SPIN-ORBITAL INTERACTION AND SINGLE-ELECTRON EXCITATIONS

СПИН-ОРБИТАЛЬНОЕ ВЗАИМОДЕЙСТВИЕ И ОДНОЭЛЕКТРОННЫЕ ВОЗБУЖДЕНИЯ

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The system of single-electron excitations, consisting in discrete changes of the spin as well as of the orbital momentum directions is analysed. The spin-orbital interaction is assumed as the main mechanism determining the dynamics of the system. It has been found that for fixed n and l the three kinds of excitations appear in the system. These excitations obey the quasi-Pauli kinematics and statistics. The energies of the excitations are of the order of 30—50 K_B. Thermodynamic analysis of the system points to the possibility of the existence of two phasetransition points. At a lower temperature the ordering parameter of the system has a singularity and at a higher temperature point, the mean value of the Z-component of the total momentum vanishes. The external periodical magnetic field leads to the appearance of the induced momenta $J^+(\omega)$ and $J^-(\omega)$. It has been found that the external stimulation is most effective at $T=0$, when the induced momenta are of the maximum value. At high temperatures the magnitude of the induced momenta decreases linearly with the increase of temperature.

The object of this paper is the formulation of a theory of single-electron excitations in hydrogen-like atoms. We assume that the L-S interaction is the main mechanism acting in the system. Such a consideration is the necessary basis for the development of the more general theory of phenomena taking place in magnetic dielectrics [2].

If the atom is placed into the external magnetic field $\mathscr{H}$, then the possible electron excitations consist in changes of the spin, the orbital and the total momentum direction. It is assumed that the energy as well as the orbital quantum number remain constant. The Hamiltonian of the considered electron system can be written as follows

$$H = H_c + H_s + H_{\alpha} \tag{1}$$

where

$$H_c = -\frac{\hbar^2}{2m_e}\Delta - \frac{Ze^2}{4\pi\varepsilon_0 r}; \quad H_s = -\mu_B \mathscr{H} S^z; \quad H_{\alpha} = R\mathbf{L}\,.\,\mathbf{S} = R\left(L^z S^z + \frac{L^+S^- + L^-S^+}{2}\right). \tag{2}$$

In the latter formula m_e is the mass of the electron, ε_0 is the permittivity, Ze is the nucleus charge, $\mu_B = 2eh/4\pi m_e$ is the doublet Bohr magneton and $R = \mu_0 e^2 c/8h\pi r_B$, where $r_B = h^2/\pi\mu_0 c^2 m_e e^2$ is the Bohr radius. The actual set of the electron states is the following

$$S_a \equiv \{|0\rangle \equiv |m_0 1\rangle; \ |1\rangle \equiv |m_f\uparrow\rangle; \ |2\rangle \equiv |m_0\downarrow\rangle; \ |3\rangle \equiv |m_f\downarrow\rangle\} \tag{3}$$

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so that the Hamiltonian (1) can be expressed in terms of the Fermi operators a^+ and a in the following way

$$H=\sum_{\mu,\nu=1}^{3} H_{\mu\nu}a_\mu^+ a_\nu\,;\quad H_{\mu\nu}=\langle\mu|H|\nu\rangle\,;\quad \mu,\nu\in(0,1,2,3). \tag{4}$$

The electron operators satisfy the condition $\sum_{\mu=1}^{3} a_\mu^+ \;\; a_\mu=1$. The matrix elements $H_{\mu\nu}$ can be easily calculated with help of (2) and (3).

In order to analyse the electron excitations we proceed to the quasi-Pauli operators $Q_\mu^+=a_\mu^+a_0$ and $Q_\mu=a_0^+a_\mu$ [1], creating and annihilating the excitations of the type μ. The Hamiltonian (4) can be expressed now in terms of the operators Q_μ^+ and Q_μ. Further analysis requires the stabilization of the Hamiltonian. It is done by the standard procedure of Lagrange's multiplicators. We note that this procedure is different for two possible cases $m_f=m_0+1$ and $m_f=m_0-1$, but in both cases the Hamiltonian reduces to the diagonal form:

$$H_{AB}=L_{AB}+\sum_{\Theta=1}^{3} P_\Theta^{+(A,B)}P_\Theta^{(A,B)}. \tag{5}$$

The operator P^+ and P are new quasi-Pauli operators, obtained by the canonical transformation of the operators Q^+ and Q. In the case $m_f=m_0+1$ denoted by the index A, we have

$$\Delta_1^{(A)}=\frac{1}{2}\{[\varphi_A^2+R^2\psi_A^2]^{1/2}-\varphi_A+R\}\,; \tag{6}$$

$$\Delta_2^{(A)}=\frac{1}{2}\{[\varphi_A^2+R^2\psi_A^2]^{1/2}+\varphi_A+R\}$$

$$\Delta_3^{(A)}=\frac{\varrho_A^2H_{\infty}^{(A)}+H_{B3}^{(A)}-R\psi_A\varrho_A}{1+\varrho_A^2}\,;\quad \varrho_A=\frac{\varphi_A-[\varphi_A^2+R^2\psi_A^2]^{1/2}}{R\psi_A}\,;\quad \psi_A=[(l_0-m_0)(l_0+m_0+1)]^{1/2}.$$

