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Electron — positron quantum droplets

A.V. Solov'yov[1,a], V.K. Ivanov[2], and R.G. Polozkov[2]

[1] Frankfurt Institute for Advanced Studies, Max-von-Laue Str. 1, 60438 Frankfurt am Main, Germany
[2] St. Petersburg State Polytechnical University, Politechnicheskaya 29, St. Petersburg 195251, Russia

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Abstract. A new physical object, electron-positron quantum droplet, is suggested. Structure, stability and dynamics of such objects are discussed. The analysis is based on the non-relativistic self-consistent local-density approximation. An essential role of many-body effects in the formation of the droplets is demonstrated. Their properties are compared with the known physical objects such as metal clusters and clusters of excitons in a solid.

PACS. 31.15.Ew Density-functional theory – 36.10.-k Exotic atoms and molecules (containing mesons, muons and other unusual particles) – 36.40.-c Atomic and molecular clusters – 36.90.+f Other exotic atoms and molecules; macromolecules; clusters – 61.46.+w Nanoscale materials

Rapid Note

1 Introduction

We discuss a novel type of quantum finite system consisting of electrons and positrons (E&P). These quantum objects are formed by a number of E&P held together by attractive Coulomb and mutual polarization forces of E&P being packed in a droplet with a compact shell structure. We discuss the stability, structure and properties of electron-positron droplets (EPD) of different size. The number of particles in EPD can be varied from several up to infinity. In the limit of large numbers such a system evolves into the electron-positron gas or plasma [1]. At small numbers the system is essentially finite and its quantum features manifest themselves more prominently. In this case the motion of E&P within the EPD volume becomes strongly quantized, similar to metal clusters. Contrary to metal clusters, in EPD the motion of both negatively and positively charged subsystems is identical and quantized. In this paper, our main attention will be devoted to the description of this new type of matter with relatively small number of particles.

EPDs can be created during the condensation or density collapse of a number of E&P initially localized in a certain volume. The necessary conditions for such a process can be met in experiments with electron and positron aligned beams of high density and of equal energy. When the beams are brought together the mutual attraction of electrons and positrons should result in the growth of particles density, formation of electron-positron plasma and subsequent creation of EPDs. Similar many-body phenomenon occurs during electron cooling of ionic beams [2]. In this case cooling of ions and subsequent growth of the density of the ionic beam is achieved by alignment of the ionic beam with the beam of electrons. The density of high energy E&P bunches in modern colliders can be as high as $n \sim 10^{21}$ cm^{-3} [3], which is only three orders of magnitude lower than the characteristic value of the electronic density in solids. Therefore, it is plausible to expect that it will be sufficient to initiate the collapse of the electron-positron density.

The alternative idea of creation of EPDs concerns the formation of these objects in the Penning traps. We expect that the condensation of E&P densities into EPDs of the finite size can take place in external electric and magnetic fields holding particles together in a trap, providing the temperature of the E&P gas is sufficiently low.

A proof of the existence of EPDs might have important consequences for various fields of science. Thus, these objects can be relevant to astrophysical problems in connection with the long standing discussion of possible presence of antimatter in the Universe [4]. In nuclear physics, similar kind of objects arise when antibaryons become bound in nuclear matter [5]. In solid state physics, the condensation of electron-hole pairs or bound states of several excitons in a form of a cluster have been experimentally observed at certain conditions [6]. There has been no self-consistent many-body theory developed for those systems so far. The formalism which we report in this paper in its application to EPDs can be utilized with the minor modifications for the treatment of the exciton clusters in semi-conductors as well.

In order to prove the existence of EPDs of a finite size we calculate the E&P energy levels structure, and analyze the stability of these objects. We evaluate the probability of the EPD annihilation and the EPD fragmentation into a number of positroniums (Ps).

