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Positron states in noble liquids: Affinity, effective mass, and mobility

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The state of the almost free positron injected into a noble liquid is considered. The pseudopotential theory of the scattering of light quantum particles in a cellular dense medium is used. The density dependences of the positron scattering length and phase shifts of partial waves are calculated for neon and argon liquids. The density dependences of the ground-state energy, effective mass, and mobility are obtained. [S0163-1829(96)07519-4]

I. INTRODUCTION

The recent development in the use of positrons as a probe of matter has stimulated interest in investigations of positron states in condensed matter.[1,2] Being injected into a liquid or solid sample, a positron during its lifetime loses an initially high energy, thermalizes itself, and comes to partial equilibrium with the medium. As a result, the positron can be observed in free or self-trapped states or in positronium. The self-trapping is more likely into clusters in dense gases.[3] In liquids it is difficult to form a cluster, and free states are more favorable thermodynamically. The affinity of the positron to a medium, V_0 (the energy of the ground state relative to vacuum), effective mass m_{eff}, and mobility in an electric field, μ, are the main parameters of the free state. A noble liquid is a medium that can be considered as a test medium for experimental and theoretical methods involving positron scattering processes. Theoretical methods developed for the study of states of excess electrons in a dense medium are applied in the present paper to positrons.

The problem of excess-electron states in liquids has attracted the attention of many researchers (see reviews[4,5]). In the last decade the behavior of excess electrons was investigated in the whole range of liquid densities. It was discovered that the ground-state energy of the electron passes through a minimum with decreasing density, while the density dependence of the electron mobility has a sharp maximum. The positions of the minimum of V_0 and the maximum of μ correspond to the same value of medium density.[6] The phenomenon has attracted great interest. The quantitative description requires the modeling of a muffin-tin potential field which the electron perceives in a medium. However, one faces a difficulty originating from the lack of knowledge of the short-range component of the electron-atom potential. It seems necessary to introduce adjustable parameters. However, the difficulty can be avoided by using a pseudopotential theory developed on the basis of the ideas of Springett, Cohen, and Hortner.[7] In Refs. 8–11 a theory was given which uses experimentally known parameters as input data: the scattering length of an electron from an isolated atom, the atomic polarizability, and the binary correlation function of a liquid. The density dependences of the energy of the electron ground state, effective mass, and mobility were calculated, in satisfactory agreement with experimental data.

The short-range positron-atom interaction differs strongly from that for electrons. The absence of exchange forces weakens the short-range repulsion. As a result, scattering lengths of positrons on isolated atoms are negative and large in magnitude. The value of the scattering length is an overall measure of the low-energy interaction, which is the result of the counterbalance of the short-range repulsion and the long-range attraction. In the framework of the pseudopotential theory[8–11] it is possible to extract information about the intensity of the short-range repulsion. This information can be used to describe positron states in a dense medium.

The present paper is organized as follows. In Sec. II, the scattering of positrons in nonpolar liquids is considered. The density dependences of the scattering lengths in liquid neon and argon are calculated. The dependences of the phase shifts of s and p partial positron waves on positron energy and liquid density are obtained. In Secs. III and IV, the density dependences of the ground-state energy and effective mass are calculated. The calculated ground-state energies are in satisfactory agreement with experimental data at the densities of rare-gas solids.[12] A number of methods exist to measure positron mobility in dense media (e.g., Refs. 1 and 2). In Sec. V, the density dependence of the positron mobility in liquid argon is calculated. We note that the ground-state energies were also calculated in Ref. 13 by using a model positron-atom potential. In the last section, all the results are discussed, validity criteria are considered, and some applications are indicated.

II. SCATTERING OF POSITRONS IN A NONPOLAR LIQUID

The necessary input data are listed in Table I. The scattering lengths from isolated atoms L_0 are taken from Ref. 14. States of liquids are described by the radial distribution functions $g(r)$ of the Lennard-Jones liquid.

When a liquid positron finds itself in a muffin-tin poten-

TABLE I. Interaction parameters.