In the case $m_f=m_0-1$, denoted by the index B, the notations are

$$\Delta_1^{(B)}=\frac{1}{2}\{[\varphi_B^2+R^2\psi_B^2]^{1/2}-\varphi_B+R\}\,; \tag{7}$$

$$\Delta_2^{(B)}=\frac{1}{2}\{[\varphi_B^2+R^2\psi_B^2]^{1/2}+\varphi_B+R\}\,;$$

$$\Delta_3^{(B)}=\frac{\varrho_B^2H_{11}^{(B)}+H_{22}^{(B)}-R\psi_B\varrho_B}{1+\varrho_B^2}\,;\quad \varrho_B=\frac{\varphi_B-[\varphi_B^2+R^2\psi_B^2]^{1/2}}{R\psi_B}\,;\quad \psi_B=[(l_0+m_0)(l_0-m_0+1)]^{1/2}.$$

The set of the quasi-Pauli states is the following:

$$S_P\equiv\{|0_10_20_3\rangle\,;\;\; |1_10_20_3\rangle\,;\;\; |0_11_20_3\rangle\,;\;\; |0_10_21_3\rangle\}. \tag{8}$$

Using the statistical operator of the canonical ensemble $\hat{\eta}=e^{(F-H)/\tau}$, where F is the free energy of the system and $\tau=k_BT$ is the temperature in energy units, it is easy to find the mean occupation number

$$\langle P_\Theta^+P_\Theta\rangle=e^{-\frac{\Delta_\Theta}{\tau}}\left(1+\sum_{b=1}^{3}e^{-\frac{\Delta_b}{\tau}}\right)\,;\quad \Theta\in(1,2,3) \tag{9}$$

and the ordering parameter of the system:

$$\sigma=1-\sum_{\Theta=1}^{3}\langle P_\Theta^+P_\Theta\rangle=\left(1+\sum_{\Theta=1}^{3}e^{-\frac{\Delta_\Theta}{\tau}}\right)^{-1}. \tag{10}$$

It turns out that in the high temperature approximation the ordering parameter has a singularity at

$\tau_c^{(A,B)}=\frac{1}{4}\sum_{\Theta=1}^{B}\Delta_\Theta^{(A,B)}$. The statistical mean value of the Z-component of the total momentum $\langle J^z\rangle$ has been calculated elsewhere, and it has been found, that it vanishes at the temperature:

$$\tau_z^{(A,B)}=\tau_c^{(A,B)}+\frac{1}{4}\,\frac{\Delta_1^{(A,B)}-\Delta_2^{(A,B)}}{m_0\pm 1/2}. \tag{11}$$

Hence we conclude that two phase transition points exist in the system: τ_c and τ_z.

Finally, the behaviour of the system under the external stimulation has been analysed. The interaction Hamiltonian was taken in the form:

$$H_{int}(t)=-\frac{1}{2}\mu_B h(t)L-\mu_B h(t)S, \tag{12}$$

where

$$h(t)=\int_{-\infty}^{\infty}d\omega h(\omega)\,e^{-i\omega t}\,;\quad h(-\omega)=h(\omega) \tag{13}$$

is the external, periodical magnetic field.

Using the linear response approximation [3] by Green's function method we calculated the induced components of the total momentum. They are estimated as follows:

$$\langle J^+(\omega)\rangle_{n.eq.}\sim\frac{\omega_2}{\tau}\,\frac{1}{\omega-\omega_2}\,; \tag{14}$$

$$\langle J^-(\omega)\rangle\sim\frac{\omega_1}{\tau}\,\frac{1}{\omega-\omega_1}.$$

As we see the external stimulation is more effective at low temperatures. The resonance effects appear for external frequencies to be equal to the frequency ω_2 of the spin excitations as well as to the frequency ω_1 of the orbital excitations.

Summarizing the results obtained we can draw the following conclusions:

a) There are three types of single-electron excitations, consting in the changes of the spin, the orbital and the total momentum directions.

b) The energy of these excitations is of the order of the L-S coupling constant, i.e. of the order of 30—50 K_B.

c) The excitations obey the quasi-Pauli kinematics and statistics.

d) There is the possibility of the existence of the phase transitions in the system. At lower temperatures the order parameter of the system has a singularity. At higher temperatures the mean value of the Z-component of the total momentum vanishes.

e) The compoents of the total momentum, induced by an external periodical magnetic field, increase sharply for external frequencies close to the spin as well as to the orbital frequencies.

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It is with deep sorrow that we inform our readers of the death of Prof. RNDr. Štefan Veis, Dr.Sc., member of our Editorial Board for many years.

He was Professor at the Department of Experimental Physics of the Mathematical and Physical Faculty (formerly Faculty of Natural Science) of Comenius University in Bratislava. It is to him we owe the advancement of the physical investigation in the field of low-temperature plasma in Czechoslovakia.

Our Editorial Board will remember him as a dedicated scientist, untiring in his efforts to solve whatever problem he had been entrusted with.

Editors and
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