendicular to the symmetry axis, the square of the projection of the total spin onto the axis parallel to the field is conserved. In these cases the system has "good" quantum numbers and, in accordance with the Wigner–Neumann theorem,[6] the levels characterized by different values of good quantum numbers may cross. For an arbitrary orientation of the field B and the symmetry axis c_3 there is only one good quantum number (parity) which is identical for all four levels and, in accordance with the Wigner–Neumann theorem, these levels cannot cross. The behavior of the spin energy levels is shown in Fig. 1.

3. We shall direct the quantization axis z along the field B and we shall take the x axis in a plane passing through B and c_3 which meet at an angle θ. The basis is represented by the functions

$$\chi_1=|++\rangle, \quad \chi_2=|+-\rangle, \quad \chi_3=|-+\rangle, \quad \chi_4=|--\rangle. \tag{2}$$

The first sign refers to an electron and the second to a muon. In this basis the Hamiltonian matrix is

$$H=\begin{pmatrix} \Omega+\omega(1-\zeta) & \Delta\Omega_1 & \Delta\Omega_1 & \Delta\Omega_2 \\ \Delta\Omega_1 & -\Omega+\omega(1+\zeta) & 2\Omega_\perp+\Delta\Omega_2 & -\Delta\Omega_1 \\ \Delta\Omega_1 & 2\Omega_\perp+\Delta\Omega_2 & -\Omega-\omega(1+\zeta) & -\Delta\Omega_1 \\ \Delta\Omega_2 & -\Delta\Omega_1 & -\Delta\Omega_1 & \Omega-\omega(1-\zeta) \end{pmatrix}; \tag{3}$$

$$\Omega=\Omega_\| \cos^2\theta+\Omega_\perp \sin^2\theta, \quad \Delta\Omega_1=(\Omega_\|-\Omega_\perp)\sin\theta\cos\theta,$$
$$\Delta\Omega_2=(\Omega_\|-\Omega_\perp)\sin^2\theta, \quad \hbar\omega=|\mu_e|B, \quad \zeta=|\mu_\mu/\mu_e|.$$

We can see that for $\theta=0$ and $\pi/2$ the matrix (3) simplifies to the terms along the principal and secondary diagonals. We can, therefore, assume that it is generally convenient to reduce the Hamiltonian (3) to the form which eliminates elements from the secondary diagonal. The unitary transformation matrix $T_1(\theta)$ is found in accordance with the familiar prescription (see, for example, Ref. 1):

$$T_1(\theta)=\begin{pmatrix} \cos\vartheta_2 & 0 & 0 & -\sin\vartheta_2 \\ 0 & \cos\vartheta_1 & -\sin\vartheta_1 & 0 \\ 0 & \sin\vartheta_1 & \cos\vartheta_1 & 0 \\ \sin\vartheta_2 & 0 & 0 & \cos\vartheta_2 \end{pmatrix}, \tag{4}$$

$$\operatorname{tg} 2\vartheta_1=(2\Omega_\perp+\Delta\Omega_2)/\omega(1+\zeta), \quad \operatorname{tg} 2\vartheta_2=\Delta\Omega_2/\omega(1-\zeta).$$

If $\theta=0$ and $\pi/2$, the Hamiltonian is diagonal in the new basis and we obtain immediately the spectrum given earlier.[1] Clearly, if the difference between the diagonal element $H'_{\alpha\alpha}$ of the Hamiltonian in the new basis $H'=T_1^{-1}(\theta)HT_1(\theta)$ and the remaining diagonal elements $H'_{\beta\beta}$ is much greater than the corresponding nondiagonal elements $H'_{\alpha\beta}$, then $H'_{\alpha\alpha}$ represents approximately an energy level. If $|H'_{\alpha\beta}| \sim |H'_{\alpha\alpha}-H'_{\beta\beta}|$, the states α and β are "mixed." It follows from our earlier analysis[1] that in fields $\omega \sim |\Delta\Omega| = |\Omega_\| - \Omega_\perp|$ with $\Omega_\| > \Omega_\perp$ the states 2 and 4 are mixed, whereas for $\Omega_\| < \Omega_\perp$ and in strong fields $\zeta\omega \sim \Omega$ the states 1 and 2 are mixed, and for $|\Delta\Omega| \sim \Omega$ the states 3 and 4 are also mixed.