	α (a_0^3)	L_0 (a_0)	σ (a_0)	r_0 (a_0)	r_1 (a_0)
Ne	2.67	-0.73	5.3	0.82	0.94
Ar	11	-4.0	6.5	1.35	1.5

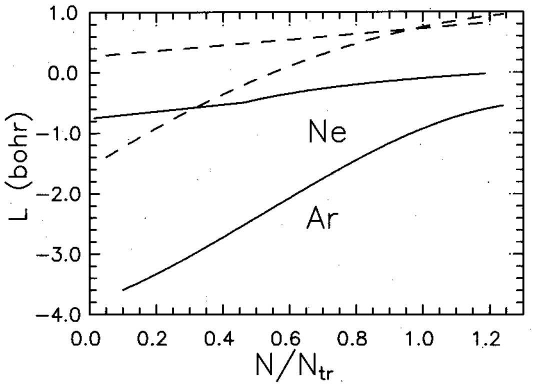

FIG. 1. Scattering lengths of positron (solid lines) and electron (dashed) in neon and argon versus ratios of the liquid densities to the densities at the triple points. The dependences are continued to the solid state.

tial field, $\overline{r}=(4\pi N/3)^{-1/3}$ is the radius of a unit cell. Within the cell the potential is represented by the positron interaction potential with an atom situated at the center of the cell, and by the mean potential of the cell environment.[8–10] The scattering length from the cell is given by the expression[8–10]

$$L(N)=\frac{L_c-\overline{rA}(1-L_c/\overline{r}\,)}{1-A(1-L_c/\overline{r}\,)}, \tag{1}$$

$$L_c=\left\{\frac{1}{\overline{r}}+\left(\frac{a_0}{\alpha}\right)^{1/2}\tan\left[\left(\frac{\alpha}{a_0}\right)^{1/2}\left(\frac{1}{r_0}-\frac{1}{\overline{r}}\right)\right]\right\}^{-1}, \tag{2}$$

$$A=\frac{2}{5}-\frac{\alpha\overline{r}}{a_0\sigma^3}f\left[I_2+\frac{9}{14}I_4\frac{\overline{r}^{\,2}}{\sigma^2}\right], \tag{3}$$

where L_c is the scattering length on the cutoff potential of the central atom of the cell, α is the atomic polarizability, and r_0 is the pseudopotential core radius. The parameter A represents the influence of the environment potential. The factor $f=(1+2\alpha\overline{r}^{-3})^{-1}$ accounts for the Lorentz-Lorenz local field.[15] The factors I_2 and I_4 account for the specifics of the interatomic correlations. If $\overline{r}\lesssim\sigma$, $I_2\simeq 1.6$ and $I_4\simeq 1.8$, where σ is the closest distance of interatomic approach.[8] If $I_2=I_4=1$, a stepwise $g(r)$ is used: if $\overline{r}\leqslant\sigma$, $g(r)=0$, and if $\overline{r}>\sigma$, $g(r)=1$. If σ in (3) is replaced by $\overline{r}$ and I_2 and I_4 by unity, Eq. (1) can be used in a dense gaseous medium where $\overline{r}>\sigma$. Of course, it is a rather crude interpolation, $L\Rightarrow L_0$.

The calculated $L(N)$ in neon and argon are presented in Fig. 1. The scattering lengths decrease in magnitude with increase in density. The scattering lengths are negative in gases due to the prevalence of the polarization attraction. With increase in density the polarization attraction is weakened as a result of the overlap of the electron-atom potentials, and the magnitude of L decreases. However, the scattering lengths remain negative. Recall that the scattering length of electrons becomes positive in liquid argon. For the Ar-positron interaction $L_0=-a_0$ and the core radius $r_0=1.35a_0$; for the Ar-electron interaction $L_0=-1.4a_0$ and the core is larger, $r_0=1.68a_0$. The pseudopotential core radius is given by