[a] e-mail: solovyov@fias.uni-frankfurt.de

2 Theoretical framework

Our analysis of the EPD properties is based on the formalism of non-relativistic density functional theory and self-consistent solution of the Kohn-Sham equations. We do that for neutral bound system consisting of N-electrons and N-positrons. Another constrain which we impose on the system is related to its sphericity. In this paper, we focus on spherical systems only, thus restruct ourselves to the EPDs with close electronic and positronic shells.

The equations for both electronic and the positronic subsystems read in the atomic system of units ($\hbar = m_e = |e| = 1$) as

$$\left(\frac{\hat{\mathbf{p}}^2}{2} + V_{eff}^{e,p}(\mathbf{r})\right)\varphi_i^{e,p}(\mathbf{r}) = \epsilon_i^{e,p}\,\varphi_i^{e,p}(\mathbf{r}), \tag{1}$$

where $\varphi_i^{e,p}(\mathbf{r})$ are the electronic and positronic wave functions respectively. The effective potential $V_{eff}^{e,p}(\mathbf{r})$ for each subsystem is formed by the core potential of the opposite charge distribution, Coulomb repulsion and exchange-correlation potential

$$V_{eff}^{e,p}(\mathbf{r}) = V^{e-p,p-e}(\mathbf{r}) + \int d\mathbf{r}\,'\,\frac{\rho^{e,p}(\mathbf{r}\,')}{|\mathbf{r}-\mathbf{r}\,'|} + V_{xc}^{e,p}(\mathbf{r}), \tag{2}$$

where

$$V^{e-p,p-e}(\mathbf{r}) = \int d\mathbf{r}\,'\,\frac{\rho^{p,e}(\mathbf{r}\,')}{|\mathbf{r}-\mathbf{r}\,'|}, \tag{3}$$

$$\rho^{e,p}(\mathbf{r}) = e^{e,p}\sum_{i=1}^{N}|\varphi_i^{e,p}(\mathbf{r})|^2. \tag{4}$$

Here N is the number of electrons (positrons) in the system, $\rho^e(\mathbf{r}) < 0$ and $\rho^p(\mathbf{r}) > 0$, $e^e = -1$, $e^p = 1$.

Many-body correlations are taken into account within the local density approach with the Perdew and Wang (PW91) parametrization for the exchange-correlation functional [7]. Note that in the system, which we consider, the shell structure arises in a self-consistent way. Due to the charge symmetry between E&P the solution of equations (1) and the corresponding shell structure are identical for the two subsystems. Numerically, this condition was fulfilled by the iterative solution of the Kohn-Sham equations for both systems. Via this procedure the single-particle energies ε_i and the wave functions $\varphi_i(\mathbf{r})$ have been obtained. Note that no assumption about the jellium background has been made neither for the electron nor for the positron background, which makes this system quite different from metallic clusters.

The exchange-correlation potential includes three parts- the local exchange interaction between equivalent particles, and the correlation interaction between equivalent and non-equivalent particles:

$$V_{xc}^{e,p}(r) = V_x^{e-e,p-p}(r) + V_c^{e-e,p-p}(r) + V_c^{e-p,p-e}(r). \tag{5}$$

The ground state of EPS is reached via the iterative solution of equations (1–5). Numerically it was shown that the E&P densities are equal as it follows from the charge symmetry of the two subsystems:

$$|\rho^e(r)| = |\rho^p(r)|. \tag{6}$$

The EPS total energy is equal to

$$E = E^e + E^p - E^{e-p}. \tag{7}$$

Here, the total energy for each subsystem is obtained within the LDA [7]:

$$E^{e,p} = \sum_{i=1}^{N}\epsilon_i^{e,p} - \frac{1}{2}E^{e-p} + E_{xc}^{e,p} - \int \rho^{e,p}(r)V_{xc}^{e-e,p-p}(r)dr, \tag{8}$$