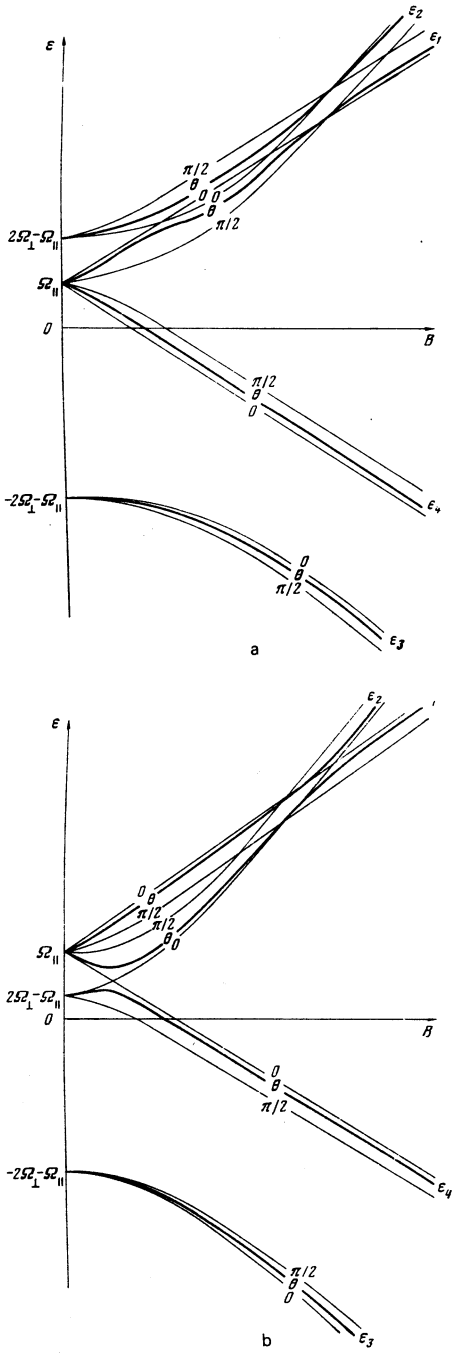

FIG. 1. Energy level scheme of the spin Hamiltonian of the O muonium: a) $\Omega_\| < \Omega_\perp$; b) $\Omega_\| > \Omega_\perp$. In accordance with the Wigner–Neumann theorem, there is no level crossing for $\theta \neq 0, \pi/2$.

The elements of the Hamiltonian H' have thus the form

$$H_{11}'=\Omega+\Delta\Omega_2 \sin 2\vartheta_2+\omega(1-\zeta)\cos 2\vartheta_2, \tag{5}$$
$$H_{22}'=-\Omega+(2\Omega_\perp+\Delta\Omega_2)\sin 2\vartheta_1+\omega(1+\zeta)\cos 2\vartheta_1, \tag{6}$$
$$H_{33}'=-\Omega-(2\Omega_\perp+\Delta\Omega_2)\sin 2\vartheta_1-\omega(1+\zeta)\cos 2\vartheta_1, \tag{7}$$
$$H_{44}'=\Omega-\Delta\Omega_2 \sin 2\vartheta_2-\omega(1-\zeta)\cos 2\vartheta_2. \tag{8}$$

The nonzero nondiagonal elements are

$$H_{12}'=H_{21}'=\Delta\Omega_1[\cos(\vartheta_1+\vartheta_2)+\sin(\vartheta_1-\vartheta_2)], \quad (9)$$

$$H_{42}'=H_{24}'=-\Delta\Omega_1[\cos(\vartheta_1-\vartheta_2)+\sin(\vartheta_1+\vartheta_2)], \quad (10)$$

$$H_{13}'=H_{31}'=-\Delta\Omega_1[\cos(\vartheta_1+\vartheta_2)-\sin(\vartheta_1-\vartheta_2)], \quad (11)$$

$$H_{13}'=H_{31}'=\Delta\Omega_1[\cos(\vartheta_1-\vartheta_2)-\sin(\vartheta_1+\vartheta_2)]. \quad (12)$$

The muon polarization is $\mathbf{P}(t)=\frac{1}{4}\mathrm{Tr}[\sigma_\mu\rho(t)]$, where σ_μ are the spin operators and $\rho(t)$ is the spin density matrix of muonium. If electrons in the investigated crystal are totally depolarized, the density matrix at the moment $t=0$ has the form

$$\rho(0)=\sigma_{\mu i}P_i(0)+{}^1/_4 I, \quad (13)$$

where $P_i(0)$ is the initial polarization of a positive muon and I is a unit matrix. Then, the polarization of a positive muon in muonium located in an octahedral void, whose symmetry axis makes an angle θ with the field B, can be described at any moment t by

$$P_i(t)=S_{ik}(\cos\theta,\ t)P_k(0), \quad (14)$$

$$S_{ik}(\cos\theta,\ t)={}^1/_4\,\mathrm{Sp}\,[\sigma_{\mu i}\exp(i\hbar^{-1}H't)\sigma_{\mu k}\exp(-i\hbar^{-1}H't)]. \quad (15)$$

