Levinson's theorem and a bound state of a positron in electron gas

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Abstract

Positrons embedded in metals annihilate predominantly with conduction electrons. The annihilation rate reduces with decreasing density for the whole range of metallic densities. Controversial suggestions have been made on the annihilation rates at very low electron gas densities. We calculate the effective screened interaction between the positron impurity and electrons within a simplified jellium model where the electrons are treated as bosonic particles and show that the electrons attracted to the positron can form a bound cluster. The resonance states of the effective interaction are analyzed by calculating the scattering phase-shifts. We find that the maximum of the phase-shift at zero energy approaches to π when $r_s \approx 14$. According to the Levinson's theorem this indicates a bound state.

Key words: positron impurity; Levinson's theorem; bound state; Jastrow theory

1. Introduction

The positron annihilation into metals and semiconductors has been studied a long period of time. Microscopic many-body theories[1–3] give reasonable results in metallic densities where the usual electron gas density parameter $2 < r_s < 6$. At lower densities, however, these methods fail to converge because the electron density at the positron position becomes very large. Only the zero density limit where the positronium ion (p^-) is formed can be treated with confidence. In this work we study the possibility of a bound state at finite densities when $r_s > 10$ by calculating the effective screened positron-electron interaction. Our method is based on the microscopic variational approach with the Jastrow wave function, which is well described in the literature[4,5]. From the Levinson's theorem[6] we know that if the s-wave phase shift at zero energy is π, then the potential has a bound state whereas in the case of no bound states it goes linearly to zero in the long wavelength limit.

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2. Results

Our variational method consists of a positron impurity embedded in the electron gas and the ionic background is taken into account within the jellium model. We minimize the chemical potential of the impurity with respect to the radial distribution function $g^I(r)$, which describes the distribution of electrons around the positron. The whole system is neutralized by the jellium charge. We want to isolate the screening of the charge from the fermionic effects and that is why we treat electrons as bosons. As a result we get the Euler equation for $g^I(r)$,

$$-\frac{\hbar^2}{2m_{\rm red}}\nabla^2\sqrt{g^I(r)} + V_{\rm eff}(r)\sqrt{g^I(r)} = 0 \qquad (1)$$

where $m_{\rm red} = m_e m_p/(m_e + m_p)$ is the reduced mass with electron and positron masses and $V_{\rm eff}(r) = -e^2/r + w_{\rm ind}(r)$ is the effective interaction. The first term in it is the attractive Coulomb interaction and the second term the interaction induced by the many-body effects. In the HNC-approximation the Fourier transform of $w_{\rm ind}(r)$ can be written in the form

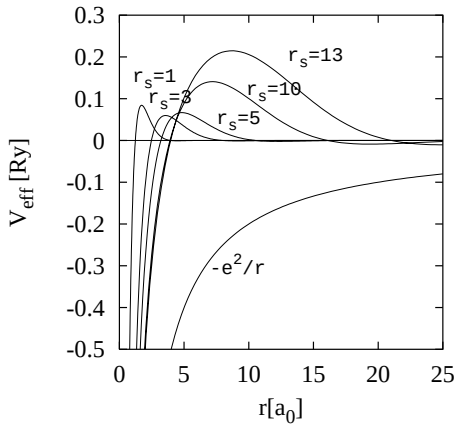

Fig. 1. The effective positron-electron potential for the r_S-values indicated in the figure. For comparison we show the bare Coulomb potential (lowest line).

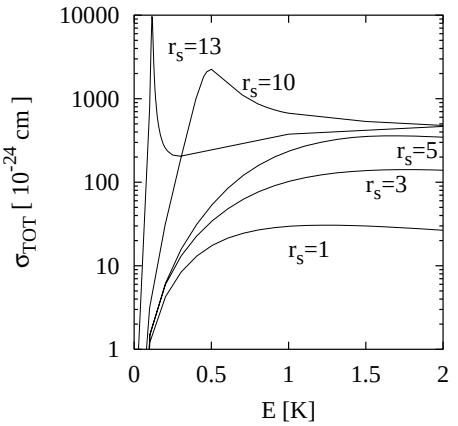

Fig. 2. The total cross section of the s-wave scattering for the same r_s-values as in Fig. 1. All curves go to zero at $E = 0$.

$$\tilde{w}^I_{\rm ind}(k) = -\frac{\hbar^2 k^2}{4m_e}\frac{S^I(k)(S(k)-1)}{S(k)}\left[1+\frac{m_e}{m_p}+\frac{1}{S(k)}\right].$$

The static structure function $S^I(k)$ is the Fourier transform of $g^I(r) - 1$ and $S(k)$ is the structure function of the electron gas. Eq. (1) satisfies the perfect screening condition, which requires that $S^I(0) = 1$. The Euler equation (1) is a non-linear differential equation and is solved iteratively with the boundary condition $g^I(\infty) = 1$. After the convergence is reached the solution determines both $g^I(r)$ and $V_{\rm eff}(r)$. The radial distribution function is strongly peaked around the impurity and the height of the peak at $r = 0$ can be measured by the positron annihilation rate measurements.

Our main interest in this work is in the effective interaction $V_{\rm eff}(r)$. Its behaviour for several r_s values is shown in Fig. 1. It is a short-ranged function, because of the perfect screening condition, additionally the many-body effects over-screen the Coulomb attraction creating a barrier at distances where electrons cluster. These potentials can not have bound states because of the fixed boundary conditions. Yet, we can calculate s-wave scattering and within that approximation the total cross section. As shown the attraction of the potential at short distances increases with decreasing density and due to the potential barrier a resonance state is formed. The energy of the resonance state approaches to zero as shown in Fig. 2 where we plot the total cross section for several r_s-values in the logarithmic scale. The approaching bound state can also be seen from the maximum of the s-wave scattering phase shifts shown in Fig. 3. According to Levinson's theorem if the phase shift of the resonance state in the zero energy limit is equal to π then the system has one bound state. The exact r_s-value where the bound state is formed is difficult to reach because of the iteration procedure is allowed to converge only for non-bound

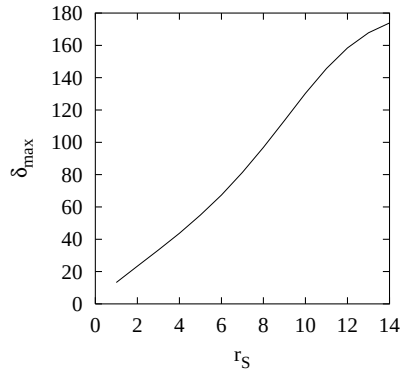

Fig. 3. The maximum of the s-wave phase shift.

systems and that is why the phase shift is bending near the critical value.

Acknowledgements

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