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Positron-electron annihilation rates in an electron gas studied by variational Monte Carlo simulation

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Abstract. – The studies of the electron-positron (e-p) interaction in condensed matter using the quantum Monte Carlo (QMC) simulations brought only fragmentary or incorrect results and have been suspended for a longer time. In the present work using the variational quantum Monte Carlo (VQMC) method correct and reasonable annihilation rates for a positron in an electron gas (EG) in a wide range of electron densities have been obtained. This has been achieved owing to an appropriate construction of the trial function which takes into account the 3-particle correlations (*i.e.* the dependence of the e-e interaction on the distance from the positron) and Friedel oscillations of the e-p correlation function. The annihilation rates have been found by "direct determination" of e-p contact densities on the basis of the variational trial function. We also have found the scheme for calculating of the momentum-dependent enhancement factors (MDEF), quantities not achievable within the MC method until now.

Positron annihilation finds applications in many areas of the human activity [1, 2]. The necessary experimental studies of this effect require the development of the theory of e-p interactions. Because of their complex nature, this is a great challenge for many-body theories as well as for a "computer experiment" such as QMC. Some unexplained discrepancies between theory and experiment, even for simple metals, manifest an incomplete understanding of this interaction in condensed matter [3, 4]. *E.g.*, it is still not clear why the annihilation rates for simple metals resulting from the most advanced theories (*e.g.* refs. [5–8]) are markedly higher than the corresponding experimental values. Early attempts, and some of the recent ones [3,4] to explain these facts by the effects of positron-lattice and positron-core interactions did not yield satisfactory results. In turn, theories based on more simplified assumptions [9] (cf. ref. [10]) fit the experiment better. The difference between results of different theories for, *e.g.*, $r_s = 2$ or $r_s = 3$ exceeds 10%. It is evident that the new experimental techniques which ensure much higher resolution will require better and more confidential theoretical data for the interpretation. Therefore one should turn back to the essentials and study the interesting properties of e-p interactions on the basis of the positron+electron gas model as the basic and simplest approach to any metal. Commonly, the results gained with such a model are widely used in several more advanced methods of investigation of the real metals.

In principle, the QMC is a useful tool for solving some problems in many-body theories [11] and could be promising in positron physics (it finds already applications in positron chemistry). However, the known realizations of this method [12–14] applied to e-p systems in solids were, apart from providing interesting results concerning e-p correlation energy (cf. also ref. [15]), unable to yield satisfactory results for e-p contact densities (and positron annihilation rates)

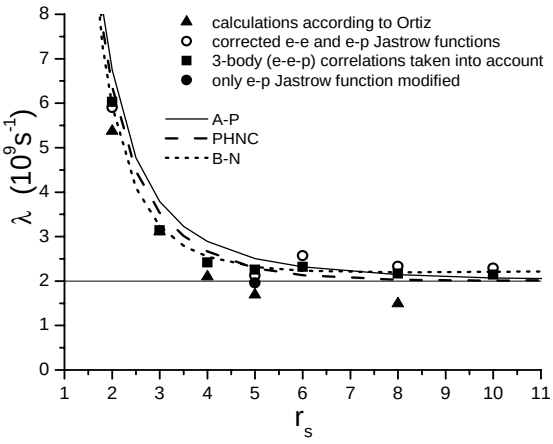

Fig. 1 – Annihilation rates *vs.* r_s calculated in this work (symbols). The solid, dashed and dotted lines correspond to refs. [5,6] and [10], respectively (ref. [10] utilizes some results of ref. [6]).

and have not been published. Moreover, they have given no advice on how to get MDEF. Both the mentioned quantities are very important and directly correspond to experimental data. The calculations within the VMC concerning e-p contact densities have been inaccurate, becoming even incorrect for $r_s > 4$ (the resulting annihilation rates fall down below $2 \cdot 10^9\,\mathrm{s}^{-1}$, see the triangles in fig. 1; such a result is unacceptable since in a homogeneous medium the electronic density on the positron is always greater than that on the positron in vacuum, the limit is the contact density value of the Ps atom).

