Atomic diamagnetism within a dense plasma

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In this paper we have studied the influence of plasma electron polarization around a charged atomic impurity on the diamagnetic response behavior of the impurity ion, when subject to large-scale magnetic fields within high-density plasmas. As a typical example, we consider the two-electron ion C^{4+} $(Z=6)$ in its ground state $1s^2{:}^1S$. Calculation performed within the Hartree-Fock approximation under the framework of the ion sphere model for the plasma-embedded impurity ion suggests that, in a high-density regime, the diamagnetic shift of the ground state is a bivariate function of the magnetic field and the plasma electron density. Also, it is shown that the magnitude of the diamagnetic susceptibility of the impurity ion increases with increasing plasma electron density, implying that the ion becomes more diamagnetic as a direct consequence of the increased orbital radii of its bound charges under enhanced density-induced screening.

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Interest in a theoretical simulation of plasma screening effects on the electronic structures of and on the processes involving multiply charged atomic systems immersed in high density plasmas has remained unabated over the years [1]. This is primarily because there are now a number of ongoing laboratory programs to study nonequilibrium plasmas where an electron density of $n_e \sim 10^{23}\,\mathrm{cm}^{-3}$ (in short-pulse laser breakdown of solid targets) or even $n_e \sim 10^{26}\,\mathrm{cm}^{-3}$ (in inertial confinement fusion experiments) can be achieved. A theoretical modeling of the atomic properties within such dense plasmas should be essential for elucidating experimentally confirmed dense plasma effects, such as the lowering of the ionization potential [2] and the red shift of emission line frequencies [3] of plasma-embedded atomic ions. It would also aid in understanding the basic behavior of atomic systems interacting with a surrounding hot, dense, and ionized matter. In this context the issue of the magnetic response properties of atomic systems against the backdrop of a high density plasma naturally follows because, dense laser-produced plasmas are well-known cradles of self-generated large-scale magnetic fields for which a number of mechanisms have been proposed. The most important of these are (i) a magnetic field due to nonparallel electron density and temperature gradients, i.e., the $\nabla n \times \nabla T$ mechanism [4]; (ii) a magnetic field due to ponderomotive forces [5]; (iii) the inverse Faraday effect mechanism [6]; and (iv) the dynamo mechanism [7]. Magnetic fields of the order of $10^4 - 10^9$ G may be generated, depending on the mechanism responsible for them. However, generation by different mechanisms is a simultaneous process—only some mechanisms are dominant under certain experimental conditions, while others are not.

Hydrogenlike ions, being the simplest and most abundant atomic species in laser-produced plasmas, have been almost archetypal so far for considering atomic processes in dense plasmas. Still, in such plasmas many-electron ions of heavier elements can exist in different stages of ionization and, in particular, He and Li-like ions are not uncommon. Being of considerably more complicated structures, these ions can contribute significantly to our understanding of the behavior of plasma-embedded atomic systems; however, theoretical as well as experimental studies on such ions in dense plasma environments have been rather sparse up to now. In this calculation we consider a multiply ionized two-electron ion C^{4+} $(Z=6)$ in its singlet ground state configuration $1s^2{:}^1S$. For such a system interacting with a magnetic field $\mathbf{B}$ (at the site of the ion in question), derivable from the vector potential $\mathbf{A}$ via the relation $\mathbf{B} = \nabla \times \mathbf{A}$, the linear momenta of the bound electrons of the ion are changed as $\mathbf{p} \rightarrow (\mathbf{p} + e\mathbf{A}/c)$. So the interaction Hamiltonian may now be expressed as

$$H_1 = \Sigma_{i=1,2}[-(e/mc)\mathbf{A}_i \cdot \mathbf{p}_i + (e^2/2mc^2)A_i^2]. \qquad (1)$$

With the assumption of a uniform magnetic field and after some simplifications [8], Eq. (1) reduces to

$$H_1 = \Sigma_{i=1,2}[(e/2mc)\mathbf{B} \cdot \mathbf{l}_i + (e^2/8mc^2)|\mathbf{B} \times \mathbf{r}_i|^2]. \qquad (2)$$

