Self-energy of a positronium atom near a metal surface

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The attractive interaction energy between a positronium atom and a metal surface has been numerically evaluated using our earlier-derived expression. In this derivation the interaction energy is obtained by considering the multipolar excitations of the positronium atom and excitations of the surface plasmons. It is shown that the interaction energy saturates to a constant value at the surface, and near the surface the interaction energy is considerably weaker than that given by the well-known semiclassical Lifshitz result.

The interaction energy between a metal surface and a positronium atom, which we assume to be on the vacuum side of the surface, is well known to be due to the induced excitations of the positronium atom and the surface plasmons of the metal electrons. The energy, which is known as the van der Waals interaction energy, has been studied extensively using semiclassical models[1,2] and more recently within a quantum framework.[3–5] For a sufficiently large distance z between the positronium atom and the metal surface, Lifshitz,[6] using a semiclassical approach, showed that the interaction energy varies as $1/z^3$. But close to the surface the quantum nature of the positronium atom becomes important as is demonstrated by Manson and Ritchie[3] and by Paranjape and Pathak.[4,5] The quantum effect weakens the interaction energy from its Lifshitz value. Using the dipolar approximation (i.e., restricting to the dipolar excitations of the positronium atom), Manson and Ritchie[3] showed that near the surface the interaction energy varies as $1/z$. However, Paranjape and Pathak[4,5] demonstrated that in addition to the dipolar excitations, the higher-order multipolar excitations of the positronium atom are important near the surface. These authors extended the calculation of Manson and Ritchie[3] to include these higher-order excitations of the positronium atom to show that the interaction energy instead of diverging at the surface, as shown by the earlier authors, in fact converges to a constant value. Paranjape and Pathak,[4] however, did not provide the numerical estimates of the interaction energy at or near the surface due to computational difficulties of evaluating a seven-dimensional integral and an infinite sum over the multipolar excitations of the positronium atom. These difficulties have now been overcome, and it is the purpose of this report to give quantitative values for the interaction energy using the analytical results given in our earlier publication.

In the following we give the essential results from our earlier paper[4] for the sake of completeness, while the details of calculation can be found in this publication. The numerical values for the interaction energy as a function of the separation between the positronium atom and the metal surface are presented. In conclusion, we give a short discussion of our numerical estimates of the interaction energy and compare these estimates with the works of Manson and Ritchie[3] and of Lifshitz.[6]

The interaction energy $E(\mathbf{r})$ of a positronium atom at $\mathbf{r}$ due to the metal surface is derived by Manson and Ritchie[3] using the self-energy analysis. The analysis, based upon the second-order perturbation theory, gives the interaction energy $E(\mathbf{r})$ as

$$E(\mathbf{r})=\sum_{n,l,\mathbf{k}}\frac{1}{8\pi^3}\exp[-i\mathbf{r}\cdot(\mathbf{k}_0+\mathbf{k})] \times\frac{\langle\phi_0,0,0\,|\,H'\,|\,n,l,\phi_k\rangle\langle l,n\,|\,H'\,|\,0,0\rangle}{E_0-E_n+e_0-e_k-\varepsilon_l+i\delta}\,, \tag{1}$$

where the interaction Hamiltonian of the positronium atom interacting with the metal surface (surface plasmons) is given by

$$H'=\sum_{\mathbf{Q}}\Gamma_{\mathbf{Q}}[\exp(-Q\,|\,Z_+\,|\,+i\mathbf{Q}\cdot\mathbf{R}_+) -\exp(-Q\,|\,Z_-\,|\,+i\mathbf{Q}\cdot\mathbf{R}_-)](a_{\mathbf{Q}}+a^{\dagger}_{-\mathbf{Q}})\,. \tag{2}$$