If the unitary transformation T_2 which diagonalizes approximately the Hamiltonian H' is known, the tensor $S_{ik}(\cos\theta, t)$ becomes

$$S_{ik}(\cos\theta,t)=\sum_{\alpha,\beta}\langle\alpha|\sigma_{\mu i}|\beta\rangle\langle\beta|\sigma_{\mu k}|\alpha\rangle\exp(i\omega_{\beta\alpha}t), \quad (16)$$

where $\hbar\omega_{\beta\alpha}=\varepsilon_\beta-\varepsilon_\alpha$; $\varepsilon_\alpha=(T_2^{-1}H'T_2)_{\alpha\alpha}$ are the approximate energy levels. The actual form of the matrix T_2 will be found later for various limiting cases. It follows from Eq. (16) that the nondiagonal components of the tensor $S_{ik}(\cos\theta, t)$ are related by

$$S_{xy}=-S_{yx},\quad S_{xz}=S_{zx},\quad S_{zy}=-S_{yz}. \quad (17)$$

4. If the magnetic field is such that $\omega\sim\Omega$ and $|\Delta\Omega|\sim\Omega$, the tensor (16) is given by cumbersome formulas, so that we shall confine our attention to the limiting cases: A) $\omega\ll|\Delta\Omega_2|, \Omega$ and B) $\omega\gg\Omega$.

A. It is clear from Eqs. (11) and (12) that the nondiagonal elements H_{13}' and H_{34}' are of the second order of smallness and, therefore, we shall neglect them. The order of the elements H_{12}' and H_{42}' depends on the sign of $\Delta\Omega_2$. For $\Delta\Omega_2>0$, we have $H_{42}'\approx(\Omega_\perp-\Omega_\parallel)\sin2\theta$, $H_{21}'\approx\omega\cot\theta$; if $\Delta\Omega_2<0$ then $H_{42}'\approx\omega\cot\theta$, $H_{21}'\approx(\Omega_\parallel-\Omega_\perp)\sin2\theta$. We shall show that the nature of the polarization is independent of the sign of $\Delta\Omega_2$.

We shall consider the specific case when $\Delta\Omega_2<0$. We shall apply the standard method of approximate diagonalization of a symmetric matrix.[7] We shall make the unitary transformation

$$T_2=\frac{1}{2^{1/2}}\begin{pmatrix}\cos\theta & -2^{1/2}\sin\theta & 0 & -\cos\theta\\ \sin\theta & 2^{1/2}\cos\theta & 0 & -\sin\theta\\ 0 & 0 & 2^{1/2} & 0\\ 1 & 0 & 0 & 1\end{pmatrix}. \quad (18)$$

To within terms quadratic in the field, we obtain

$$\hbar^{-1}\varepsilon_{1,4}=\Omega_\parallel\pm\omega\cos\theta,\qquad \hbar^{-1}\varepsilon_{2,3}=\pm2\Omega_\perp-\Omega_\parallel. \quad (19)$$

Using the form of the matrix T_2, we obtain the components of the tensor S_{ik}:

$$S_{zz}={}^1/_2[\cos^2\theta(1+\cos4\Omega_\perp t)+2g(t)\sin^2\theta], \quad (20)$$

$$S_{xx}={}^1/_4\sin2\theta[2g(t)-1-\cos4\Omega_\perp t], \quad (21)$$

$$S_{xx}={}^1/_2[\sin^2\theta(1+\cos4\Omega_\perp t)+2g(t)\cos^2\theta], \quad (22)$$

$$S_{yy}=g(t), \quad (23)$$

$$S_{yx}=f(t)\cos\theta,\quad S_{yz}=f(t)\sin\theta, \quad (24)$$

where for compactness we have introduced the functions

$$g(t)=\cos2\Omega_\perp t\cos2\Omega_\parallel t\cos(\omega_{14}t/2), \quad (25)$$

$$f(t)=\cos2\Omega_\perp t\cos2\Omega_\parallel t\sin(\omega_{14}t/2). \quad (26)$$

Employing the characteristic equation for $\zeta\omega\ll\Omega$ [see Eq. (10) in Ref. 1], we find that to within quadratic terms the quantity ω_{14} is given by

$$\omega_{14}=2\omega[\cos^2\theta+\Omega_\perp{}^2\omega^2/(\Omega_\parallel{}^2-\Omega_\perp{}^2)^2]^{1/2}. \quad (27)$$

The expression (27) for ω_{14} is valid for any angle θ subject to the condition $\omega\ll|\Omega_\parallel-\Omega_\perp|$. The formulas (20)–(24) describe the behavior of the polarization[1] also for $\theta=0$, when the condition $\omega\ll|\Delta\Omega_2|$ is not obeyed. We may expect the range of validity of these formulas to be really limited only by the condition $\omega\ll|\Omega_\parallel-\Omega_\perp|$ and they should work well for any angle θ.