The first term linear in $\mathbf{B}$ is known as the *linear Zeeman term*, which depends on the orbital angular momentum $\mathbf{l}_i$ (actually on $\mathbf{l}_i + 2\mathbf{s}_i$, considering the spin of the electrons). For the singlet ground state $1s^2{:}^1S$ of the two-electron closed-shell ion under consideration, the total orbital angular momentum as well as the total spin angular momentum are zero, and therefore the linear Zeeman term vanishes. So in Eq. (2) the term quadratic in $\mathbf{B}$, known as the *diamagnetic term* (sometimes also called the *quadratic Zeeman term*), solely determines the system's response to an external magnetic field. At this point we may note in passing that atomic diamagnetism has its macroscopic manifestation in the form of *Lenz's law* of electromagnetic induction in classical electromagnetism. The diamagnetic effect in an atomic system is usually of a highly subtle nature, and requires precise theoretical estimation, for which sophisticated *ab initio* methods of atomic calculations are available. It is this effect which is investigated in this paper under laser-plasma conditions for the magnetic field and plasma electron density.

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For modeling an atomic system within a dense plasma environment, we resort to an ion sphere (alternatively called the "Wigner-Seitz sphere") model, which is a reasonable approximation for describing the effects of static screening within a dense, strongly coupled plasma. It makes qualitatively correct predictions at high densities, and has been widely used to investigate atomic processes in such plasmas [1,9]. In this model, a heliumlike ion with nuclear charge Z and $n_b(=2)$ number of bound electrons is surrounded by a sphere of radius $R_0=[3(Z-2)/4\pi n_e]^{1/3}$ containing exactly $n_f(=Z-2)$ uniformly distributed free plasma electrons to neutralize the charge of the ion, where n_e is the plasma electron density. Under these assumptions, the electrostatic potential energy "seen" by the bound electrons due to free plasma electrons is given by

$$V(r_i;R_0)=[(Z-2)/2R_0]e^2[3-(r_i/R_0)^2], \quad r_i<R_0, \tag{3}$$

The total potential and its first derivative vanish at the ion sphere radius $r_i=R_0$. Beyond the ion sphere boundary the distribution of the positive charge is assumed to neutralize the negative electron distribution exactly, thereby producing an electrically neutral background. Therefore, with the additional potential energy due to free plasma electrons, the unperturbed nonrelativistic Hamiltonian of the plasma-embedded atomic ion is given by

$$H_0=\Sigma_{i=1,2}[(p_i^2/2m)-(Ze^2/r_i)+V(r_i;R_0)]+e^2/r_{12}. \tag{4}$$

However, such a static screened potential model of a plasma-embedded atomic system, although often considered as a convenient starting point, disregards the dynamic screening effects within a plasma.

In solving for the unperturbed Hamiltonian in Eq. (4), and for estimating the first-order energy correction E_1 due to the perturbation term in the interaction Hamiltonian of Eq. (2), we have adopted *atomic units* (au), in which $e=m=\hbar=1$, the unit of length a_B (the Bohr radius) is equal to $(\hbar^2/\mathrm{me}^2)=0.529177$ Å, and the unit of energy is 2 Ry $=(me^4/\hbar^2)=27.2116$ eV. A variational Hartree-Fock-Roothaan solution to the unperturbed equation by the basis set expansion technique [10] is performed in order to obtain the unperturbed ground-state wave functions and energy levels of H_0 at different values of the ion sphere radius R_0 (or, equivalently, at different plasma electron densities n_e). It is justified to assume that, for such highly stripped low-Z atomic systems the Hartree-Fock level of description should be considerably accurate as a result of a heavy suppression of the (intra-atomic) electronic correlation contributions to the energy and other properties, due to the predominance of the Ze^2/r terms over the lone $1/r_{12}$ term in H_0 with an increasing nuclear charge Z. It was checked that this suppression renders the calculations at still higher levels, such as with the multiconfiguration Hartree-Fock approach, almost redundant in the present case from the point of view of numerical accuracy. The unperturbed solutions for the ground state $(1s^2{:}^1S)$ wave function Φ_0 (normalized) and the ground state energy E_0 of the ion C^{4+} implicitly depend on the plasma electron density n_e. With increasing density and density-induced screening, the total binding is gradually reduced—the ground state energy increases. This is displayed in Fig. 1. However, the *energy* of a state is *not* observable; it would be more appropriate to speak of *energy differences* instead. Therefore, we calculate the ionization energy of C^{4+} ion, which is the energy required for single ionization of the atomic system concerned, and is given by the difference between the ground state energy of a C^{5+} ion and that of a C^{4+} ion, i.e., $E_{\mathrm{ion}}=E_0[C^{5+}1s{:}^2S]-E_0[C^{4+}1s^2{:}^1S]$. As depicted in Fig. 2, the ionization energy exhibits a downward trend as the plasma electron density increases. To our knowledge, no other density-dependent data on heliumlike ions are available in the literature. However, in view of the lowering of the ionization energy (which is more commonly referred to as *continuum lowering* in the literature) of hydrogenic ions in dense plasmas, as obtained experimentally as well as from previous theoretical consid-

