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# New approach to electron–positron interaction in jellium

By H. Stachowiak

Institute for Low Temperature and Structure Research, Polish Academy of Sciences, 50–950 Wrocław, P. O. Box 937, Poland.

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*In honor of Martin Peter's 60th birthday.*

*Abstract.* A new formalism is proposed for the description of positron behaviour in jellium. It is shown how to cope with the non-orthogonality of the wave functions overlooked in the Kahana approach and poorly accounted for by Lowy and Jackson, including at the same time the positron recoil neglected by these last authors. Also a form of the Pauli exclusion principle is proposed which is free of the inaccuracies occuring in the Kahana formalism. It is shown that within this scheme its application has no influence on the screening cloud distribution, unlike in the above mentioned approaches.

## 1. Introduction

In order to study experimentally the electronic structure of metallic materials by positron annihilation a reliable information about the effect of $e^+ - e^-$ interaction (EPI) is needed. Before entering into details let us refer to the article of Arponen and Pajanne [1] (cf. also [2]) where a review of theories treating this problem is presented.

Successive elaboration of spectrometers for two-dimensional correlation of annihilation photons in the S. Berko group at Brandeis, the M. Peter group in Geneva and the R. N. West group in Norwich provided the possibility to study EPI in more detail. Comparison of theoretical and experimental results for EPI [3, 4] shows marked discrepancies, though theoretical approaches basing on the formalism proposed first by Kahana [5] seem to give the best agreement with experiment. Among the most significant measurements let us mention the Kingston and Geneva experiments for alkalis [6 to 8], the Brandeis studies of copper [9] and the results from Norwich for zinc [10, 11].

This shows that the theory of EPI needs further studies. In this article, using the results of the theory of liquids [12, 13], we will comment on the competing approaches of Kahana on one side and Lowy and Jackson on the other [14 to 16], proposing a new formalism going beyond the approximations forming the basis of these theories. Some preliminary applications of this formalism will be presented.

## 2. Basic assumptions

Following the results of the theory of liquids [12, 13] Gondzik and Stachowiak [17] assumed the wave function of the one positron-many electrons system in the form

$$\Psi_L(\mathbf{r}_p, \mathbf{r}_1 \ldots \mathbf{r}_N) = \prod_{i=1}^{N} w(|\mathbf{r}_i - \mathbf{r}_p|) \prod_{i \neq j}^{N} f(|\mathbf{r}_i - \mathbf{r}_j|)\Phi(\mathbf{r}_1 \ldots \mathbf{r}_N) \tag{1}$$

where $\Phi$ is the Slater determinant for free electrons, $r_p$ denotes positron coordinates. Note that the theory of liquids distinguishes between the trial function $w(r)$ used in equation (1) and the square root of the electron density distribution.

This formalism can be generalized by assuming the wave function $\Psi$ of the system in the form of a Slater determinant built out of functions

$$\psi_{\mathbf{k}}(\mathbf{r}_e, \mathbf{r}_p) = w(|\mathbf{r}_e - \mathbf{r}_p|)\varphi_{\mathbf{k}}(\mathbf{r}_e, \mathbf{r}_p). \tag{2}$$

If $w(r)$ in (2) is assumed constant we get back to the formalism of both Kahana and Lowy and Jackson (cf. [18]).

Let us remark that the Jastrow type trial function (1) has been pretty successful in describing the screening of the positron in an electron gas. This is an argument for applying perturbation theory and assuming that the $\varphi_k$ function in (2) differs little from a plane wave:

$$\varphi_{\mathbf{k}}(\mathbf{r}_e, \mathbf{r}_p) = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k}\mathbf{r}_e} + v_{\mathbf{k}}(\mathbf{r}_e, \mathbf{r}_p), \tag{3}$$

where $\Omega$ is the volume of the sample. Terms of higher order in $v_k$ will be consequently neglected. This is the advantage of the present formalism over the approaches of Kahana and Lowy and Jackson which use higher orders of perturbation theory.

The function of equation (2) obeys generally the equation

$$\left[-\frac{1}{2}\nabla_e^2 - \frac{1}{2}\nabla_p^2 + V(|\mathbf{r}_e - \mathbf{r}_p|)\right]\psi_{\mathbf{k}} = \frac{k^2}{2}\psi_{\mathbf{k}} \tag{4}$$

while $w(r)$ can be assumed in different ways. E.g. we can make it satisfy the equation for $[\rho(|\mathbf{r}_e - \mathbf{r}_p|)]^{1/2}$ from Ref. [17]. Let is satisfy the equation

$$[-\nabla^2 + V_0(s)]w(s) = 0. \tag{5}$$

We assume that

$$v(s) = V(s) - V_0(s) \tag{6}$$

is small and terms involving it in higher order can be dropped.