B. We shall now consider the range of strong fields $\omega\gg|\Delta\Omega|, \Omega$; then ϑ_1 and ϑ_2 are small. If $\zeta\omega\ll\Omega$ and $|\Delta\Omega|\ll\Omega$, the polarization is described by the familiar formulas for two-frequency precession[8-11] but the transition frequencies are given by the diagonal elements (5)–(8) of the Hamiltonian H'. If $|\Delta\Omega|\sim\Omega$, the formulas for the polarization have the simpler form in the range $\zeta\omega\sim\Omega$. In this case we have $|H_{24}'|\ll|H_{22}'-H_{44}'|$ and $|H_{13}'|\ll|H_{11}'-H_{33}'|$, and we can ignore the nondiagonal elements (10) and (12).

We are thus left with the elements H_{12}' and H_{34}'. Then, the Hamiltonian H' can be reduced to the diagonal form by the transformation

$$T_2=\begin{pmatrix}\cos\vartheta_3 & -\sin\vartheta_3 & 0 & 0\\ \sin\vartheta_3 & \cos\vartheta_3 & 0 & 0\\ 0 & 0 & \cos\vartheta_4 & -\sin\vartheta_4\\ 0 & 0 & \sin\vartheta_4 & \cos\vartheta_4\end{pmatrix}, \quad (28)$$

where $\tan2\vartheta_3=\Delta\Omega_1/(\Omega-\zeta\omega)$, and $\tan2\vartheta_4=\Delta\Omega_1/(\Omega+\zeta\omega)$. The approximate energy levels are then defined as follows:

$$\hbar^{-1}\varepsilon_{2,1}=\omega\pm[\Delta\Omega^2+(\Omega-\zeta\omega)^2]^{1/2},\quad \hbar^{-1}\varepsilon_{4,3}=-\omega\pm[\Delta\Omega_1{}^2+(\Omega+\zeta\omega)^2]^{1/2}. \quad (29)$$

The components of the tensor $S_{ik}(\cos\theta, t)$ are

$$S_{zz}=2\left[\frac{(\Omega-\zeta\omega)^2+\Delta\Omega_1{}^2\cos\omega_{21}t}{\omega_{21}{}^2}+\frac{(\Omega+\zeta\omega)^2+\Delta\Omega_1{}^2\cos\omega_{43}t}{\omega_{43}{}^2}\right], \quad (30)$$

$$S_{xz}=2\left[\frac{\Delta\Omega_1(\Omega-\zeta\omega)}{\omega_{21}{}^2}(\cos\omega_{21}t-1)+\frac{\Delta\Omega_1(\Omega+\zeta\omega)}{\omega_{43}{}^2}(\cos\omega_{43}t-1)\right], \quad (31)$$

$$S_{yz}=[(\Delta\Omega_1/\omega_{21})\sin\omega_{21}t+(\Delta\Omega_1/\omega_{43})\sin\omega_{43}t], \quad (32)$$

$$S_{xx}=2\left[\frac{\Delta\Omega_1{}^2+(\Omega-\zeta\omega)^2\cos\omega_{21}t}{\omega_{21}{}^2}+\frac{\Delta\Omega_1{}^2+(\Omega+\zeta\omega)^2\cos\omega_{43}t}{\omega_{43}{}^2}\right], \quad (33)$$

$$S_{yx}=\{[(\Omega-\zeta\omega)/\omega_{21}]\sin\omega_{21}t+[(\Omega+\zeta\omega)/\omega_{43}]\sin\omega_{43}t\}, \quad (34)$$

$$S_{yy}={}^1/_2(\cos\omega_{21}t+\cos\omega_{43}t). \quad (35)$$

We can see that for $|\Omega\pm\zeta\omega|\gg|\Delta\Omega_1|$ the formulas (30)–(35) reduce to the familiar expressions for two-frequency precession with the corresponding hyperfine constant Ω depending on the angle θ.

5. We shall now consider the behavior of the longitudinal (parallel to an external magnetic field B) and transverse (perpendicular to B) polarizations of a muon in the three simplest special cases.