$$r_0=\sqrt{\alpha/a_0}[\pi+\arctan(L_0^{-1}\sqrt{\alpha/a_0})]^{-1}. \tag{4}$$

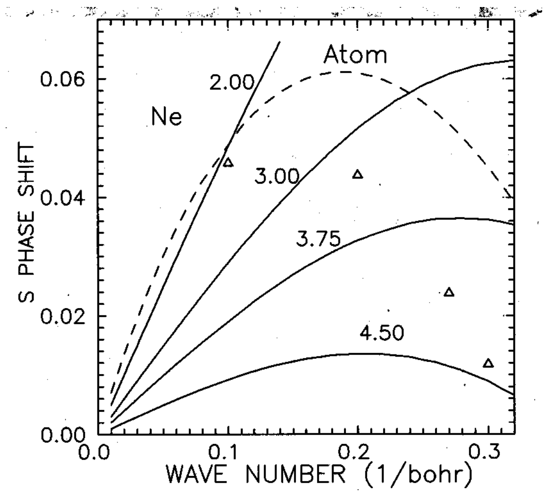

FIG. 2. Phase shift δ_0 in Ne versus wave number of positron. Liquid densities N are given in units of 10^{22} cm^{-3}. Isolated atom (Ref. 14): points; our calculation: dotted line.

In Fig. 2 the phase shifts of the positron s wave scattered in neon are shown. The calculated $\delta_0(k)$ for the isolated Ne atom reproduces the dependence obtained in Ref. 14 as a result of sophisticated calculations. It should be noted that our calculations, which use no adjusted parameters, are more accurate at small positron energies $\epsilon=\hbar^2k^2/2m$, where k is the positron wave number. For small wave numbers in a dilute gas the role of the polarization is very important:[10]

$$\delta_0=-kL_0-\pi\alpha k^2(3a_0)^{-1}+(2\alpha r_0k^3/3a_0)\ln(1.36/kr_0). \tag{5}$$

In dense media the polarization potential loses its tail, and the k^2 term vanishes. For small wave numbers the values of δ_0 can be calculated using the formula[16]

$$\delta_0=-kL-(\alpha\overline{rk}^3/3a_0)[(1+2x\ln x+x/4-3x^2/2)+(2/7)y^3f(I_2+0.7I_4y^2)], \tag{6}$$

where $x=r_0/\overline{r}$ and $y=\overline{r/\sigma}$. The relationship between the first and second terms in Eq. (6) varies strongly with the density because L depends strongly on the density.

If $\overline{kr}$ is comparable to unity the phase shifts should be calculated numerically.

Figure 2 shows that the phase shifts are positive even at the density of the solid state, $N=4.5\times10^{22}$ cm^{-3}. As to the phase shift of the scattered electron wave, it becomes negative with increasing density.[10,11] Hence the attraction of positron to atom predominates over the repulsion at the whole range of energies.

The phase shifts in argon (Fig. 3) are larger due to the larger values of the L magnitudes. The validity of the present formulas requires the fulfillment of the inequality $|L|k\ll 1$. So if the values of δ_0 are comparable to unity their reliability is doubtful. For this reason, the calculated $\delta_0(k)$ values disagree at $k\geqslant 0.1a_0^{-1}$ with the Nakanishi and Schrader data[14] for the isolated argon atom.

The pseudopotential approach gives the following expression for the p-wave phase shift on an isolated atom at small k:[16]

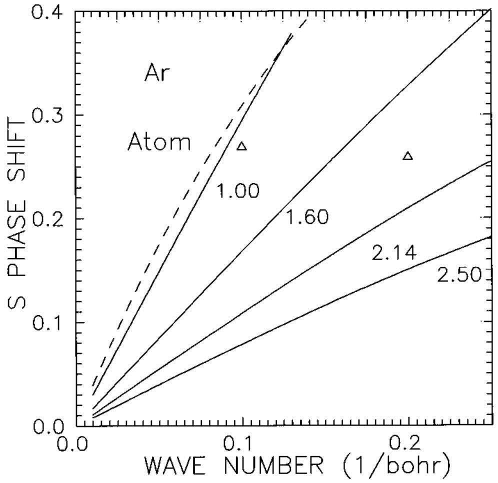

FIG. 3. Phase shift δ_0 in Ar. Designations as in Fig. 2.

$$\delta_1 = \alpha k^2 a_0^{-1}[\pi/15 - kr_1/6] - (kr_1)^3/3, \tag{7}$$

where r_1 is the radius of the hard core of the pseudopotential for the p wave, which is different from r_0. Comparison with the $\delta_1(k)$ from Ref. 14 allows one to determine r_1. For Ne $r_1 = 0.94a_0$; for Ar $r_1 = 1.5a_0$. Of course, r_1 is larger than r_0.

