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Calculation of the Effective G-Factor for the $\left(ns^2S_{1/2}\right)\to\left(np^2P_{3/2}\right)\to\left(n's^2S_{1/2}\right)$ Transitions in Hydrogen-Like Atoms and Its Application to the Atomic Cesium

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Abstract

We have calculated the effective g-factor $\left(g^*\right)$ for the $\left(ns^2S_{1/2}\right)\to\left(np^2P_{3/2}\right)\to\left(n's^2S_{1/2}\right)$ transitions in hydrogen-like atoms and applied it to atomic cesium. We have identified that not only the g* factor in this case is an integer number g* = 1, but also the existence of possible entangled states related to the above transitions. Furthermore we have used the above result to calculate the transition energies which are in complete agreement (within the 1% margin error). Such results can give access to the production of new laser lights from atomic cesium.

Keywords: Photonic Transitions, Hydrogen-Like (Hydrogenic) Atoms, Landé G-Factor, Quantum Entanglement

1. Introduction

The study and accurate determination of the excited-state properties of atomic and molecular systems, such as the fine and hyperfine coupling constants and oscillator strengths play an important role in testing high-precision atomic theories and quantum mechanics.

In particular the investigation of hydrogen-like atoms and its applications in modern technology go beyond the hydrogen atom itself. Amongst hydrogenic atoms, cesium with its low ionization potential and simplicity of its outer shell structure has attracted a lot of attention. In particular cesium has been involved in a number of significant studies within the field of laser cooling as well as in the development of atomic clocks. Furthermore investigations of parity violation [1] in cesium have been able to yield high precision results.

Recently it was also shown that cesium atoms are ideal candidates for optical computers, since cesium vapor is optically highly nonlinear, as well as possessing sensitivity much greater than most semiconductors [2]. In addition a new series of scientific experiments on the properties and behavior of cesium atoms have been used to prove fundamental connections between chaos theory [3] and quantum entanglement.

The aim of the present study is to investigate the effective g-factor (g^*) for the $\left(ns^2S_{1/2}\right)\to\left(np^2P_{3/2}\right)\to\left(n's^2S_{1/2}\right)$ transitions in hydro-gen-like atoms and apply it to atomic cesium. We identify that the effective g factor has an integer value of g*=1 as well as the existence of possible entangled states related to the above transitions. We show that the allowed transitions occur vertically from one crossing point to another with respect to g* variable. Moreover calculations of their corresponding energy values reveal complete agreement with our previous results [4] (within the 1% margin of error), giving access to new laser lights from atomic cesium.

We start by modeling a one-electron hydrogen-like atom in the presence of a magnetic field $\vec{B}=B\hat{z}$. We assume the sources of the magnetic field [5,6] to be the proton's magnetic moment, μ_p and the electron's magnetic moment μ_e (or μ_j) which has two components, namely, the orbital part, μ_l and the spinning part μ_s. We note that the Coulomb potential in both cases requires planar orbits for the electron, therefore the direction of $\vec{\mu}_p$ is taken to be in z-direction.

Moreover it was recently shown by Saglam *et al.* [5,6] that the quantized magnetic flux through the electronic orbits of the Dirac hydrogen atom corresponding to the quantum state $\left|n,l,m_j\right\rangle$ is given by $\Phi\left(n,l,m_j\right)=\left(n-l-m_j\right)\Phi_0$ where $\Phi_0=\frac{hc}{e}=4.14\times10^7 G\cdot cm^2$ is the flux quantum. Since the above relationship is independent of $\left(\mu_p,\mu_e\right)$, it can be easily generalized to hydrogen-like atoms. Note that in such a cases μ_p would be replaced by the magnetic moment of the positively charged ion core. The above calculated flux results in very high magnetic field values (such as $10^7 G-10^8 G$) inside a hydrogen-like atom. Therefore when such an atom is placed in an external magnetic field $\vec{B}=B\hat{z}$ its effect would be to orient $\vec{\mu}_p$ in the z-direction and $\vec{\mu}_e$ in the opposite direction. Nevertheless the total magnetic field inside the atom will still be of the same order with the initial value $10^7 G-10^8 G$ because of the fact that $B<<10^7 G$. Such high magnetic field values have not been achieved experimentally so far.