Case 1: Field **B** *directed along the* [100] *axis.* The directions of the symmetry axes of all four inequivalent octahedral voids make the same angle with the field defined by $\cos\theta=3^{-1/2}$. Consequently, only one O muonium is observed. The polarization of all four octahedral voids can be written in the form

$$P_z(t)=P_z(0)S_{zz}(3^{-1/2},\ t), \tag{36}$$

$$P_+(t)=P_+(0)\,[S_{xx}(3^{-1/2},\ t)+S_{yy}(3^{-1/2},\ t)+2iS_{yx}(3^{-1/2},\ t)\,]. \tag{37}$$

In general, the polarization has a fairly complex time dependence and is governed by all six possible transition frequencies (Fig. 1), but in weak and strong fields the formulas simplify considerably. As expected from Eqs. (20) and (22)–(24), all the components have oscillatory terms in weak fields ($\omega\ll|\Omega_\parallel-\Omega_\perp|$) and these terms exhibit beats of frequency $\omega[\frac{1}{3}+\Omega_\perp^2\omega^2/(\Omega_\parallel^2-\Omega_\perp^2)^2]^{1/2}$. The constant term of the longitudinal and transverse component is $\frac{1}{6}$. If $|\Delta\Omega|\lesssim10^8$ sec^{-1}, this behavior may be observed in fields $B\lesssim10$ G.

In strong fields the polarization is given by Eqs. (30) and (33)–(35). It is interesting to note that in fields $\zeta\omega\sim\Omega$ the longitudinal component has two terms oscillating at frequencies ω_{21} and ω_{43}. One frequency (ω_{21}) has a minimum at $\zeta\omega=\Omega=(\Omega_\parallel+2\Omega_\perp)/3$ and its value is $\omega_{\min}=2^{3/2}|\Omega_\parallel-\Omega_\perp|/3$; the corresponding amplitude is $\frac{1}{2}$. The amplitude associated with the frequency ω_{43} decreases monotonically. If $\zeta\omega\gg\Omega$, the longitudinal component of the polarization is unity. The transverse polarization is given by Eqs. (33)–(35); they also contain the constant term and the precession is described by two frequencies ω_{21} and ω_{43}. In a field $\zeta\omega=(\Omega_\parallel+2\Omega_\perp)/3$, the constant term is close to $\frac{1}{2}$ and the precession is described only by the frequency ω_{43}; the only oscillations at the frequency $\omega_{\min}$ have the amplitude $\frac{1}{4}$.

Case 2: Field **B** *directed along the* [111] *axis.* In this case the symmetry axis of one octahedral void is parallel to the field and the directions of the symmetry axes of the three other inequivalent octahedral voids make the same angle with the field and this angle is defined by $\cos\theta=\frac{1}{3}$. For this orientation of a crystal in the field there should be two varieties of the O muonium. The total polarization of the O muonium is given by

$$P_z(t)=\tfrac{1}{4}P_z(0)\,[S_{zz}(1,\ t)+3S_{zz}(\tfrac{1}{3},\ t)\,], \tag{38}$$

$$P_+(t)=\tfrac{1}{4}P_+(0)\,\{S_{xx}(1,\ t)+iS_{yx}(1,\ t)+\tfrac{3}{2}[S_{xx}(\tfrac{1}{3},t)+S_{yy}(\tfrac{1}{3},\ t)+2iS_{yx}(\tfrac{1}{3},\ t)\,]\}. \tag{39}$$

In general, there are 11 transition frequencies. The above formulas simplify in weak and strong fields. For a void with the symmetry axis parallel to the field there are only high-frequency oscillatory terms and no beats in weak fields. The constant term in the longitudinal and transverse components of the polarization is $\frac{1}{6}$ and the amplitude of the oscillatory term exhibiting beats of frequency $\omega[\frac{1}{9}+\Omega_\perp^2\omega^2/(\Omega_\parallel^2-\Omega_\perp^2)^2]^{1/2}$ is $\frac{2}{3}$. The precession term (with beats) of the transverse polarization has the amplitude $\frac{1}{24}$.

In strong fields the longitudinal component is given by Eq. (30). For muonium in an octahedral void characterized by $\mathbf{B}\parallel c_3$ the polarization is constant and close to unity and, therefore, its contribution to the total longitudinal polarization (38) is $\frac{1}{4}$. The second term in Eq. (38) has components oscillating at two frequencies. In a field $\zeta\omega=(\Omega_\parallel+8\Omega_\perp)/9$ the term of frequency ω_{21} has the maximum amplitude $\frac{3}{8}$ and the frequency has its minimum at $\omega_{\min}=2^{5/2}|\Omega_\parallel-\Omega_\perp|/9$.