In Eqs. (1) and (2) the state associated with the center of mass of the positronium atom is denoted by a plane-wave state $|\phi_K\rangle=(2\pi)^{-3/2}\exp(i\mathbf{k}\cdot\mathbf{r})$ with the associated energy $e_k=\hbar^2k^2/2m$, $|n\rangle$ is the quantum state of the surface plasmons with energy $E_n=\hbar\omega_Q(n+1/2)$, a_Q and $a_Q^{\dagger}$ are, respectively, the destruction and creation operators for the surface plasmons with wave vector $\mathbf{Q}$ assumed to be parallel to the surface, $|l\rangle$ represents the internal state of the positronium atom having the energy $(\varepsilon_0+\varepsilon_l)$. The unperturbed state of the positronium atom is assumed to be at the ground state for the internal coordinates, but the state of the center-of-mass motion of the positronium atom is assumed to be the plane-wave state represented

by $\phi_0=(2\pi)^{-3/2}\exp(-i\mathbf{k}_0\cdot\mathbf{r})$, where the wave vector $\mathbf{k}_0$ is taken to be normal to the surface so that in cylindrical coordinate system $\mathbf{k}_0\equiv(0,k_0)$. The intermediate states for the center-of-mass motion are represented by the wave vector $\mathbf{k}\equiv(\kappa,k_3)$. The coordinates of the center of mass of the positronium atom are deduced by $(\mathbf{R},Z)$ in cylindrical coordinates with Z measured positively away from the surface on the vacuum side. The relative coordinates of the positronium atom are given by $(\mathbf{R}',Z')$ so that the positional coordinates for the positron and the electron are given by $\mathbf{R}_+=\mathbf{R}\pm(\mathbf{R}'/2)$ and $Z_\pm=Z\pm(Z'/2)$. The coupling constant is defined by $\Gamma_Q=e^2\pi\hbar\omega_Q/L^2Q$, where e is the charge of the electron and L is the periodic length parallel to the surface.

In Eq. (1) the summations over $\mathbf{k}$ and n and the integral over the angle made by the vector $\mathbf{Q}$ with respect to an arbitrary vector parallel to the surface, are accomplished as was shown in our earlier publication,[4] to give

$$
\begin{aligned}
E(z)=\frac{-Q_s^2e^2}{2}\sum_l\int dQ\int d\mathbf{r}'\int d\mathbf{r}''\psi_0^*(\mathbf{r}')\psi_l(\mathbf{r}')\psi_0(\mathbf{r}'')\psi_l^*(\mathbf{r}'')
&\times\left[J_0\left[\frac{Q}{2}\,|\,\mathbf{R}'-\mathbf{R}''\,|\,\right]\right.\\
&\times\left\{\exp(-Q\,|\,z''_+\,|\,)\left[\exp(-Q\,|\,z'_+\,|\,)\left[\frac{\Theta(z'_+)}{D_1}+\frac{\Theta(-z'_+)}{D_1^*}\right]\right.\right.\\
&\qquad+\frac{Q}{\alpha}\exp(-\alpha\,|\,z'_+\,|\,)\\
&\qquad\left.\left.\times\left[\frac{\Theta(z'_+)\exp(-ik_0\,|\,z'_+\,|\,)}{D_2}+\frac{\Theta(-z'_+)\exp(ik_0\,|\,z'_+\,|\,)}{D_2^*}\right]\right]\\
&\quad+\exp(-Q\,|\,z''_-\,|\,)\left[\exp(-Q\,|\,z'_-\,|\,)\left[\frac{\Theta(z'_-)}{D_1}+\frac{\Theta(-z'_-)}{D_1^*}\right]\right.\\
&\qquad+\frac{Q}{\alpha}\exp(-\alpha\,|\,z'_-\,|\,)\\
&\qquad\left.\left.\left.\times\left[\frac{\Theta(z'_-)\exp(-ik_0\,|\,z'_-\,|\,)}{D_2}+\frac{\Theta(-z'_-)\exp(ik_0\,|\,z'_-\,|\,)}{D_2^*}\right]\right]\right\}\\
&-J_0\left[\frac{Q}{2}\,|\,\mathbf{R}'+\mathbf{R}''\,|\,\right]\\
&\times\left\{\exp(-Q\,|\,z''_-\,|\,)\left[\exp(-Q\,|\,z'_+\,|\,)\left[\frac{\Theta(z'_+)}{D_1}+\frac{\Theta(-z'_+)}{D_1^*}\right]\right.\right.\\
&\qquad+\frac{Q}{\alpha}\exp(-\alpha\,|\,z'_+\,|\,)\\
&\qquad\left.\left.\times\left[\frac{\Theta(z'_+)\exp(-ik_0\,|\,z'_+\,|\,)}{D_2}+\frac{\Theta(-z'_+)\exp(ik_0\,|\,z'_+\,|\,)}{D_2^*}\right]\right]\\
&\quad+\exp(-Q\,|\,z''_+\,|\,)\left[\exp(-Q\,|\,z'_-\,|\,)\left[\frac{\Theta(z'_-)}{D_1}+\frac{\Theta(-z'_-)}{D_1^*}\right]\right.\\
&\qquad+\frac{Q}{\alpha}\exp(-\alpha\,|\,z'_-\,|\,)\left[\frac{\Theta(z'_-)\exp(-ik_0\,|\,z'_-\,|\,)}{D_2}\right.\\
&\qquad\left.\left.\left.\left.+\frac{\Theta(-z'_-)\exp(ik_0\,|\,z'_-\,|\,)}{D_2^*}\right]\right]\right\}\right],
\end{aligned}
\tag{3}
$$