Introducing (2) into (4) we get the equation for $v_k$ in the form

$$\left[-\frac{1}{2}\nabla_e^2 - \frac{1}{2}\nabla_p^2 - \frac{k^2}{2}\right]v_{\mathbf{k}} = \frac{w'}{w}\frac{\vec{s}}{s\sqrt{\Omega}} ike^{i\mathbf{k}\mathbf{r}_e} - \frac{1}{\sqrt{\Omega}} v(s)e^{i\mathbf{k}\mathbf{r}_e}. \tag{7}$$

The wave function $\Psi$ of the system can be simplified if one switches to the variables (cf. [18, 19])

$$\mathbf{s} = \mathbf{r}_e - \mathbf{r}_p, \qquad \mathbf{s}_i = \mathbf{r}_i - \mathbf{r}_p. \tag{8}$$

Then the wave function of the system $\Psi(s_1 \ldots s_N)$ is built out of the functions

$$\psi_{\mathbf{k}}(\mathbf{s}) = w(s)\left[\frac{1}{\sqrt{\Omega}} e^{i\mathbf{k}\mathbf{s}} + v_{\mathbf{k}}(\mathbf{s})\right]. \tag{9}$$

Equation (7) can be solved in Born approximation (cf. [20]) yielding

$$v_{\mathbf{k}}(\mathbf{s}) = \frac{1}{\Omega^{3/2}} \sum_{\mathbf{q}} \frac{\Phi_1(q) k \cos\Theta + \Phi_2(q)}{(\mathbf{k}+\mathbf{q})^2/2 + q^2/2 - k^2/2} e^{i(\mathbf{k}+\mathbf{q})\mathbf{s}} \tag{10}$$

where

$$\Phi_1(q) = \frac{4\pi}{q^2} \int_0^\infty ds \frac{d}{ds} (\ln w(s))[\sin qs - qs \cos qs], \tag{11}$$

$$\Phi_2(q) = -\frac{4\pi}{q} \int_0^\infty ds\, sv(s) \sin qs. \tag{12}$$

$\Theta$ is the angle between $\mathbf{k}$ and $\mathbf{q}$.
The wave function of the system can now be written in the form

$$\psi(\mathbf{s}_1 \ldots \mathbf{s}_N) = \prod_{i=1}^{N} w(s_i)\Phi' \tag{13}$$

where $\Phi'$ is a Slater determinant built out of functions

$$\varphi_{\mathbf{k}}(\mathbf{s}) = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k}\mathbf{s}} + v_{\mathbf{k}}(\mathbf{s}) \tag{14}$$

## 3. Electron density distribution and Pauli exclusion principle

In the approximation used in this paper one can replace $v_k(s)$ by $\bar{v}_k(s)$:

$$\bar{v}_{\mathbf{k}}(\mathbf{s}) = \frac{1}{\Omega^{3/2}} \sum_{\substack{\mathbf{q} \\ |\mathbf{k}+\mathbf{q}|>k_F}} \frac{\Phi_1(q) k \cos\Theta + \Phi_2(q)}{(\mathbf{k}+\mathbf{q})^2/2 + q^2/2 - k^2/2} e^{i(\mathbf{k}+\mathbf{q})\mathbf{s}} \tag{15}$$

since this leads to omitting in $\Psi$ terms quadratic in the perturbation (cf. [18]). In the case of constant $w(s)$ (15) corresponds to applying the Pauli exclusion principle. Unlike in the case of a proton the functions $\psi_k$ of equation (9) are not orthogonal, no matter whether we insert in (9) $\bar{v}_k$ from equation (15) or $v_k$ from equation (10) (this last because of positron recoil, cf. [14] and [18]). For a proton applying the form $\bar{v}_k$ given by equation (15) destroys the orthogonality of the $\psi_k$ functions. However in the present formalism, unlike in previous approaches, we can operate relatively easily with nonorthogonal $\psi_k$ functions. Indeed, applying

the formula for the electron density distribution

$$\rho(s_1) = N \frac{\int |\Psi|^2 \, d\tau_1}{\int |\Psi|^2 \, d\tau} \quad \text{where} \quad d\tau = \prod_{i=1}^{N} d\mathbf{s}_i, \qquad d\tau_1 = \frac{d\tau}{d\mathbf{s}_1} \tag{16}$$

one gets

$$\rho(s) = 2 \sum_{|k|<k_F} \psi_{\mathbf{k}}^*(\mathbf{s}) \psi_{\mathbf{k}}(\mathbf{s}) - 2 \sum_{\substack{\mathbf{k} \neq \mathbf{k}' \\ \text{occ}}} A_{\mathbf{k}'\mathbf{k}} \psi_{\mathbf{k}'}^*(\mathbf{s}) \psi_{\mathbf{k}}(\mathbf{s}) \tag{17}$$

where

$$A_{\mathbf{k}'\mathbf{k}} = \int d\mathbf{s}' \psi_{\mathbf{k}}^*(\mathbf{s}') \psi_{\mathbf{k}'}(\mathbf{s}') \tag{18}$$

if only terms linear in the non-orthogonality of the $\psi_{\mathbf{k}}$ functions are kept.