The p scattering on isolated atoms does not differ significantly from the scattering on the pure polarization potential. However, the role of the polarization is weakened in a dense medium. At small k we have[16]

$$\delta_1 = (\alpha k^3 \overline{r}/9a_0)[(1 - 3x/2 + x^3/2) + (2/7)y^3 f(I_2 + 0.7I_4 y^2) - (kr_1)^3/3], \tag{8}$$

where $x = r_1/\overline{r}$ and $y = \overline{r}/\sigma$. The density variations of δ_1 are shown in Figs. 4 and 5. The decrease of δ_1 with the density increase does not lead to a change in sign as occurs for electron scattering.[11,16] The attraction dominates the interaction at the whole density range.

The role of higher l waves is not significant. At small $k\overline{r}$ for d waves we have $\delta_2 = ak^5\overline{r}^3/675a_0$. If the set of phase shifts is determined one can calculate the energy spectrum, the scattering cross section, and the mobility.

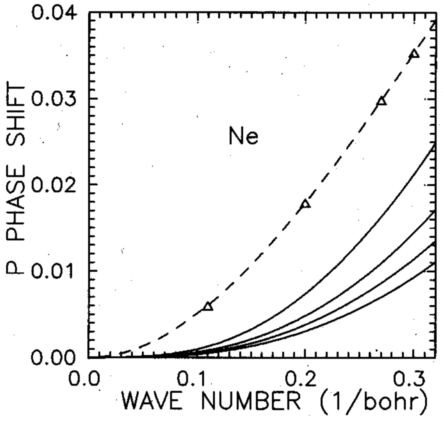

FIG. 4. Phase shift δ_1 in Ne. Designations as in Fig. 2.

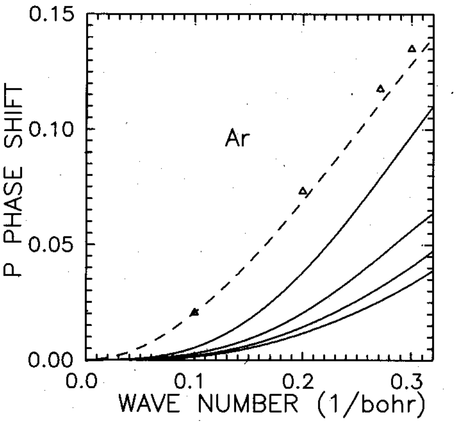

FIG. 5. Phase shift δ_1 in Ar. Designations as in Fig. 2.

III. ENERGY OF THE GROUND STATE

The energy of the ground state is given by[7]

$$V_0 = u_0 + T_0, \quad u_0 = -3\alpha e^2 I_0 (2\sigma \overline{r}^3)^{-1} f, \tag{9}$$

where u_0 is the mean polarization energy and T_0 is the energy of the ground state in the Wigner-Seitz cell. For the Lennard-Jones fluid $I_0 \cong 1.2$.[8] In gases one should replace σ by $\overline{r}$, and the factor I_0 by unity.

For calculations of T_0 we use the solution of the Schrödinger equation in the Wigner-Seitz cell which was obtained in Ref. 11 for the case $L < 0$. If $(|L|/\overline{r})^3 \ll 1$ we have

$$T_0 = -\hbar^2 \kappa_0^2/2m, \quad \tanh[\kappa_0 \overline{r} + \mathrm{Im}\ \delta_0(i\kappa_0)] = \kappa_0 \overline{r}. \tag{10}$$

Here $\delta_0(i\kappa 0)$ is the analytic continuation of the function δ_0, defined on the plane of complex wave numbers, from the axis of real wave numbers k to the axis of imaginary wave numbers $i\kappa$. If $\delta_0(k) = -Lk + Ak^3$, then

$$\delta_0(i\kappa) = -iL\kappa - iA\kappa^3. \tag{11}$$

In the limit of small densities, Eq. (10) can be reduced to the optical approximation, $T_0 = (3/2)\hbar^2 L \overline{r}^{-3}/m$.