The total magnetic field inside the atom will be called the local magnetic field, B^*. The investigation of the effective g-factor $\left(g^*\right)$ requires to study the Zeeman effect in detail, therefore the eigenstates must be distinguished in the Zeeman sense including the quantum number $m_j=m_l+m_s$ [7-8]. Using a non relativistic Hamiltonian [9] we proceed to investigate the Zeeman fine energies. It can be shown that for the above magnetic field values the spin-orbit coupling and the quadrupole moment energy can be neglected. Considering diamagnetic and paramagnetic effects the energy eigenvalues become

$$\left[E\left(n,l,m_j,B^*\right)=-\frac{C}{n^2}-\mu_B B^*\left(m_l+g^* m_s\right)\right]$$

corresponding to the $\left|n,l,m_j\right>$ eigenstate. Note that the magnetic field B is replaced by the local magnetic field B^* and the Lande-g factor is replaced by the effective Lande-g factor, g^* which is treated here as a varying parameter. It should be noted that the same expression is also applicable in the case of an atom subject to a laser beam, where due to the photon's magnetic moment [11] and hence the large intrinsic magnetic field comparable with the above large values [12], the same diamagnetic and paramagnetic effects are present inside the atom.

To proceed further, by using the above energy relation we define a new dimensionless function

$$f\left(m_l,\pm g^*\right)=\left[E\left(n,l,m_j,B^*\right)+\frac{C}{n^2}\right]\Big/\hbar\omega_c^*=-\frac{m_l}{2}\mp\frac{g^*}{4}$$

which allows us to investigate the effective-g-factor values $\left(g^*\right)$ more easily. For $s(l=0)$ and $p(l=1)$ levels where we have $m_l=0,\pm1$, the plotting of $f\left(m_l,\pm g^*\right)$ as a function of g^* shows that crossings of these lines correspond to either $g^*=1$, $(s-p)$ crossings or $g^*=2$, which corresponds to $p-p$ crossings. As the subject of the present work is to investigate the effective g-factor $\left(g^*\right)$ for the $\left(ns^2S_{1/2}\right)\to\left(np^2P_{3/2}\right)\to\left(n's^2S_{1/2}\right)$ transitions in hydrogen-like atoms, our graphic clearly shows that for the above transitions we have: $g^*=1$. At these crossing points, two states with opposite spin have the same energy value. We believe that these crossing points correspond also to the entangled states [12]. After finding the effective g-factor value which is equal to one $\left(g^*=1\right)$, we set $g^*=1$ in the energy expressions $E\left(n,l,m_j,B^*\right)$. Substituting the value of $\mu_B=\frac{e\hbar}{2mc}$ and $m_s=\pm1/2$, we find:

$E\left(n,m_j,B^*\right)=-\frac{C}{n^2}-\frac{m_l\hbar\omega_c^*}{2}\mp\frac{\hbar\omega_c^*}{4}$. Here the constant C is the characteristic of each hydrogen-like atom and calculated from the ionization energies. Applying the above results to atomic cesium and calculating the corresponding Zeeman fine energies at the s-p crossings, reveals complete agreement with experiment [4,13] (within the 1% margin of error). The above treatment can give access to new laser lights from atomic cesium.

The outline of the present study is as follows: In Section 2 we calculate the energy levels of the non-relativistic hydrogen-like atom in the presence of an effective(local) magnetic field, $\vec{B}^*$. From the above energy relation we calculate the effective g-factor for the $\left(ns^2S_{1/2}\right)\to\left(np^2P_{3/2}\right)\to\left(n's^2S_{1/2}\right)$ transitions. In Section 3 we apply the present energy results to atomic cesium. In Section 4 we present the concluding remarks.