The formula (17) is derived in the following way: $|\Psi|^2$ can be written formally in the form

$$|\Psi|^2 = \sum_{P'} (-1)^{P'} \prod_{i=1}^{N} \psi_{\mathbf{k}_i(P'2)\sigma_i(P'2)}^*(\mathbf{s}_i) \times \psi_{\mathbf{k}_i(P'1)\sigma_i(P'1)}(\mathbf{s}_i) \tag{19}$$

where $\sigma_i$ indicates spin quantum numbers. In case of exact orthogonality of $\psi_k$ wave functions the only terms remaining after integration over $d\tau$ are those with

$$\mathbf{k}_i(P'2) = \mathbf{k}_i(P'1), \qquad \sigma_i(P'2) = \sigma_i(P'1) \tag{20}$$

for all values of $i$. The same concerns integration over $d\tau_1$. In this way one gets the usual formula for $\rho(s_1)$.

In case of weak non-orthogonality of the $\psi_{\mathbf{k}}$ functions, the non-orthogonal terms in the denominator will be small to second order and can be neglected. In the numerator terms in (19) containing a single permutation with regard to the relations (20) will give a contribution linear in the non-orthogonality. This leads to equation (17).

While performing actual computations using equation (17), we will consider as small the factor $w^2(s) - 1$, because it is limited in space and the term $v_k$ following from perturbation. Neglecting consequently terms of higher order of smallness we can write $\rho(s)$ in the form

$$\rho(s) = w^2(s)\rho_0 + \delta\rho^3(s) - \delta\rho^1(s) - \delta\rho^2(s) \tag{21}$$

where

$$\delta\rho^1(s) = 2 \sum_{\substack{\mathbf{k} \neq \mathbf{k}' \\ \text{occ}}} A_{\mathbf{k}'\mathbf{k}}^1 \psi_{\mathbf{k}'}^*(\mathbf{s}) \psi_{\mathbf{k}}(\mathbf{s}), \tag{22}$$

$$\delta\rho^2(s) = 2 \sum_{\mathbf{k}\neq\mathbf{k}',\mathrm{occ}} A^2_{\mathbf{k}'\mathbf{k}} \psi^*_{\mathbf{k}'}(\mathbf{s})\psi_{\mathbf{k}}(\mathbf{s}), \tag{23}$$

$$\delta\rho^3(s) = \frac{2w^2(s)}{\Omega^{1/2}} \sum_{\mathbf{k}\mathrm{occ}} [v_{\mathbf{k}}(\mathbf{s})e^{-i\mathbf{k}\mathbf{s}} + v^*_{\mathbf{k}}(\mathbf{s})e^{i\mathbf{k}\mathbf{s}}], \tag{24}$$

$$A_{\mathbf{k}'\mathbf{k}} = A^1_{\mathbf{k}'\mathbf{k}} + A^2_{\mathbf{k}'\mathbf{k}}, \tag{25}$$

$$A^1_{\mathbf{k}'\mathbf{k}} = \frac{1}{\Omega} \int d\mathbf{s}'[w^2(s') - 1]e^{i(\mathbf{k}'-\mathbf{k})\mathbf{s}'}, \tag{26}$$

$$A^2_{\mathbf{k}'\mathbf{k}} = \frac{1}{\Omega^{1/2}} \int d\mathbf{s}'[v_{\mathbf{k}'}(\mathbf{s}')e^{-i\mathbf{k}\mathbf{s}'} + v^*_{\mathbf{k}}(\mathbf{s}')e^{i\mathbf{k}'\mathbf{s}'}]. \tag{27}$$

Performing calculations with $\bar{v}_k$ (Equation (15)) instead of $v_k$ one gets for the electron density distribution $\tilde{\rho}(s)$ the formula

$$\tilde{\rho}(s) = w^2(s)\rho_0 + \delta\tilde{\rho}^3(s) - \delta\tilde{\rho}^1(s) - \delta\tilde{\rho}^2(s). \tag{28}$$

One obtains

$$\delta\tilde{\rho}^1(s) = \delta\rho^1(s), \qquad \delta\tilde{\rho}^2(s) = 0, \qquad \delta\tilde{\rho}^3(s) = \delta\rho^3(s) - \delta\rho'(s). \tag{29}$$

Obvious calculations show that

$$\delta\rho'(s) = \delta\rho^2(s). \tag{30}$$

Thus application of the Pauli exclusion principle in the form (15) has no influence on the computed electron density distribution provided non-orthogonal terms are included according to equation (17).

## 4. Conclusions

From the results presented above it appears that performing within the formalism presented in this paper extensive calculations of EPI characteristics of the kind of Lowy and Jackson [14 to 16] or Rubaszek and Stachowiak [18] (cf. [3]) is quite feasible and should give additional insight in the still open problem of $e^+ - e^-$ interaction in jellium.

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