where $\Theta(x)=1$ for $x>0$ and zero otherwise, J_0 is the Bessel function of the first kind, ψ_l is the lth excited state, $\psi_0(r)$ is the unperturbed ground state of the positronium atom,

$$D_1=[\alpha^2+(k_0+iQ)^2],\quad D_2=[Q^2+(k_0-i\alpha)^2]\ ,$$
$$Q_s^2=(2\omega M/\hbar),\quad Q_1^2=(2M\varepsilon_1/\hbar^2)\ ,$$
$$\alpha^2=Q_s^2+Q_1^2+Q^2-k_0^2,\quad Z'_{\pm}=[Z\pm(Z'/2)],\quad Z''_{\pm}=[Z\pm(Z''/2)]\ .$$

The integrations and summation in Eq. (3) are evaluated numerically using the hydrogenlike wave functions, appropriately modified to represent the wave functions of the positronium atom. All the degenerate states corresponding to the first four excited states of the positronium atom are included in the summation over l. The sum is sufficiently convergent so that there was no need to go beyond the states $l>4$. The seven-dimensional integral in Eq. (3) was evaluated by the application of the Monte Carlo technique using 10000 sampling points. The Monte Carlo technique was tested on a similar problem[7] in which we evaluated the interaction energy of the electrons in the helium atom. In this test problem, a six-dimensional integral similar to the one occuring in Eq. (3) is evaluated. Since the exact value of the six-dimensional integral in the test problem is known, it is possible to estimate the reliability of the Monte Carlo method by comparing the computational result with the exact result. The comparison allowed us to achieve an accuracy of 3% or better in the numerical evaluation of the interaction energy $E(Z)$, given by Eq. (3). The result is depicted in Fig. 1 which gives the variation $E(Z)$ with separation Z for two speeds of the positronium atom and for an aluminium surface. The corresponding Lifshitz's results which are independent of the speed of the positronium atom, are also drawn comparison.