where the Coulomb attractive energy of E&P subsystems is

$$E^{e-p} = E^{p-e} = \iint \frac{\rho^{e,p}(\mathbf{r})\rho^{p,e}(\mathbf{r}\,')}{|\mathbf{r}-\mathbf{r}\,'|}d\mathbf{r}d\mathbf{r}\,' \tag{9}$$

and the exchange-correlation energy reads as follows

$$E_{xc}^{e,p} = \int \rho^{e,p}(r)\varepsilon_{xc}^{e,p}(r)dr \tag{10}$$

with ε_{xc} being equal to

$$\varepsilon_{xc}^{e,p}(r) = \varepsilon_x^{e,p}(r) + \varepsilon_c^{e,p}(r) + \varepsilon_c^{e-p,p-e}(r). \tag{11}$$

Note that the Coulomb repulsion energy of E&P subsystems in (7) reads as

$$E^{e-e,p-p} = \frac{1}{2}\iint \frac{\rho^{e,p}(\mathbf{r})\rho^{e,p}(\mathbf{r}\,')}{|\mathbf{r}-\mathbf{r}\,'|}d\mathbf{r}d\mathbf{r}\,'. \tag{12}$$

Accounting for the equality of the E&P densities in the ground state, see (6), one derives

$$E^{e-e} + E^{p-p} = -E^{e-p}. \tag{13}$$

3 Energetics of the EPD

We have calculated the E&P energy level structure for the EPD with the number of electrons and positrons equal to $N = 2, 8, 18, 20$. These numbers correspond to the EPD with the closed $1s^2, 1p^6, 1d^{10}$ and $2s^2$ shells for each subsystem. The calculated radial dependences of the equilibrium densities and the corresponding self-consistent potentials are presented in Figure 1.

The EPD structure has many features common to atomic clusters of simple metals, like Na or K, in which strong delocalization of valence electrons takes place. Although, there are important differences. In metallic clusters the motion of valence electrons is quantized and creates the shell structure while the positively charged ions form the background. In the simplest case, the jellium model for metal clusters suggests the homogeneous distribution of the ionic density within the cluster volume [8]. In the more advanced jellium-type models for metal

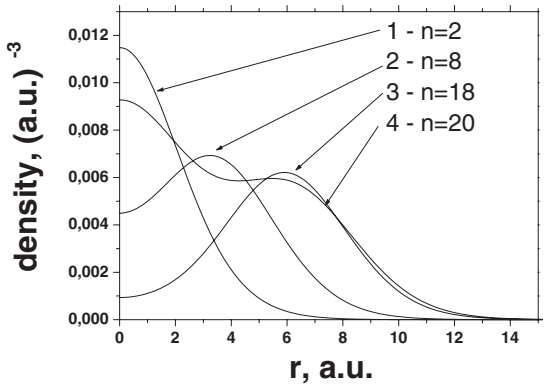

Fig. 1. The radial distribution of density in the EPD with $N = 2, 8, 18, 20$ calculated by the self-consistent solution of the Kohn-Sham equation.

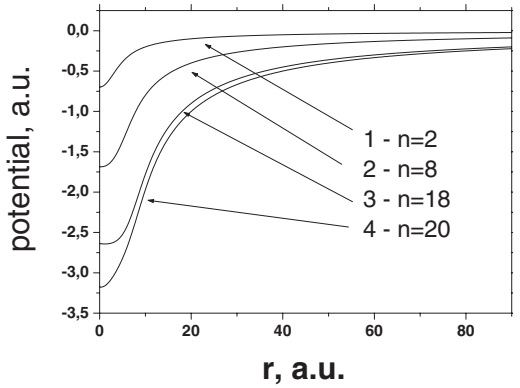

Fig. 2. The effective potential in the EPD with $N = 2, 8, 18, 20$ calculated by the self-consistent solution of the Kohn-Sham equation.

Table 1. Total energies per particle and averaged distances between particles for EPD with $N = 2, 8, 18, 20$.