2. Calculation of the Energy Levels of Hydrogen-Like Atoms in the Presence of a Uniform Magnetic Field

Let us consider the non-relativistic Hamiltonian [9] for a one-electron hydrogen-like atom in the presence of an external magnetic field, $\vec{B}=B\hat{z}$:

$$H=\frac{1}{2m}p^2-\frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r}+\xi(r)\vec{L}.\vec{S}+\frac{\mu_B}{\hbar}\left(\vec{L}+g\vec{S}\right)\cdot\vec{B}+\frac{e^2}{8mc^2}\left(\vec{B}\times\vec{r}\right)^2 \quad (1)$$

The first term corresponds to the kinetic energy operator, the second term is the Coulomb potential, the third term is the spin-orbit coupling, the forth term is the dipole moment energy and the last term is the quadrupole moment energy. As was discussed in [9] for fields up to $10^4 T$ the spin-orbit coupling and the quadratic terms can be neglected so the Hamiltonian is reduced to:

$$H_{reduced} = \frac{1}{2m}p^2 - \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r} + \frac{\mu_B}{\hbar}\left(\vec{L} + g\vec{S}\right)\cdot\vec{B} = H_0 + H_B \tag{2}$$

where H_0 is the Hamiltonian for a free electron and $H_B = \frac{\mu_B}{\hbar}\left(\vec{L} + g\vec{S}\right)\cdot\vec{B}$ is the perturbing Hamiltonian Using Dirac notation, we denote the eigenstates of H_0 by $\left|n,l,m_l\right\rangle$ thus writing:

$$H_0\left|n,l,m_l\right\rangle = E_n\left|n,l,m_l\right\rangle = -\frac{C}{n^2}\left|n,l,m_l\right\rangle \tag{3}$$

where $E_n = -\frac{C}{n^2}$ is the energy of the free hydrogen-like atom (here the constant C is determined through the ionization energy).

If we denote the eigenstates of the Hamiltonian, $H_{reduced}$ by $\left|n,l,m_j\right\rangle$ where $m_j = m_l + m_s$, the energy eigenvalues $\left[E\left(n,l,m_j,B\right) = E_n + E_{Zeeman}\right]$ will contain the Zeeman correction which is first order in B, *i.e.*:

$$\begin{aligned} H_{reduced}\left|n,l,m_j\right\rangle &= \left(H_0 + H_B\right)\left|n,l,m_j\right\rangle \\ &= E\left(n,l,m_j,B\right)\left|n,l,m_j\right\rangle \end{aligned} \tag{4}$$

Here the field dependent part $H_B = \frac{\mu_B}{\hbar}\left(\vec{L} + g\vec{S}\right).\vec{B}$ corresponds to the Zeeman energy, E_{Zeeman} *i.e.*:

$$\begin{aligned} H_B\left|n,l,m_j\right\rangle &= E_{Zeeman}\left|n,l,m_j\right\rangle \\ &= -\mu_B B\left(m_l + gm_s\right)\left|n,l,m_j\right\rangle \end{aligned} \tag{5}$$

Substitution of the Equations (3) and (5) in Equation (4) gives the energy eigenvalue, $E\left(n,l,m_j,B\right) \equiv E\left(n,m_j,B\right)$ including the Zeeman correction:

$$E\left(n,m_j,B\right) = -\frac{C}{n^2} - \mu_B B\left(m_l + gm_s\right) \tag{6}$$

where $\mu_B = \frac{e\hbar}{2mc}$ is the Bohr magneton and g is the Lande-g factor which is equal to 2 for a free electron. For an atom or ion in a free space the Lande-g factor [14] is given by:

$$g = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} \tag{7}$$

When an atom is subject to a laser beam because of the photon's magnetic moment [11] and hence the large intrinsic magnetic field [12], we will have diamagnetic and paramagnetic effects [10] inside the atom. Therefore the magnetic field inside the atom must be replaced by the local magnetic field B^* [15]. The Lande-g factor is also replaced by the effective Lande-g factor, g^* which is treated as a varying parameter [16,17]. Therefore the magnetic field B and the Lande-g factor in Equation (6) must be replaced by the effective values, B^* and g^* respectively, such that:

$$E\left(n,m_j,B^*\right) = -\frac{C}{n^2} - \mu_B B^*\left(m_l + g^* m_s\right) \tag{8}$$

Substituting the value of $\mu_B = \frac{e\hbar}{2mc}$ and $m_s = \pm\frac{1}{2}$ in Equation (8), we find:

$$E\left(n,m_j,B^*\right) = -\frac{C}{n^2} - \frac{m_l\hbar\omega_c^*}{2} \mp \frac{g^*\hbar\omega_c^*}{4} \tag{9}$$

Where $\omega_c^* = \frac{eB^*}{mc}$ is the cyclotron frequency corresponding to B^*.