The purpose of the present work is to stimulate progress in this field. Calculations of annihilation rates are indispensable for investigating defects and electronic structure of solids with positrons. The present paper shows that the most important deficiencies of the QMC method can be removed and reasonable values of positron annihilation rates in the EG are obtainable. Some details of the method and preliminary calculations have been presented earlier in conference proceedings [16].

The total Hamiltonian $\boldsymbol{H}$ (in atomic units) for the system of N electrons and 1 positron is

$$\boldsymbol{H} = -\frac{1}{2}\sum_i^N \nabla^2_{\boldsymbol{x}_i} - \frac{1}{2}\nabla^2_{\boldsymbol{x}_+} + \sum_{i<j}^N \frac{1}{|\boldsymbol{x}_i - \boldsymbol{x}_j|} - \sum_i^N \frac{1}{|\boldsymbol{x}_i - \boldsymbol{x}_+|} + \Lambda, \tag{1}$$

where the indices i and j correspond to the electrons, $+$ corresponds to the positron, and Λ is a constant potential ensuring charge neutrality of the system. In order to simulate an infinite system, one has to assume periodic boundary conditions. The positron–many-electron trial wave function (the symbol X denotes the set of electron coordinates $X = \{\boldsymbol{x}_1, \boldsymbol{x}_2, ...\boldsymbol{x}_N\}$) can be written as

$$\Psi(\boldsymbol{x}_1, \boldsymbol{x}_2, ...\boldsymbol{x}_N, \boldsymbol{x}_+) = D(X^\uparrow)D(X^\downarrow)\varphi(\boldsymbol{x}_+)J(X), \tag{2}$$

where $D(X^\uparrow)$ and $D(X^\downarrow)$ are Slater determinants (plane waves) for $N/2$ spin-up $\uparrow$ and $N/2$ spin-down $\downarrow$ electrons, respectively. $\varphi(x_+)$ is the positron wave function (plane wave, constant for the lowest energy state in a homogeneous medium), and J is the Jastrow-Feenberg–type factor

$$J = \prod_i \exp[v_{ep}(r_{i+})] \prod_{i<j} \exp[v_{ee}(r_{ij})] \prod_{i<j} \exp[v_{eep}(r_{ij}, r_{i+}, r_{j+})], \tag{3}$$

where $r_{ij} = |\boldsymbol{x}_i - \boldsymbol{x}_j|$ and $r_{i+} = |\boldsymbol{x}_i - \boldsymbol{x}_+|$. The general form of the functions v (v_{ee}, v_{ep}) is expressed (according to ref. [17]) as follows:

$$v(r) = \overline{v}(r) + v^1(r), \tag{4}$$

where $r \equiv r_{ij}$ (or r_{i+} for e-p interactions). The functions $\overline{v}(r)$ taking into account cusp conditions are formulated as in ref. [17]. The form of $v^1(r)$ is assumed on the basis of the comparison of figures for the variational and diffusion results for the electron-electron (e-e) correlation functions in ref. [17] and is aimed to correct already in variational calculations the shape (and properties) of e-e correlation hole:

$$v^1_{ee}(r) = A_{ee}\,(1 + cr^2)\,e^{-\alpha r^2 - \gamma r^4}\,\cos(d\,r)\,, \tag{5}$$

where A,c,d,α,γ are variational parameters. This function does not change the cusp conditions, the variational parameter γ makes the function (and its derivatives) vanishing well before r approaches the boundary of the simulation cell. A more complicated form of the correction $v^1(r)$ can be applied to the e-p part of the Jastrow factor (the parameters are different):

$$v^1_{ep} = A_{ep}\,e^{-\alpha r^2_{i+} - \gamma r^4_{i+}}\,\cos[(d + ce^{-\delta r_{i+}})r_{i+}]. \tag{6}$$

The argument of the cosine is the function that makes the period of Friedel-type oscillations changing with r. It is a quite important feature of e-p correlation function (*e.g.* ref. [6]) and should be taken into account already when constructing the Jastrow factors. Introducing such oscillations in eq. (6) leads to lowering the total energy of the system by $\sim 0.5\%$.