The results given by the figure allow us to draw the following conclusions. Firstly we observe that the variation of the potential energy $E(Z)$, over the size (~ 1 Å) of the positronium atom, is small compared with the binding energy of the positronium atom. Hence, the distortion produced by the interaction potential in the unperturbed hydrogenic ground-state wave function of the positronium atom is expected to be small. The use of the perturbation theory is therefore justified. Secondly we see from the figure that $E(Z)$ saturates to a constant value at the surface. The saturation is a consequence of our consideration of the multipolar excitations of the positronium atom. As we remarked earlier, the restricted consideration of only the dipolar excitations led to a divergent value for the interaction energy as was shown in the work of Manson and Ritchie.[3] Finally we note that, in this paper, we have considered the interaction energy between the positronium atom and the surface modes of the metal electrons (surface plasmons), but we have neglected the interaction of the positronium atom with the bulk electrons (bulk plasmons). The later interaction is important near the surface when the positronium wave function significantly overlaps the bulk electrons. For Z less than the effective Bohr radius a_0, such an overlap is indeed large. Therefore, our theory (and also the theory of Manson and Ritchie) is inadequate to give reliable values for the potential energy of the positronium atom at these small distances.

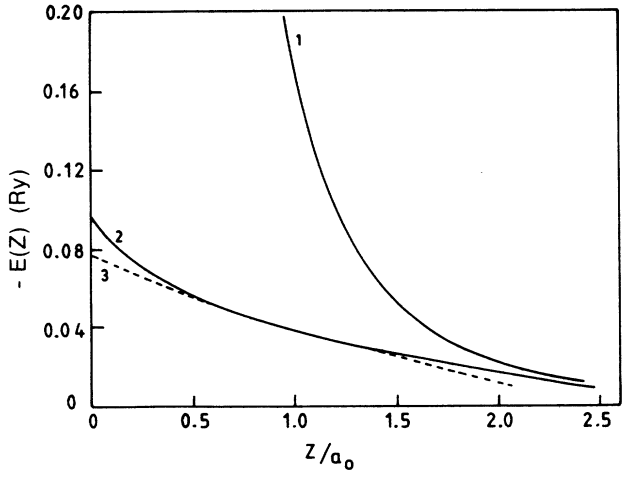

FIG. 1. The variation of $E(Z)$ with Z. Curve 1 gives the Lifshitz result. Curves 2 and 3 show the results of our calculation for a positronium with zero energy and with energy 4 eV, respectively.

For values of $Z>a_0$, the results obtained by us are expected to be reasonably accurate since the interaction of the positronium atom with the bulk electrons is small. Furthermore, our consideration of the multipolar excitations of the positronium atom should give more accurate values of $E(Z)$ than the values obtained, under restrictive conditions, by Manson and Ritchie.[4] The ratio of the interaction energy $E(Z)$ as given by Eq. (3) to the value given by the Lifshitz's result is different from unity for $Z>a_0$ and is significantly smaller than the corresponding ratio obtained by Manson and Ritchie.[3] For example, at $Z=2a_0$ the ratio obtained in this report is close to 0.6 while the same result for the calculation of Manson and Ritchie[3] is close to 0.94 if the positronium atom is considered to be at 4 eV. Our results also show that the potential energy experienced by the positronium atom is weaker as its speed is increased. This is evident from our figure where we have shown $E(Z)$ for 4-eV and zero-energy positronium atoms.

For values of $Z<a_0$, the potential energy $E(Z)$ is strongly influenced by the interaction between the positronium atom and the electrons of the bulk metal. The overlap of the positronium atom wave function with the electrons of the bulk metal is large, and consequently the use of hydrogenic wave function for the positronium atom is also not justified at these distances. Unfortunately, we are unable to make a quantitative estimate of this interaction since our Hamitonian [Eq. (2)] excludes the interaction. The effect on $E(Z)$ of the interaction between the positronium atom and the metal electrons has been analyzed recently in some detail by Platzman and

Tzoar[8] and by Takada and Kohn.[9] These authors show that near the surface a strong repulsion occurs between the positronium atom and those electrons of the metal having the same spin as the spin of the electron forming the positronium. The results obtained by these authors and the results obtained in this publication together should provide a reasonably accurate variation of $E(Z)$ for all positive values of Z.

The results obtained in this report are of some relevance to the experimental work of Lynn and Welch[10] who demonstrated the production of thermal energy positronium atoms as a result of the interaction between a low-energy positron and a metal surface.

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