Calculated results are shown in Fig. 6. They agree satis-

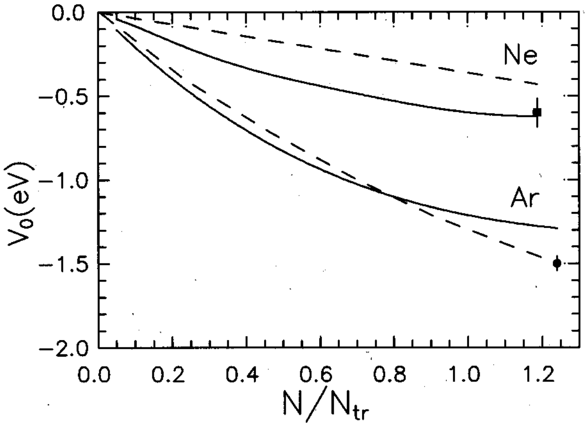

FIG. 6. Dependences of the energy V_0 in argon and neon on the ratios of densities to the densities at the triple points. Experimental data (Ref. 12): points. Calculated data (present paper): solid lines; (Ref. 13): dotted lines.

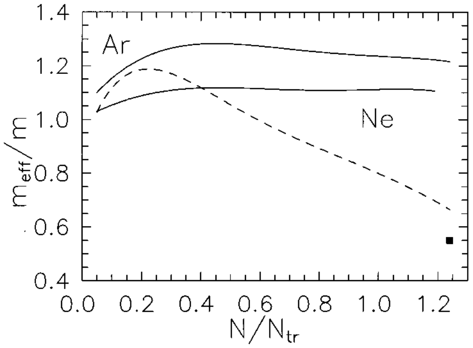

FIG. 7. Density dependences of the reduced effective mass of free positrons in Ar and Ne (solid lines) and the reduced effective mass of electrons in Ar (dotted line). Experiment (Ref. 21): electron in Ar.

factorily with the experimental data in solids.[12]

In the whole density range there is good agreement with the calculation.[13] In Ref. 13 the short-range positron-atom potential was written explicitly using some adjusted parameters, the environment potential $u(r)$ was calculated as usual, and the Schrödinger equation in the Wigner-Seitz cell was solved numerically. Unfortunately, in Ref. 13 the phase shifts of the scattered positron waves are not displayed. It would be interesting to compare them with our data.

IV. EFFECTIVE MASS

The effective mass of the almost free positron is given by the Bardeen formula[17,18]

$$(m_{\rm eff}/m)^{-1}=\psi^2(\overline{r})[d\ \ln\ \chi_1(\overline{r})/d\ \ln\ \overline{r}-1], \qquad (12)$$

where $\psi(\overline{r})$ is the wave function of the positron ground state in the unit cell and $\chi_1(\overline{r})$ is the single-site radial p-wave function. Both the functions are taken at the cell boundary. In the case of negative L, we have[11]

$$\psi(\overline{r})=A(\kappa_0\overline{r})^{-1}\sinh[\kappa_0(\overline{r}-L)],$$

$$A^2=(4/3)(\kappa_0\overline{r})^{-3}\{\sinh[2\kappa_0(\overline{r}-L)]+\sinh(2\kappa_0L)-2\kappa_0\overline{r}\}, \qquad (13)$$

$$d\ \ln\ \chi_1/d\ \ln\ \overline{r}=-(\kappa_0\overline{r})^2\ \tanh[\kappa_0\overline{r}+{\rm Im}\ \delta_1(i\kappa_0)]\times\{\tanh[\kappa_0\overline{r}+{\rm Im}\ \delta_1(i\kappa_0)]-\kappa_0\overline{r}\}^{-1}-1.$$

In Fig. 7 calculated results are given and compared with the effective masses of electrons.

The value of the reduced effective mass can either exceed unity or be lower. If the attraction predominates over the repulsion, $m_{\rm eff}/m$ exceeds unity.[11] In the opposite case, $m_{\rm eff}/m<1$. Really, the measured effective mass of the positron in liquid sodium is equal to $(1.9\pm0.4)m$.[19] The effective mass in solid aluminum is equal to $1.1m$.[20] The last value was calculated by another method, which uses the expansion of the wave function over plane waves, but not over the cellular functions.