The two varieties of the anomalous muonium appear most clearly in strong fields $\zeta\omega\sim\Omega$, where only two low frequencies of each muonium may be observed. For each muonium in a void characterized by $\mathbf{B}\parallel c_3$ there should be a precession stopping point in a field $\zeta\omega=\Omega_\parallel$ and the behavior of polarization should be as described in detail in Ref. 1: For the other O muonium the signal is stronger and has a constant component whose maximum value corresponds to $\zeta\omega=(\Omega_\parallel+8\Omega_\perp)/9$. The precession occurs then only at the frequency ω_{43} and the component with the frequency $\omega_{\min}$ oscillates with the amplitude $\frac{3}{16}$.

Case 3: Field **B** *parallel to the* [110] *axis.* In this case the symmetry axes of two octahedral voids are perpendicular to the field and the directions of the other two voids make the same angle θ with the field: $\cos\theta=(\frac{2}{3})^{1/2}$. In this case there should be once again two varieties of anomalous muonium. The total polarization is given by the formulas

$$P_z(t)=\tfrac{1}{2}P_z(0)\,[S_{zz}(0,\ t)+S_{zz}((^2/_3)^{1/2},\ t)\,]. \tag{40}$$

$$P_+(t)=\tfrac{1}{4}P_+(0)\,\{S_{xx}(0,\ t)+S_{yy}(0,\ t)+S_{xx}((^2/_3)^{1/2},\ t)+S_{yy}((^2/_3)^{1/2},\ t)+2i[S_{yx}(0,\ t)+S_{yx}((^2/_3)^{1/2},\ t)\,]+e^{i2\varphi}[S_{xx}((^2/_3)^{1/2},\ t)-S_{yy}((^2/_3)^{1/2},\ t)+(S_{xx}(0,\ t)-S_{yy}(0.\ t))/3]\}. \tag{41}$$

The system does not have axial symmetry and, therefore, the polarization depends on the angle φ between the planes passing through **P**(0) and **B**, and on the directions of the symmetry axes making an angle θ relative to the field. It follows from Eq. (41) that the transverse polarization has the simplest form for $\varphi=0$ and $\pi/2$, i.e., **P**(0) is parallel to the directions [001] and $[\bar{1}10]$, respectively. In weak fields the longitudinal component has two oscillatory terms which exhibit low-frequency beats. The term of frequency $\Omega_\perp\omega^2/|\Omega_\parallel^2-\Omega_\perp^2|$ has the amplitude $\frac{1}{2}$ and the term of frequency $\omega[\frac{2}{3}+\Omega_\perp^2\omega^2/(\Omega_\parallel^2-\Omega_\perp^2)^2]^{1/2}$ has the amplitude $\frac{1}{6}$.

The constant term is also $\frac{1}{6}$. The transverse polarization has an oscillatory term exhibiting beats of frequency $\Omega_\perp\omega^2/|\Omega_\parallel^2-\Omega_\perp^2|$ and the term with the beat frequency $\omega[\frac{2}{3}+\Omega_\perp^2\omega^2/(\Omega_\parallel^2-\Omega_\perp^2)^2]^{1/2}$ precesses.

In strong fields the first term of the longitudinal component (40) is close to $\frac{1}{2}$, whereas the second term is given by Eq. (30) and for $\zeta\omega=(2\Omega_\parallel+\Omega_\perp)/3$ the term oscillating at the frequency $\omega_{\min}=2^{3/2}|\Omega_\parallel-\Omega_\perp|/3$ has the maximum amplitude of $\frac{1}{4}$. The behavior of the transverse polarization is given by the precession of two varieties of O muonium. For one type of O muonium ($\mathbf{B}\perp c_3$) the behavior of the polarization is analyzed in detail in Ref. 1 and stopping of the precession occurs in a field $\zeta\omega=\Omega_\perp$. The behavior of the other O muonium is given by Eqs. (33)–(35); there are two frequencies and a constant term whose maximum corresponds to $\zeta\omega_{\min}=(2\Omega_\parallel+\Omega_\perp)/3$.