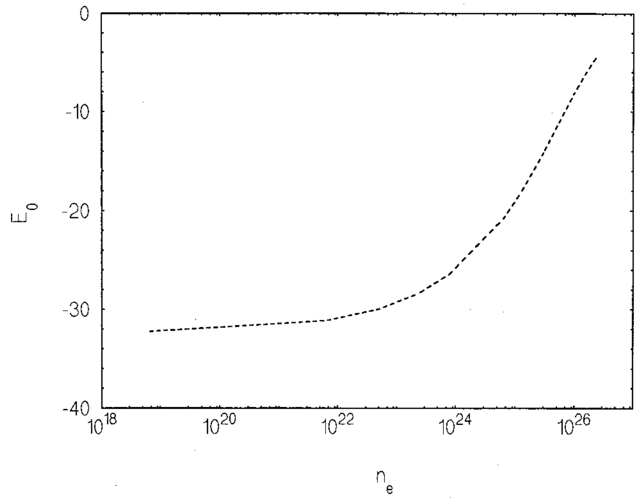

FIG. 1. Dependence of the ground state energy (E_0, in a.u.) of the C^{4+} ion on the plasma electron density (n_e, in cm^{-3}).

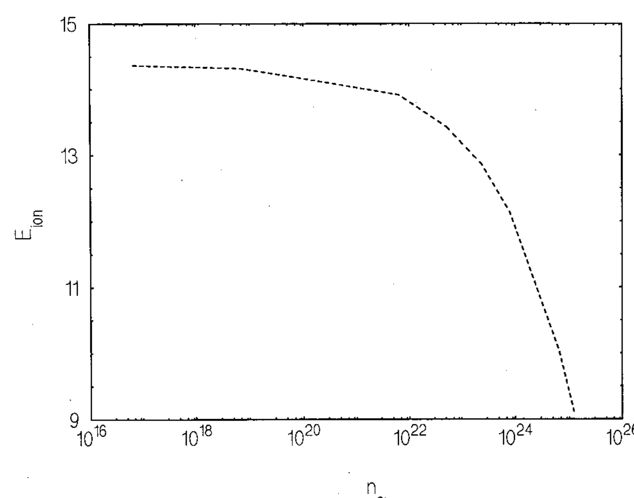

FIG. 2. Variation of the ionization energy (E_{ion}, in a.u.) of the C^{4+} ion with the plasma electron density (n_e, in cm^{-3}).

TABLE I. Diamagnetic shift E_1 (in cm^{-1}) of the ground state ($1s^2$:^1S) of a C^{4+} impurity ion in the presence of a magnetic field B (in units of 10^6 G) within dense plasmas characterized by the plasma electron density n_e (in cm^{-3}).