	$N = 2$		$N = 8$		$N = 18$		$N = 20$	
Model	$E/2N$ (a.u.)	R_s (a.u.)	$E/2N$ (a.u.)	R_s (a.u.)	$E/2N$ (a.u.)	R_s (a.u.)	$E/2N$ (a.u.)	R_s (a.u.)
HF JM	−0.049	3.29	−0.047	3.15	−0.045	3.10	−0.045	3.10
LDA JM		4.0	−0.072	4.0	−0.074	4.00	−0.074	4.00
OJM	−0.054	3.33	−0.051	3.35	−0.049	3.5	−0.049	3.5
EPD 1	−0.065	3.328	−0.07	3.121	−0.071	3.197	−0.072	3.053
EPD 2	−0.094	2.963	−0.100	2.79	−0.1014	2.859	−0.1023	2.733
Ps	−0.125		−0.125		−0.125		−0.125	

clusters, like the optimized jellium model [9], the ionic background is no-longer homogeneous. Thus, by the double variation procedure it was analytically demonstrated that the total electronic density is equal to the "'optimal" ionic charge density, $\rho_i(\mathbf{r})$, at each space point. i.e. $|\rho_e(\mathbf{r})| = |\rho_i(\mathbf{r})|$ meaning that the condition of local electroneutrality in the optimized cluster system is to be met. Contrary, in the EPD case no assumption about the background in the systems is made neither for electronic nor for positronic subsystems. Moreover, both subsystems are considered dynamical, i.e. the kinetic energy for both E&P is taken into account.

The jellium model proved to be a good theoretical framework for the description of the main properties of metal clusters like the shell structure and density, cluster stability, collective excitations of electrons and many-more, see [10] and references therein. Therefore, we believe that with the accounting for the kinetic energy terms for both subsystems and the correlation potential between them our model should be reliable enough to predict major properties of EPD.

Figure 1 shows that the electron and the positron densities are strongly dispersed in the EPD outer region. The dispersion of the electron density in the vicinity of the cluster surface is known for metal clusters as the spill out effect. In EPDs spilling out the density is much stronger than in metal clusters, because the EPD does not have fixed core determining the system geometry and the density of delocalized electrons or positrons.

The calculated total energies per particle and the averaged distance between particles for the EPDs with $N = 2, 8, 18, 20$ are presented in Table 1 and compared with the corresponding characteristics obtained for Na clusters and with the Ps binding energy. The following definitions have been used. HF JM is the ordinary Hartree-Fock jellium model for metal clusters [9]; LDA JM is the similar model developed within the LDA [8]; OJM is the optimized jellium model for metal clusters [9]; EPD 1 and EPD 2 are the results of this work obtained without and with accounting for the correlations between electronic and positronic subsystems, respectively.

Our calculations demonstrate that the EPDs have larger binding energy ($E/2N$) and higher density (smaller Wigner-Seirz radius R_s) than those for Na clusters calculated both in HF JM [13] and LDA JM [9]. The correlation interaction between E&P systems plays a very important role. It lowers significantly the EPD total energy and makes it very close to the Ps binding energy. Also, it reduces the average distance between particles, being in the range 2.8–3.0 a.u. for the EPS considered.

To estimate the EPD stability against the decay into Ps, we use the analogy between this system and metal clusters. In neutral metal clusters, the evaporation of a single atom usually means overcoming a barrier, which is typically of about 1 eV. It can be very roughly estimated by the double value of the binding energy per atom in a cluster. Applying this argument to the EPD, one can roughly estimate the evaporation energy of a single Ps from the EPD as ~ 0.2 eV, see Table 1.