It is clear from the results obtained that complex precession occurs in weak fields. When the field is orient-

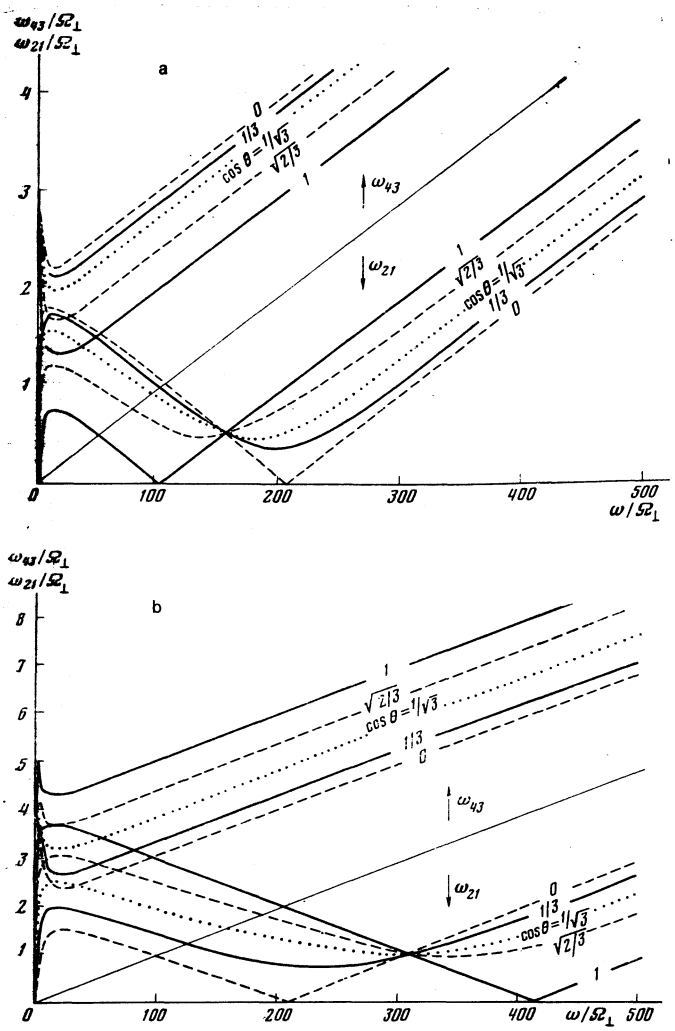

FIG. 2. Magnetic-field dependences of the observed frequency spectrum of the O muonium in strong fields. The continuous curves correspond to the field oriented along the [111] axis; the dashed curves to the field oriented along [110] and the dotted curves to the field oriented along [100]. Two frequencies ω_{21} and ω_{43} correspond to the two types of O muonium: a) $\Omega_\parallel = 0.5\Omega_\perp$; b) $\Omega_\parallel = \Omega_\perp$.

ed along the [111] axis, ten frequencies are observed: four of them correspond to the O muonium for which $\mathbf{B} \| c_3$ and six to the O muonium whose symmetry axis is not parallel to the field. It is clear from Eq. (39) that the amplitude of the latter frequencies is three times higher. If the field is directed along the [110] axis, once again there are ten precession frequencies. In strong fields ($\omega > \omega_0^0$) there are in reality only two frequencies for each variety of the O muonium. The dependences of the observed frequencies on the magnetic field are illustrated in Fig. 2.

6. The formulas (36)–(41) describe completely the experiments reported in Refs. 3–5. It should be pointed out that, in agreement with our theory, a large number of frequencies was observed in weak fields[3-5] but the results were not interpreted. It should be noted that the range of weak fields is very interesting because the experiments carried out in such fields give practically the only reliable possibility of accurate determination of the g factor of the O-muonium electron. The experiments reported in Refs. 3–5 gave $2\pi^{-1}\Omega_\perp = 92.1 \pm 0.3$ MHz, $2\pi^{-1}\Omega_\parallel = 17.1 \pm 0.3$ MHz, $g_e = -2.2 \pm 0.2$, and $g_\mu = 2.01 \pm 0.01$. It follows from the above discussion that the value of g_e cannot be regarded as finally established until experiments are carried out in weak fields.

The clearest experimental confirmation of the O-muonium hypothesis is probably the angular dependence of the precession frequencies obtained in Refs. 4 and 5 on rotation of a crystal relative to the $[01\bar{1}]$ axis oriented at right-angles to the field. It seems that the other speculative possibilities discussed in Refs. 4 and 5 are not very likely. It should be stressed that studies of relaxation processes will require experiments in longitudinal fields and then Eqs. (36), (38), (40) and (20), (30) of the present paper will be of special interest. We may conclude that a new stage of the investigation of solids by the muon method has been discovered.

As pointed out earlier, we cannot *a priori* predict the existence of several potential minima of a Mu atom, but this situation should not be specific to silicon alone, and, therefore, there is special interest in the search for several types of Mu atom in other crystals. In this connection we shall point out that the preliminary data of Graf *et al.*[3] indicate a considerable temperature dependence of the intensities of the O- and T-muonium lines. In addition to these lines there is always a muon component. As the temperature is increased, the normal (T) muonium disappears first and at $T = 295°K$ only the muon component remains. On the other hand, the intensity of the muon component rises on increase of the degree of doping of a crystal and at impurity concentrations $n = 10^{18}$ cm^{-3} only this component is observed.