	B			
n_e	0	0.5	2.0	10.0
8.055×10^{23}	0	0.000 168	0.002 69	0.0672
1.259×10^{25}	0	0.000 174	0.002 78	0.0695
1.007×10^{26}	0	0.000 208	0.003 32	0.0831
2.387×10^{26}	0	0.000 237	0.003 80	0.0949

erations, it seems that the present results are consistent at a qualitative level, at least.

Having checked the consistency of our approach, we next proceed to calculate the magnetic field-induced (diamagnetic) shift of the ground state energy of the C^{4+} ion, which may be expressed as

$$E_1 = \langle \Phi_0 | H_1 | \Phi_0 \rangle, \tag{5}$$

using first-order perturbation theory. The perturbation scheme would be appropriate for magnetic fields that are well below the limit of 1 a.u. [11] of magnetic field $\approx 2.35\times10^9$ G. This calculation considers magnetic fields in the range of 0.1–10 MG. In Table I we present the variation of the diamagnetic shift E_1 (expressed in cm^{-1}, where 1 a.u. $= 219\,474\,\mathrm{cm}^{-1}$) with magnetic field B (in MG) at several plasma electron densities n_e (in cm^{-3}). It is evident that, at any density, the shift rises quadratically with the magnetic field, as may be expected from Eq. (2). Also, at a particular value of the magnetic field, the energy shift increases with increasing plasma electron density. These behaviors are demonstrated graphically in Fig. 3, where the functional dependence of E_1 on B is represented by a family of parabolas passing through the common vertex. Here the inner ones

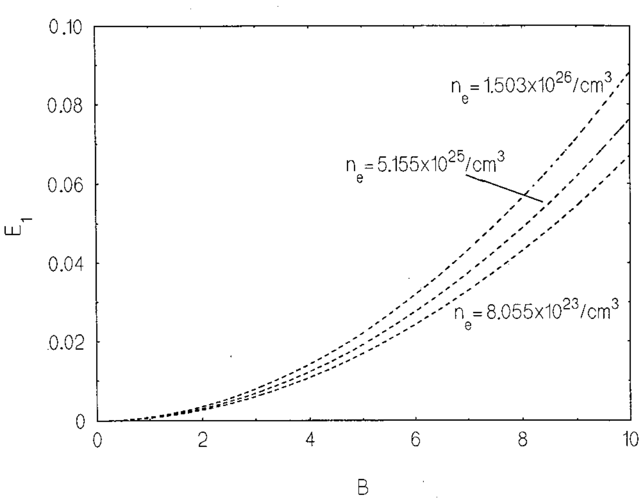

FIG. 3. Diamagnetic shift (E_1, in cm^{-1}) of the ground state of a C^{4+} ion as a function of the magnetic field (B, in MG) within dense plasmas at plasma electron densities $n_e = 8.055\times10^{23}\,\mathrm{cm}^{-3}$, $5.155\times10^{25}\,\mathrm{cm}^{-3}$ and $1.503\times10^{26}\,\mathrm{cm}^{-3}$.

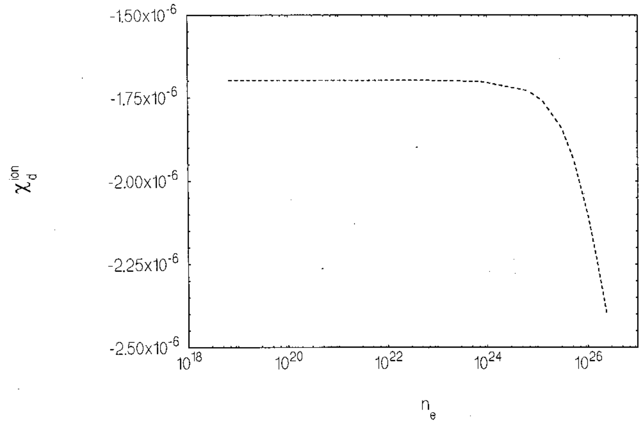

FIG. 4. Variation of the diamagnetic susceptibility (χ_d^{ion}, in a_B^3) of a plasma-embedded C^{4+} ion in its ground state against the plasma electron density (n_e, in cm^{-3}).

correspond to the cases of larger plasma electron densities. However, it is to be understood that, at two different plasma electron densities, the variation of E_1 with B refers to two different reference levels (i.e., two different positions of the unperturbed ground state) from which the corresponding shift is to be measured, because the ground state energy exhibits a strong density dependence in Fig. 1.

