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SPIN-ORBITAL INTERACTION AND SINGLE-ELECTRON EXCITATIONS

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ABSTRACT. The system of single-electron extitations, consisting in diskrete changes of the spin as well as of the orbital momentum direction is analysed.The spin-orbital interaction is assumed as the main mechanism determining the dynamics of the system. It was 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 excitations are of the order of 3o-5o K_B.Thermodynamical analysis of the system points at the possibility of the existence of two phase-transitation points.At the lower temperature the ordering parameter of the system has a singularity and at the 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 $\mathcal{J}^{+}(\Omega)$ and $\mathcal{J}^{-}(\Omega)$.It was shown that the external stimulation is most effective at T=O, when induced momenta are of the maximal value.At high temperatures the magnitude of the induced momenta desreases linarly with increase of temperature.

Spin-Orbital Interaction and Single-Electron Excitations

The object of this paper is the formulations of a theory of single-electron excitations in hydrogen-like atoms. We assume that L-S interactions are the main mechanism acting in the system. Such considerations are the necessary basis for development of the more general theory of phenomena taking place in magnetinc dielectrics.[1)]

If the atom is placed into external magnetic field $\dot{\mathcal{H}}$, then the possible electron excitations consist in changes of spin, orbital and 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

$$H = H_e + H_S + H_{cS} \tag{1}$$

where

$$H_e = -\frac{\hbar^2}{2m}\Delta - \frac{Ze^2}{r}; \quad H_S = -\mu_B \mathcal{H} S^z; \quad H_{cS} = R\vec{L}\vec{S} = R\left(L^z S^z + \frac{L^+S^- + L^-S^+}{2}\right) \tag{2}$$

In the last formula m is the mass of the electron, Ze is the nucleus charge, $\mu_B = 2\frac{\hbar e}{2mc}$ is the doubled Bohr's magneton and $R = \frac{Ze^2\hbar^2}{2m^2c^2r_B^3}$ where $r_B = \frac{\hbar^2}{me^2}$ is the Bohr's radius. The actual set of electron states is the following

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

so that Hamiltonian (1) can be expressed in terms of 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 bi easily calculated with help of (2) and (3).

In order to analyse the electron excitations we are going over to the quasi-Pauli operators $Q_\mu^+ = a_\mu^+ a_0$ and $Q_\mu = a_0^+ a_\mu$ [2)], creating and annihiliating the excitations of the type μ. The

Hamiltonian(4) can be expressed now in terms of the operators Q_μ^+ and Q_μ, The further analysis requires the stabilization of the Hamiltonian. It is don by the standard procedure of Lagrange's multiplicators. We nottice that this procedure is different for two possible cases $m_f = m_0+1$ and $m_f = m_0-1$, but in bouth cases the Hamiltonian reduces to the diagonal form:

$$H_{AB} = \mathcal{L}_{A,B} + \sum_{\Theta=1}^{3} \Delta^{(A,B)} \mathcal{P}_\Theta^{+(A,B)} \mathcal{P}_\Theta^{(A,B)} \tag{5}$$

The operators $\mathcal{P}^+$ and $\mathcal{P}$ are new quasi-Pauli operators, obtaiend by the canonical transformaton of the operators Q^+ and Q. In the case $m_f = m_0+1$, denoted by the index A, we have

$$\Delta_1^{(A)} = \frac{1}{2}\left\{\sqrt{\varphi_A^2 + R^2\psi_A^2} - \varphi_A + R\right\}; \quad \Delta_2^{(A)} = \frac{1}{2}\left\{\sqrt{\varphi_A^2 + R^2\psi_A^2} + \varphi_A + R\right\} \tag{6}$$

$$\Delta_3^{(A)} = \frac{\rho_A^2 H_{00}^{(A)} + H_{33}^{(A)} - R\psi_A\rho_A}{1+\rho_A^2}; \quad \rho_A = \frac{\varphi_A - \sqrt{\varphi_A^2 + R^2\psi_A^2}}{R\psi_A}; \quad \psi_A = \sqrt{(l_0 - m_0)(l_0 + m_0 + 1)}$$

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

$$\Delta_1^{(B)} = \frac{1}{2}\left\{\sqrt{\varphi_B^2 + R^2\psi_B^2} - \varphi_B + R\right\}; \quad \Delta_2^{(B)} = \frac{1}{2}\left\{\sqrt{\varphi_B^2 + R^2\psi_B^2} + \varphi_B + R\right\}$$

$$\Delta_3^{(B)} = \frac{\rho_B^2 H_{11}^{(B)} + H_{22}^{(B)} - R\psi_B\rho_B}{1+\rho_B^2}; \quad \rho_B = \frac{\varphi_B - \sqrt{\varphi_B^2 + R^2\psi_B^2}}{R\psi_B}$$

$$\psi_B = \sqrt{(l_0 + m_0)(l_0 - m_0 + 1)} \tag{7}$$

The set of quasi-paulion states is the following:

$$\Delta_{\mathcal{P}} \equiv \left\{ |0_1 0_2 0_3\rangle; |1_1 0_2 0_3\rangle; |0_1 1_2 0_3\rangle; |0_1 0_2 1_3\rangle \right\} \tag{8}$$

Using the statisical operator canonical ensemble $\hat{\eta} = e^{\frac{F-H}{\tau}}$ where F is free energy of the system and $\tau = k_B T$ is the temperature in energy units it is easy to find the mean occupation number

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

and the ordering parameter of the system:

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

It turns, in the high temperature approximation, that the ordering parameter has a singularity at $\tau_C^{(AB)} = \frac{1}{4}\sum_{\Theta=1}^{3}\Delta_\Theta^{(AB)}$. The statistical mean value of the Z-component of total momentum $\langle J^z \rangle$ was calculated else, and it was shown that it vanishes at the temperature:

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

So we conclude that two phase transitions points exist in the system: τ_c and τ_Z .

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

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

where

$$\vec{\ell}(t) = \int_{-\infty}^{+\infty} d\Omega\, \vec{\ell}(\Omega)\, e^{-i\Omega t}; \qquad \vec{\ell}(-\Omega) = \vec{\ell}(\Omega) \tag{13}$$

is the external, periodical magnetic field.
Using the linear response approximation [3] by the Green's functions method we calculated the induced components of the total momentum. They are estimated as follows:

$$\langle J^+(\Omega)\rangle_{n.eq.} \sim \frac{\Omega_2}{T}\,\frac{1}{\Omega-\Omega_2}; \quad \langle J^-(\Omega)\rangle \sim \frac{\Omega_1}{T}\,\frac{1}{\Omega-\Omega_1} \tag{14}$$

As we see the external stimulation is more effective at low temperatures. The resonance effects appear for external frequences equal to the frequency Ω_2 of spin excitations as well as to the frequency Ω_1 of orbital excitations.

Summarizing the results obtaiend, we can draw the following conclusions:

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

b) The energy of these excitationsis of the order of L-S coupling constant, i.e. of the order of 3o-5o K_B.

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

d) There is the possibility of the existence of two phase.

transitions in the system.At lower temperatures the order parameter of the system has a singularity.At higher temperatures the mean value of Z-component of the total momentum vanishes.

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

References

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