Let us proceed by defining a dimensionless function using the above energy expression given in Equation (9) such as:

$$f\left(m_l, \pm g^*\right) = \left[E\left(n,m_j,B^*\right) + \frac{C}{n^2}\right]\Big/\hbar\omega_c^* = -\frac{m_l}{2} \mp \frac{g^*}{4} \tag{10}$$

which does not have an explicit n dependence:

Plotting $f\left(m_l,\pm g^*\right)$ for $\left(m_l = 0,\pm 1\right)$ as a function of g^* leads to the following results (**Figure 1**):

1) The crossings of these $f\left(m_l,\pm g^*\right)$ lines correspond to $g^* = 1$ or $g^* = 2$.

2) At these crossing points, two states with opposite spin have the same energy value. We believe that these crossing points correspond to entangled states [12].

3) For the crossings (entanglements) of the [$\left(ns^2 S_{1/2}\right)$ and $\left(np^2 P_{3/2}\right)$] as well as [$\left(ns^2 S_{1/2}\right)$ and $\left(np^2 P_{1/2}\right)$] states, the effective g- factor is found to be equal to one: $g^* = 1$.

4) The crossing for the $\left(p-p\right)$ states occur at $g^* = 2$.

In the present study since we concentrate on the $\left(ns^2 S_{1/2}\right) \to \left(np^2 P_{3/2}\right) \to \left(n's^2 S_{1/2}\right)$ transitions at the crossing points, we substitute $g^* = 1$ in Equation (9) for all energy calculations. Here we note the allowed photonic transitions occur vertically from one crossing point to another one.

To find the energy eigenvalues, we start with $s(l = 0)$. We note that depending on the spin orientations we have two $\left(ns^2 S_{1/2}\right)$ states. In Dirac notation, these states are

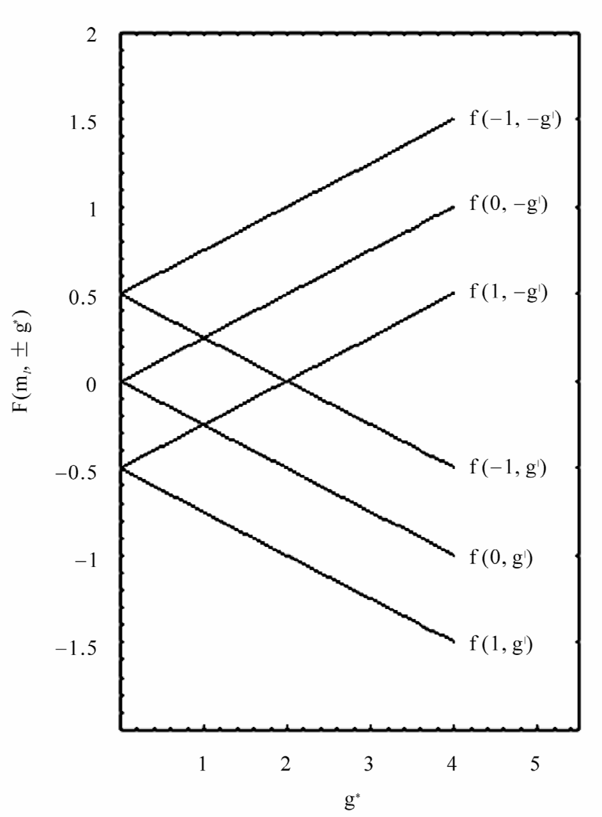

Figure 1. $f\left(m_l, \pm g^*\right) = -\frac{m_l}{2} \mp \frac{g^*}{4}$ **as a function of** g^* **for** $m_l = 0, \pm 1$ **. Identifying the effective g values (g*). The** $(s-p)$ **crossings occur at** $g^* = 1$ **; the** $(p-p)$ **crossings occur at** $g^* = 2$ **.**

$|n,0,0,\uparrow> \equiv |n,0,0,1/2>$ and $|n,0,0,\downarrow> \equiv |n,0,0,-1/2>$. From Equation (9) the corresponding energy eigenvalues at the crossing points are given by:

$$E(n,0,0,1/2) = -\frac{C}{n^2} - \frac{\hbar\omega_c^*}{4} \quad (11)$$

and

$$E(n,0,0,-1/2) = -\frac{C}{n^2} + \frac{\hbar\omega_c^*}{4} \quad (12)$$

respectively.