The very small energy shifts listed in Table I are responsible for the diamagnetism of the C^{4+} ion in its ground state. We now calculate the diamagnetic susceptibility (χ_d^{ion}) of the ion as a function of the plasma electron density n_e. χ_d^{ion} is defined as

$$E_1 = -\tfrac{1}{2}\chi_d^{\mathrm{ion}} B^2. \tag{6}$$

χ_d^{ion} is always negative, expressing that the induced magnetic moment is in a direction opposite to that of the applied magnetic field, which may be interpreted classically in terms of Lenz's law. Figure 4 illustrates the variation of χ_d^{ion} (expressed in units of a_B^3) against the plasma electron density n_e (n_e is given in cm^{-3}). As can be seen from this figure, the diamagnetic susceptibility remains almost at the free-ion value of $(-1.6984\times10^{-6})a_B^3$ up to a density of $\sim 10^{24}\,\mathrm{cm}^{-3}$. Then it becomes more negative very sharply, i.e., its magnitude increases in a smooth and steep manner within the very high density regime $n_e \sim 10^{24}$–$10^{26}\,\mathrm{cm}^{-3}$. Up to the highest density $n_e = 2.387\times10^{26}\,\mathrm{cm}^{-3}$ under consideration in the present study, the magnitude of χ_d^{ion} experiences about a 40% gain over the isolated ion value. This suggests that ionic diamagnetism increases within a dense plasma. Now, from Eq. (2), it is evident that $E_1 \propto \langle r^2 \rangle$. The mean-square orbital radius of the bound electrons of the ion increases within dense plasmas as a direct consequence of a loosening of the bound charge cloud. Therefore, the growing diamagnetic behavior of the ion may be attributed to the expansion of the ion's bound electronic orbit due to enhanced plasma electron density-induced screening effects. Figure 3 demonstrates the variation of E_1 as a function of B at different n_e values, while Fig. 4 actually expresses the dependence of E_1 on n_e when B is unity. Thus, these two figures fully specify the bivariate dependence of E_1 on B and n_e, both within a dense plasma.

In summary, this paper contains an account of the diamagnetic response behavior of a two-electron atomic system as modified by the presence of a surrounding dense plasma medium and under magnetic field conditions pertinent to laser-produced plasmas. Diamagnetism is characteristically a very feeble effect, and the resultant energy shifts are usually very small in magnitude. However, for closed-shell atomic systems in which all the electrons are paired with electrons of opposite spins, it becomes all the more important due to the absence of the linear Zeeman term in the interaction Hamiltonian of Eq. (2), and constitutes the very basic and sole response of such systems to external magnetic fields. As to the measurability of the diamagnetic shifts, the sample results presented in Table I indicate that, at a self-generated field of $\sim 10^8$ G (this is about 4% of 1 a.u. of the magnetic field, so we assume an approximate validity of a first-order perturbation calculation even for this field) the shift would amount to $\sim 6.7\ \text{cm}^{-1}$ at $n_e \sim 8.0\times 10^{23}\ \text{cm}^{-3}$ and $\sim 9.5\ \text{cm}^{-1}$ at $n_e \sim 2.4\times 10^{26}\ \text{cm}^{-3}$ respectively. Hence the diamagnetic shift and the plasma-density-induced increase of this shift both lie within the microwave region (approximately 0.03–10 cm^{-1}), and so it appears that both may possibly be amenable to experimental detection at sufficiently high fields and high densities. However, it is worthwhile to point out that the present calculation aims to demonstrate the gross features of plasma-density effects on atomic diamagnetism in a simple way, assuming the validity of the ion-sphere model under a magnetic field. In a more rigorous approach taking into consideration the field-induced distortion of the free-electron distribution within the ion sphere as a perturbation, it is very likely that the tabulated set of data would be modified, preserving the demonstrated trend only in a qualitative way.

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