According to Table 1, the emission of Ps from the EPD can either be the exotermic or endothermic process, depending on the balance between the increase of the binding energy of E&P in the ejected Ps and the lowering of the binding energy in the remaining open shell EPD caused by its deformation. The emission of Ps from the EPD occurs via the fission barrier originating due to the restructuring of both electronic and positronic energy levels in the system. Similar situation takes place in the fission of multiply charged metal clusters [10,11]. The height of this barrier has to be comparable with the binding energy of two Ps. The Ps dimer has been recently described and the binding energy 0.4 eV for this system has been reported, see [1] and references therein. This value gives a very rough estimate for the value of barrier to be overcame during the Ps emission process.

The fact that the binding energy of E&P in the EPD turns out to be smaller than the Ps binding energy, see Table 1, implies the possibility of Mott phase transition in the system and formation of a cluster of Ps with a well defined lattice structure. For a medium of ortho-Ps this also means the possibility of transition into Bose-Einstein condensate state at sufficiently low temperatures.

4 EPD annihilation probability

Let us now evaluate the probability of the two-photon annihilation process:

$$W = 4\pi r_0^2 c \sum_{mn} \iint |\varphi_n^e(\mathbf{r})|^2 |\varphi_m^p(\mathbf{r}\,')|^2 \delta(\mathbf{r} - \mathbf{r}\,') d\mathbf{r} d\mathbf{r}\,'. \tag{14}$$

Integrating (14) over the angular variables, one derives

$$W = r_0^2 c \sum_{n'l'} N_{l'} \sum_{nl} N_l \int P_{n'l'}^{(p)2}(r) P_{nl}^{(e)2}(r) dr \tag{15}$$

where $r_0 = e^2/m_e c^2$, $P_{n'l'}^{(p)}(r)$ and $P_{nl}^{(e)}(r)$ are the radial parts of the positron and the electron wave functions; $N_l = 2(2l+1)$, $N_{l'} = 2(2l'+1)$ are the occupation numbers for the E&P subshells respectively. This expression is proportional to the probability of two photon annihilation of para-positronium: $W_{\mathrm{Ps}} = r_0^2 c/2$.

It is interesting to compare the probability (15) with the probability of the two photon annihilation in a system of equivalent number of positroniums, i.e. to calculate the ratio $R = W/(NW_{\mathrm{Ps}})$. Integrating (15) one derives the following ratios: $R_{N=2} = 0.68$; $R_{N=8} = 2.27$; $R_{N=18} = 4.787$ and $R_{N=20} = 4.517$. These estimates demonstrate that the EPD life time against annihilation is comparable with the Ps life time, which means it is very large at the atomic units scale, and it grows fast with increase of the EPD size.

Accounting for the annihilation in EPD of sufficiently large size should lead to the additional polarization of the medium within the EPD and as a result to the additional attraction between E&P. This effect should reduce the EPD total energy. For the EPD of larger size, one may expect that accounting for the additional attraction in the system caused by the annihilation could make it energetically more stable than the Ps condensate. Investigation of this interesting phenomenon could be a subject for further work. Another interesting question concerns the calculation of probability of immediate annihilation of several E&P into one high energy photon as well as all other possible annihilation channels in the system including its explosion.

5 Conclusion

In this paper, we have not discussed collective dynamics of particles in the EPD, which is another interesting topic for further consideration. Indeed, one can extend our model and add to the Hamiltonian of the system a part responsible for the collective dynamics of the EPD in a similar way as it was done for metal clusters within the dynamical jellium model [12] accounting for collective breathing, dipole and quadrupole deformation modes. EPD at finite temperatures can be treated using the technique developed in [12].

We have performed our calculations for the closed shell EPDs. The extension of this consideration for open shell systems implies accounting for deformations similarly to how it was done for clusters in the Hartree-Fock deformed jellium model [13]. Our theory is based on the non-relativistic density functional formalism. Treatment of the EPDs on the basis of the Hartree-Fock-Dirac equation and the consistent many-body perturbation theory is another interesting problem to be solved in the future.

Summarizing, we have described a new physical object, electron-positron quantum droplet, and suggested a broad spectrum of problems for further investigation.

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