It is as yet difficult to draw definite conclusions but we may point out that in addition to the obvious interpretation variants associated with the differences between the rates of relaxation of the O- and T-muonium polarizations, we must allow also for the interesting possibility of the actual disappearance of one of the types of muonium at higher temperatures. If the barrier between the potential wells is relatively small, muonium may overcome this barrier at higher temperatures in a time much shorter than the lifetime of the positive muon. The relaxation processes will be considered in the next paper.

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Translated by A. Tybulewicz

Higher orders and structure of the perturbation-theory series for the anharmonic oscillator

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(Submitted 25 July 1978)
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A simple method of calculating higher orders of perturbation theory (PT) in powers of g for the D-dimensional isotropic oscillator with arbitrary anharmonicity $gv(r)$ is developed. The method is based on transforming from the Schrödinger equation to the Riccati equation (2.3). In the important particular case of power nonlinearity $v(r) = r^{2N}$, $N = 2,3,4,...$, all the terms $\xi_k(r)$ of the PT series (2.4) become polynomials, and this simplifies considerably the calculation of the higher orders of PT. A new variant of PT is proposed, which converges at all values of the coupling constant g: $0<g<\infty$. The structure of the PT series for the energy levels is investigated for potentials with a power increase $[v(r)\sim r^{\nu}]$ and exponential increase $[v(r)\sim\exp(br^{2\nu})]$ at infinity. It is shown that, in the latter case with $0<\nu<1$, the PT series is asymptotic for $g\to 0$ but is not summable by the Borel method. For $\nu\geq 1$ a PT series in integer powers of g does not exist, and the energy difference $E(g)-E(0)$ vanishes more slowly than g as $g\to 0$. The energy correction $E(g)-E(0)$ for small values of g is calculated. The character of the singular point of $E(g)$ at $g=0$ changes at $\nu=1$.

PACS numbers: 03.65.Ge

1. INTRODUCTION

Many papers (see, e.g., Refs. 1–15) have been devoted to the study of the anharmonic oscillator

$$H=\sum_{i=1}^{D}(p_i^2+x_i^2)+g\Big(\sum_{i=1}^{D}x_i^2\Big)^N \tag{1.1}$$

($N=2,3,4,\ldots$). This is explained by the fact that this problem not only has important applications in solid-state theory and molecular physics but is also of fundamental interest in connection with certain problems in quantum field theory. In a series of papers,[1-5] Bender and Wu investigated the structure of the perturbation-theory (PT) series for the energy levels

$$E(g)=\sum_{k=0}^{\infty}E_k(-g)^k \tag{1.2}$$

and showed that the coefficients of the PT series increase factorially as $k\to\infty$:

$$E_k\approx(k\alpha)!a^kk^b\Big(c_0+\frac{c_1}{k}+\frac{c_2}{k^2}+\ldots\Big). \tag{1.3}$$

Lipatov[16] established that the coefficients of the PT series for the Gell-Mann–Low function in scalar field theory with the interaction

$$H_{\cdot\cdot}=\int\frac{d^Dx\,g\varphi^n}{n!},\qquad D=\frac{2n}{n-2}$$

behave analogously. In view of this analogy, the anharmonic oscillator is a convenient model upon which we can elucidate a number of questions of importance for field theory (e.g., the summability of the PT series by different methods of summation of divergent series, the structure of the expansion (1.3) in powers of $1/k$, and so forth).

The present paper is devoted to an investigation of the PT series for the anharmonic oscillator. In Sec. 2 a simple method of systematic calculation of the terms of the PT series, based on transforming from the Schrödinger equation to the nonlinear Riccati equation, is described. The application of this method to the D-dimensional oscillator with anharmonicity gr^{2N} enables us to obtain a large number of coefficients of the PT series with ease.

In Sec. 3 a new variant of PT is proposed, in which the expansion is performed not in powers of g but in the deviation of the wave function from its asymptotic form for $r\to\infty$. This makes it possible, with the aid of a small number of approximations, to obtain the level energies $\bar{E}_k(g)$ with good accuracy for all $0<g<\infty$. The analytic properties of the $\bar{E}_k(g)$ as functions of g are close to the properties of the exact solution. In Sec. 4 the energy discontinuity $\Delta E(g)$ across the cut as $g\to -0$ is calculated in the semiclassical approximation for arbitrary anharmonicity $v(r)$.

The structure of the PT series for the energy eigen-

 0038-5646/78/1201012-09$02.40