Accordingly, the reduced effective masses in neon and argon exceed unity. In the limit of small densities, Eq. (12) leads to $m_{\rm eff}/m=1$. However, it is clear that our results are accurate only at high densities when the density fluctuations do not disturb the cellular structure. At small densities the calculated dependences should be considered as an interpolation.

In argon the effective mass of an injected electron passes through unity with density variation. This occurs near the density where the scattering length changes sign. In solid argon the calculated effective mass of the electron is close to the measured value of Ref. 21. For positrons, measured data are absent. It is worth noting that the calculated values do not contradict the indirect information given in Refs. 12 and 22.

V. MOBILITY OF FREE THERMAL POSITRONS

In the framework of the Cohen and Lekner kinetic theory[23] the mobility is given by the Lorentz-like formula

$$\mu=\tfrac{2}{3}(2e^2/\pi Tm)^{1/2}[4\pi L^2(N)S(0)N]^{-1} \qquad (14)$$

where $S(0)$ is the long-wavelength structure factor of a liquid, which accounts for interatomic correlations. The theory is based on the requirement that the subsequent scattering events are independent. It means that the mean free path of the positron, $l=[4\pi L^2NS(0)]^{-1}$, must be larger than other characteristic lengths. The most important parameter is the ratio of the wavelength of the thermal positron, $\lambda_T=\hbar(2mT)^{-1/2}$, to the free path length,

$$\xi=\lambda_T[4\pi L^2(N)S(0)N]. \qquad (15)$$

It has to be small. In this case, accurate values of μ are given by[24]

$$\mu=\mu_0(1-\pi^{1/2}\xi). \qquad (16)$$

However, if the parameter ξ becomes comparable to unity, the kinetic theory cannot be applied. A light quantum particle interacts with a number of atoms at every moment.

In such a regime, the mobility can be estimated by the Ioffe-Regel formula.[25] The mean free path of a quantum particle cannot be shorter than the wavelength λ_T. Hence λ_T should be inserted in Eq. (14) instead of the kinetic mean free path l. This results in

$$\mu\approx\tfrac{2}{3}(2e^2/\pi mT)^{1/2}(\hbar/\sqrt{2mT}). \qquad (17)$$

The calculated mobility of positron in liquid argon is presented in Fig. 8. The mobility is compared with the electron mobility.[26] Near the triple point the electron mobility decreases with decreasing density because of the growth of the liquid compressibility, which is proportional to $S(0)$. However, at smaller densities the density dependence of the scattering length becomes the strongest in Eq. (14). The scattering length decreases and even passes through zero at $N^*=1.2\times10^{22}$ cm^{-3} (Fig. 1). Therefore the mobility increases with decreasing density until the density N^*, where it passes through a maximum.

The magnitude of the positron scattering length grows monotonically with decreasing density. This leads to the decrease of the mobility. Moreover, due to the large magnitude of $L(N)$ the scattering becomes nonbinary, and the correction factor $(1-\pi^{1/2}\xi)$ decreases. Finally, near the density $N\approx1.7\times10^{22}$ cm^{-3} the mobility mechanism changes. At

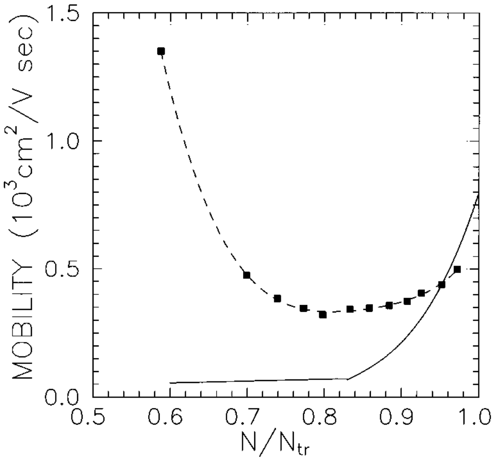

FIG. 8. Mobilities of thermal positron and electron on the Ar isobar 5.5 MPa. Positron [Eqs. (14) and (17)]: solid line; electron (Ref. 26): squares and dotted line.

lower densities the mobility magnitude corresponds to that low level which is estimated by the Ioffe-Regel formula (17).