From Equations (11) and (12) we see that the state $|n,0,0,\uparrow> \equiv |n,0,0,\frac{1}{2}>$ has the lowest energy so it is identified as the ground state.

Next we consider the $p(l=1)$ states, which are six states in total. The spin up states $|n,1,1,\frac{1}{2}>$, $|n,1,0,\frac{1}{2}>$ and $|n,1,-1,\frac{1}{2}>$ states are denoted by $np^2P_{3/2}$ while the spin down states $|n,1,1,-1/2>$, $|n,1,0,-1/2>$ and $|n,1,-1,-1/2>$ are written as $np^2P_{1/2}$. Using Equation (9) the corresponding energy eigenvalues are:

$$E(n,1,1,1/2) = -\frac{C}{n^2} - \frac{\hbar\omega_c^*}{2} - \frac{\hbar\omega_c^*}{4} = -\frac{C}{n^2} - \frac{3\hbar\omega_c^*}{4} \quad (13)$$

$$E(n,1,1,-1/2) = -\frac{C}{n^2} - \frac{\hbar\omega_c^*}{2} + \frac{\hbar\omega_c^*}{4} = -\frac{C}{n^2} - \frac{\hbar\omega_c^*}{4} \quad (14)$$

$$E(n,1,0,1/2) = -\frac{C}{n^2} - \frac{\hbar\omega_c^*}{4} \quad (15)$$

$$E(n,1,0,-1/2) = -\frac{C}{n^2} + \frac{\hbar\omega_c^*}{4} \quad (16)$$

$$E(n,1,-1,1/2) = -\frac{C}{n^2} + \frac{\hbar\omega_c^*}{2} - \frac{\hbar\omega_c^*}{4} = -\frac{C}{n^2} + \frac{\hbar\omega_c^*}{4} \quad (17)$$

$$E(n,1,-1,-1/2) = -\frac{C}{n^2} + \frac{\hbar\omega_c^*}{2} + \frac{\hbar\omega_c^*}{4} = -\frac{C}{n^2} + \frac{3\hbar\omega_c^*}{4} \quad (18)$$

3. Application to Atomic Cesium

The ionization energy for cesium is $3.89\ eV$, while the smallest amount of energy that allows a transition from the ground state to the nearest excited state is $1.38\ eV$. Therefore in Equation (11) setting the lowest energy to $-3.89\ eV$ we can write:

$$E(6,0,0,1/2) = -\frac{C}{6^2} - \frac{\hbar\omega_c}{4} = -3.89\ eV \quad (19)$$

From Equation (12) and Equation (17) the nearest excited state energy is given by $\left(-\frac{C}{6^2} + \frac{\hbar\omega_c}{4}\right)$. Since the smallest amount of energy that allows a transition from the ground is $1.38\ eV$, then the energy of this level will be

$$-\frac{C}{6^2} + \frac{\hbar\omega_c}{4} = -(3.89 - 1.38) = -2.51\ eV \quad (20)$$

From Equations (19) and (20), we find that the unknowns: $C = 115\ eV$ and $\frac{\hbar\omega_c^*}{2} = 1.38\ eV$. Thus for the cesium atom Equation (9) is written as:

$$E(n,l,m_j,B) = E\left(n,l,m_l \pm \frac{1}{2},B\right) = -\frac{115}{n^2} - 1.38m_l \mp 0.69g^* \quad (21)$$

where the range of m_l takes the values (-1,0,1) for the present transitions. In **Figure 2** we plot the energies given in Equation (21) for quantum numbers: $n=6$ and $n=10$.

