Collective levels in heavy atoms

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It is shown that the spectrum of the excitations of the shell of a heavy atom contains two optically active collective levels of small width. By the same token, the question of the real existence of collective excitations of an atom is answered in the affirmative.

The question of the collective levels (CL) of an electron shell of a heavy atom,[3)] which are similar to plasma oscillations in macroscopic media, was raised long ago[1] (see also the review).[2] Its solution, however, was hindered by the lack of data on the width Γ of these levels. It is clear from general considerations[2] that in an atom, unlike in a homogeneous medium, the ratio of Γ to the level energy ω does not contain formally any small parameters. Therefore only a numerical calculation could cause this ratio to be small and by the same token lead to the conclusion that CL actually exist. We present below the results of such a calculation and their discussion.

1. For a microscopic description of a nonuniform electron shell of a heavy ($Z \gg 1$) atom we can use the random-phase approximation in conjunction with a quasiclassical analysis of the single-particle states; the accuracy of such an approximation is determined by the parameter $Z^{-2/3}$. This leads to an expression for the longitudinal dielectric constant of the system[4,2]

$$\epsilon(\omega, \mathbf{x}_1, \mathbf{x}_2) = \delta(\mathbf{x}_1 - \mathbf{x}_2) + \frac{p_0(\mathbf{x}_1)}{\pi^2}\left\{\frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|} + i|\omega| \int_{-\infty}^{0} dt\, \overline{\frac{\exp(-it\omega)}{|\mathbf{x}(t) - \mathbf{x}_2|}}\right\}. \quad (1)$$

Here $\mathbf{x}(t)$ is the classical trajectory of the electron in a Thomas-Fermi field $U(\mathbf{x})$, i.e., the solution of the equation $\ddot{\mathbf{x}} = -\nabla U$ with initial conditions $\mathbf{x}(0) = \mathbf{x}_1$ and $\dot{\mathbf{x}}(0) = p_0(\mathbf{x}_1)\mathbf{n}$; $p_0 = [2(\mu - U)]^{1/2}$ is the limiting momentum; the bar denotes averaging over the directions of the unit vector $\mathbf{n}$; the limiting energy in the neutral atom is $\mu = 0$; we use atomic units in this article. The frequency and the damping of the CL are determined by the real and imaginary parts of the eigenvalue of the equation

$$\int d\mathbf{x}_2\, \epsilon(\omega, \mathbf{x}_1, \mathbf{x}_2)\phi(\mathbf{x}_2) = 0, \quad (2)$$

where, subject to the appropriate normalization, ϕ is the change of the electron density upon excitation of the atom.

The approximations used in the derivation of (1) are valid only at the center of an atom of radius $R \sim Z^{-1/3}$. We consider only CL localized within this region, imposing the boundary condition on (2) in the form $\phi(R) = 0$. The evidence of the localization of the CL will be the plateaus in the plots of $\omega(R)$ and $\Gamma(R)$ (see Fig. 1 below). The second obvious boundary condition is of the form $\phi(0) < \infty$.

2. In the concrete calculations we used the Tietz approximation[5]

$$U = Z/[r(1 + \xi)^2], \quad \xi = r/a, \quad a = (9\pi/16)^{1/3}.$$

In such a field, the trajectories are closed self-intersecting curves (with period of motion T). It is easy to show that the imaginary part of ϵ, which leads to the damping of the CL, is connected with the poles of ϵ at the points $\omega T = 2\pi k$ (k is an integer). This condition corresponds to resonance with single-particle quasiclassical transitions—a direct analog of the usual Landau damping in a homogeneous system.

The Landau damping, being proportional to Z (see[2] and Eq. (3) below), plays literally the most important role. In addition, there is radiative damping which is undoubtedly small in comparison with ω. A more important damping mechanism is connected with the emergence of the excitation to the outer shells of the atoms; to describe it would be necessary to resort to special methods. It is clear, however, that the corresponding width does not depend on Z and is therefore small in comparison with ω, although it can become comparable with the value of Γ calculated in this paper, a value that

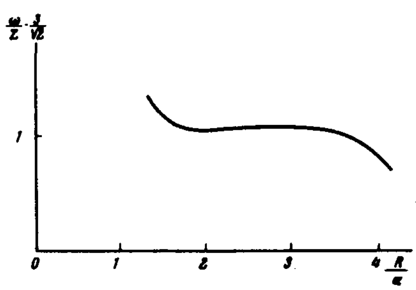

FIG. 1.

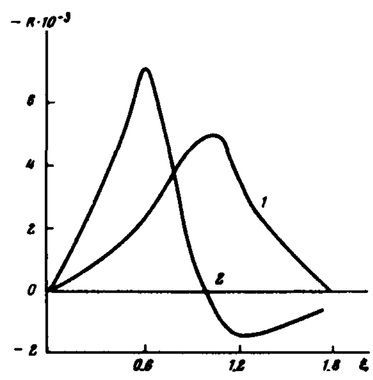

FIG. 2.

turns out to be anomalously small (see Eq. (3) below).

3. The numerical calculation was made with the BESM-6 computer of the Computation Center of the USSR Academy of Sciences, using the complemented-vector method.[6] As a result of a search for CL with relatively small widths, we observed two such levels, pertaining to the dipole type ($\phi(\mathbf{x}) = R(r)\cos\theta$)

$$\omega_1 = 13.74\, Z \text{ eV} \quad \Gamma_1 = 3\cdot 10^{-3}\, Z \text{ eV} \quad \omega_2 = 36.04\, Z \text{ eV} \quad \Gamma_2 \cong 10^{-4}\, Z \text{ eV}. \tag{3}$$

These values correspond to a plateau on the $\omega(R)$ or $\Gamma(R)$ curve (see Fig. 1, which shows only the former curve; the latter is similar in shape). Figure 2 shows the corresponding eigenfunctions of Eq. (2).

It is interesting to note that the physical picture of the CL corresponds, roughly speaking, to oscillations of the shell as a unit relative to the nucleus (this picture was discussed long ago by E.L. Feĭnberg); in fact, however, the shell is deformed somewhat and remains immobile near the nucleus and on the periphery of the atom.

4. The question of the experimental manifestation of the CL is not simple and calls for a special discussion. It is possible that the CL may manifest themselves as narrow resonances in the photoabsorption cross sections, and can also lead to the characteristic "Bohr" picture of the atomic reactions.[2]

A detailed exposition of the results of this article, as well as of the calculations of the CL oscillator strengths, will be the subject of separate articles.

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3) We have in mind only the "truly" CL, which constitute a separate branch of the excitation spectrum (oscillations of a charged liquid drop) and have specific quantum numbers. We do not consider collective effects in single-particle transitions, effects investigated in many recent papers (see, e.g.,[3]).

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