VI. DISCUSSION

The range of validity of the pseudopotential theory is determined by some requirements. The theory does not use an explicit form of the short-range component of the positron-atom potential. Only the phase shifts of the partial waves scattered from the pseudopotential core are necessary. In dense media these phase shifts are the same as the ones in dilute gases. But then the theory does not describe the behavior of positrons inside the volume occupied by the pseudopotential core, $(4\pi/3)r_0^3$. The space of the pseudopotential core must be smaller than the unit cell volume, $r_0^3 \ll \overline{r^3}$. Additionally, one must require the validity of another inequality, $|L(N)|^3 \ll \overline{r^3}$. On the contrary, it would not be possible to use the approach of the potential of zero radius in the Wigner-Seitz cell.

These inequalities are violated as the density decreases toward a dense gas. Moreover, at these densities the cellular model of liquids fails. Fortunately, the pseudopotential theory reproduces the results of the gaseous approach in the limit of very small densities. Hence, in the intermediate range of densities, the theory provides a reasonable interpolation, but does not pretend to an accurate description.

The theory is suitably applied to neon and argon liquids. At the triple point of argon $r_0^3/\overline{r^3}=0.068$ and $|L|^3/\overline{r^3}=0.068$.

The theory used in the present paper assumes smallness of the calculated phase shifts. This hinders the application of the theory to the heavier noble liquids, especially to xenon. Due to the high atomic polarizability the scattering length from an isolated xenon atom is the maximal one, $L_0 \approx -7.5a_0$ (Ref. 3). As a result, the scattering lengths in liquid xenon are comparable to $\overline{r}$. However, with further increase of density the polarization attraction is weakened so much that near the triple point the magnitude of $L(N)$ becomes small. Finally, at the triple point the scattering length is positive, $L(N_{\rm tr}) \cong 0.16a_0$. Let us use it to calculate an annihilation rate λ_1 of thermal positrons at the triple point of xenon.

The annihilation rate is given by

$$\lambda_1 = \pi(e^2/mc)^2 cNZ_{\rm eff}, \quad Z_{\rm eff} = 4\pi \int_0^{\overline{r}} \rho_a(r)\psi(r)^2 r^2 dr, \tag{18}$$

where c is the light velocity, $Z_{\rm eff}$ is the effective charge of the atom in a liquid,[3] $\rho_a(r)$ is the density distribution of atomic electrons, and $\psi(r)$ is the wave function of the positron in the Wigner-Seitz cell.

$$\psi(r) = A(k_0 r)^{-1} \sin[k_0(r-L)], \quad \tan[k_0(\overline{r}-L)] = k_0\overline{r}.$$

The measured magnitudes of $Z_{\rm eff}$ in Xe are given in Ref. 27. Being as high as 300 at low densities, the value of $Z_{\rm eff}$ becomes equal to 13 at the triple point. This reinforces the statement that the effects of the polarization attraction are almost nullified near the triple point. To calculate the effective charge, suppose for simplicity that

$$\rho_a(r) = Z(4\pi r_a^3/3)^{-1}\theta(r-r_a), \quad r_a = 1.33Z^{-1/3}, \tag{19}$$

where Z is the nuclear charge and r_a is the Thomas-Fermi radius of atom. A straightforward integration[28] yields

$$Z_{\rm eff} = Z\xi(r_a)/\xi(\overline{r}), \tag{20}$$

$$\xi(y) = y^{-2}(1-L/y)\{1-[2k_0(y-L)]^{-1} \sin[2k_0(y-L)]\}.$$

Equation (20) is valid in the density range where the self-trapping of positrons in clusters is strongly hindered. It is related undoubtedly to the vicinity of the triple point. The calculated $Z_{\rm eff}=16$ compares well to the measured value $Z_{\rm eff}=13$.