Plotting the energies corresponding to Equation (21) against g^* for $n = 6,7,8,9,10$ gives crossings at $g^* = 1$ as expected. We observe 10 main crossing points which are denoted by the letters: A, A' B, B', C,

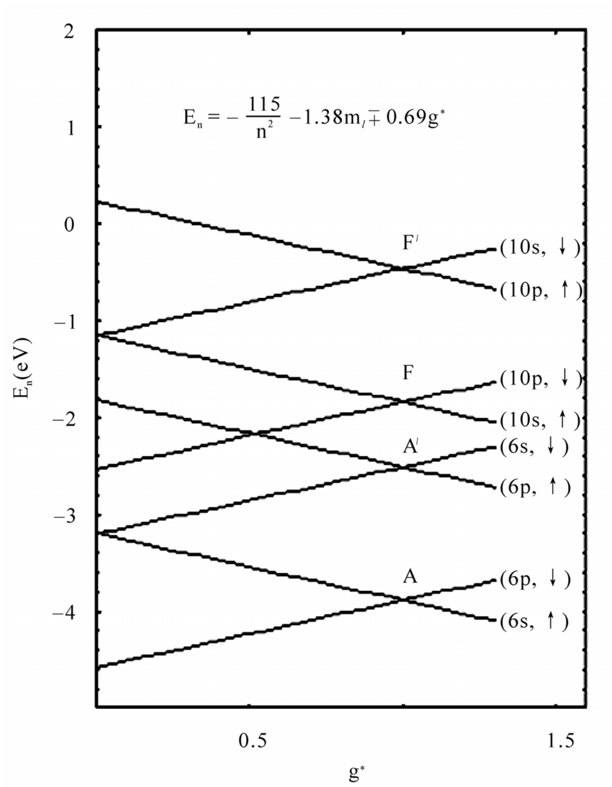

Figure 2. The plots of $E(n, m_l, g^*)$ with respect to g^* for the $(6s, 6p)$ and $(10s, 10p)$ states for atomic cesium. As it is seen the crossings occur at $g^* = 1$ and transitions take place vertically with respect to g^*.

C', D, D' and F, F'. Their energies and related states are given in **Table 1**.

To excite electron from A to A' ,which corresponds to a $(6s^2S_{1/2}) \rightarrow (6p^2P_{3/2})$ transition, the required energy is $E_{A'} - E_A = -2.51 - (-3.89) = 1.38\ eV$. To excite electron from A' to F, which corresponds to $(6p^2P3/2) \rightarrow (10s^2S_{1/2})$ transition, the required energy is $E_F - E_{A'} = -0.45 - (-2.51) = 2.06\ eV$. When the electron relaxes back to the ground state the energy of the corresponding laser will be given by:
$E_F - E_A = -0.45 - (-3.89) = 3.44\ eV$. These values are in good agreement with experiments involving cesium lasers [4].

4. Conclusions

We have calculated the effective g-factor (g^*) for the $(ns^2S_{1/2}) \rightarrow (np^2P_{3/2}) \rightarrow (n's^2S_{1/2})$ transitions in hydrogen-like atoms and applied it to atomic cesium. We have found that the value of g^* is exactly equal to 1 for the above mentioned photonic transitions. Application of the present results to atomic cesium gives complete agreement (within the 1% margin of error) with the previous experimental results. We have also shown the existence of possible entangled states related to the above transitions. Applications of the above treatment can give access to the production of new laser lights from atomic cesium.

Table 1. Energies and the raleted states at the crossing points for *n* = 6,7,8,9,10.

Energies	Mixture of states
$E_A = -3.89\ eV$	$\|6,0,0,\uparrow>$ and $\|61,1,\downarrow>$
$E_{A'} = -2.51\ eV$	$\|6,0,0,\downarrow>$ and $\|6,1,-1,\uparrow>$
$E_B = -3.04\ eV$	$\|7,0,0,\uparrow>$ and $\|7,1,1,\downarrow>$
$E_{B'} = -1.66\ eV$	$\|7,0,0,\downarrow>$ and $\|7,1,-1,\uparrow>$
$E_C = -2.49\ eV$	$\|8,0,0,\uparrow>$ and $\|8,1,1,\downarrow>$
$E_{C'} = -1.11\ eV$	$\|8,0,0,\downarrow>$ and $\|8,1,-1,\uparrow>$
$E_D = -2.09\ eV$	$\|9,0,0,\uparrow>$ and $\|9,1,1,\downarrow>$
$E_{D'} = -0.71\ eV$	$\|9,0,0,\downarrow>$ and $\|9,1,-1,\uparrow>$
$E_F = -0.45\ eV$	$\|10,0,0,\uparrow>$ and $\|10,1,1,\downarrow>$
$E_{F'} = 0.93\ eV$	$\|10,0,0,\downarrow>$ and $\|10,1,-1,\uparrow>$

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