The scattering length determines the state of a light quantum particle at thermal energies. At elevated energies a set of phase shifts of l waves becomes necessary to calculate the positron scattering cross section. However, for a short-range potential $\delta_l \sim (k^2)^l$, and the higher partial waves become important one after another with increase in energy. In liquid neon and argon up to the energy $\epsilon \cong 0.7$ eV it is sufficient to take into account the phase shifts of s and p waves. The phase shift of the d wave can be reasonably estimated using the cutoff polarization potential, $\delta_2 = \alpha k^5 \overline{r^3}/675a_0$. Accounting for it results in a small correction only.

The contrast between the electron and positron states in liquid argon is remarkable. The scattering length of positrons is negative for the whole density range. The electron scattering length at the triple point is positive. Hence at the triple point the Ramsauer minimum in the scattering cross section exists for positrons, but not for electrons.

The positron mobility can be calculated using the effective cross sections. The mobility of a slow free positron in argon is shown in Fig. 8. Being enhanced at the triple point, the mobility decreases with decreasing density. This may be considered as a precursor of the self-trapping of slow positrons in dense gases.[3]

Positron motion in an electric field is studied by investigating the drift of injected positrons to a surface; see Refs. 1 and 2. During the positron lifetime $\tau \cong 10^{-9}$ s the drift length is of the order of 1 μm. There are several methods to obtain the positron mobility from measured data, and we hope that our prediction induces experimentalists to make measurements in noble liquids.

As we can see in Fig. 6, the ground-state energy V_0 (relative to the vacuum) is negative. But, in contrast to the case of an excess electron, the ground-state energy of the positron decreases monotonically with increasing N. The calculated V_0 agrees satisfactorily with the calculated results of Ref. 13. At the densities of solids the calculated V_0 compare well to the measured data.

In media with a strong interparticle interaction the structure of the energy spectrum is influenced very weakly by thermal effects. Temperature dependences would be displayed due to the temperature dependence of the liquid structure. In our theory the peculiarities of structure should be represented by the integral factors I_0, I_2, and I_4.[8] However, the factors are almost insensitive to temperature variation in the whole range of liquid states. As to the temperature dependence of the mobility, it is considerable due to the presence of the liquid structure factor in Eq. (14).

In Ref. 11 we discussed the problem of fluctuations of the potential field due to density fluctuations, which our mean-field theory does not take into account. They should be important if the mean values of the scattering length are small and the corresponding densities are not too high. As in the case of electrons, the positron behavior in xenon is sensitive to fluctuations. In liquid xenon the scattering length passes through zero. Also, the scattering length magnitude becomes small in neon near the triple point. A theoretical approach that properly accounts for the fluctuations is based on the Feynman path-integral approach, which is employed in Refs. 29–31 for studying excess electrons and adopted to positrons in Ref. 32. In principle, the path-integral approach with Monte Carlo or molecular dynamic calculations can yield results with high precision which take account of the inherent disorder of liquids. We hope that our results will induce further calculations in this manner.

The reduced effective masses, presented in Fig. 7, exceed unity, as must be in the case of prevalence of the attraction in the particle-medium interaction.[11] Such behavior follows from the Bardeen formula, which is definitely valid for the description of an almost free quantum particle in a cellular medium. We can use the calculated m_{eff} to estimate the binding energy of positronium in solid argon. The binding energy is described by the hydrogenlike formula for the Wannier exciton[33]

$$E_B = \frac{\text{Ry}}{\epsilon^2}\frac{m^*}{m}, \quad m^* = \frac{m_{\text{eff}} m_{\text{eff}}^{-}}{m_{\text{eff}} + m_{\text{eff}}^{-}}, \tag{21}$$

where m^* is the reduced mass equal to the positronium effective mass, m_{eff} and m_{eff}^{-} are the effective masses of the positron and electron, and ϵ is the dielectric constant of the medium. In solid argon $\epsilon^{-2} = 0.36$. Using the measured value $\overline{m}_{\text{eff}} = 0.53$ (Ref. 21) and the calculated $m_{\text{eff}} = 1.3$, we obtain $E_B = 1.85$ eV. The comparison with the experimental[22] $E_B = 2.5$ eV should be considered as satisfactory. It should be noted that the approach of the continuous medium can be applied here under some stipulations. The positronium wave function is not spread so much as to cover a large number of atoms of the medium.

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