The 3-particle correlation (electron-electron-positron) can be taken into account in the following way:

$$v_{eep} = A_{eep}\,(e^{-\alpha r^2_{i+}} + e^{-\alpha r^2_{j+}})e^{-\gamma r^4_{ij}}\,(d + r^2_{ij}e^{-\delta r_{ij}}). \tag{7}$$

The above function is applied only to the electrons of antiparallel spins. The form of the r_{ij}-dependent part of the function v_{eep} is based on the approximate form of the difference between e-e pair correlation functions for two different electron densities. The part depending on r_{i+} and r_{j+} is the function that drives the amplidude of this difference depending on the distance of the two considered electrons from the positron. It corresponds to the following mechanism: if one of the electrons is to some extent screened by the positron, the amplitude of the e-e correlation function becomes smaller. From another point of view, when we concentrate on the positron, one can find an analogue in the local density approximation in the density functional theory where the e-p interaction depends on the local electron density.

The e-p correlation function $g(r)$ is a quantity directly connected with the positron annihilation rate. For the EG the annihilation rate λ can be obtained from the formula

$$\lambda(r_s) = \frac{12}{r_s^3} g(r_s, 0), \tag{8}$$

where $g(r_s, 0)$ is the contact density (the value of $g(r)$ at $r = 0$ for a given electron density).

In order to determine the e-p pair-correlation function and MDEF for the considered system it is useful to introduce a new set of coordinates [16, 18] that do not change the form of (2):

$$R = \frac{1}{N+1}\left(\boldsymbol{x}_+ + \sum_{i=1}^{N} \boldsymbol{x}_i\right), \quad \xi_i = \boldsymbol{x}_i - \boldsymbol{x}_+. \tag{9}$$

Conventionally, for the EG and for the positron in an electron gas the methods of calculation of $g(r)$ within MC simulations are based on collecting, during the simulation process, the

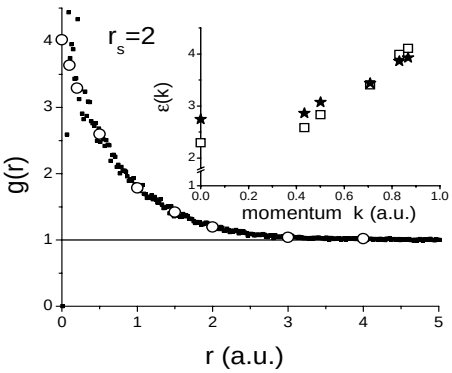

Fig. 2

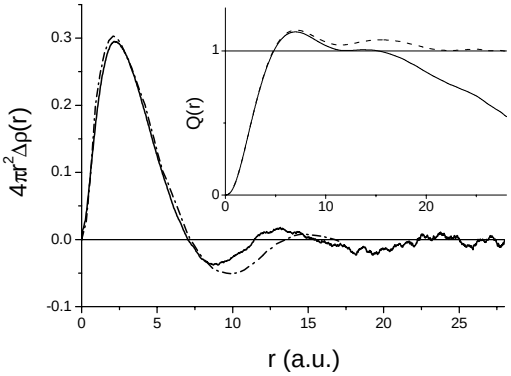

Fig. 3

Fig. 2 – Positron-electron correlation function according to formula (10) (circles). The dots represent the values obtained with the conventional method [12]. In the inset: momentum-dependent enhancement factor. The open squares and stars correspond to the assumption that Φ_k represents the system of noninteracting ($J = 1$) or interacting electrons, respectively.

Fig. 3 – Screening cloud distribution $4\pi r^2\Delta\rho$ around a positron for $r_s = 6$. The solid and dashed lines correspond to this work and ref. [6], respectively. The inset: the screening charge $4\pi r^2 \int_0^r [g(r) - 1]\mathrm{d}r$ up to the distance r from the positron. The solid and dashed lines correspond to the normalisation to N and $N - 1$ electrons, respectively.

statistics of the number of particles whose distances from the positron drop into spherical layers of volume $\Delta V_r = 4\pi r^2\Delta r$ [12–14]. This procedure yields values that are greatly diffused in the neighbourhood of $r = 0$ (fig. 2, dots). Commonly, to find reasonable values, a fitting (cf. ref. [19]) that uses some additional knowledge is necessary. This procedure could make some effects (or values) which are connected exclusively to the given simulation disturbed, dimming the result (and evaluation) of the simulation itself. *E.g.*, the character of the assumed oscillations may have an influence on the value of $g(r)$ in the cusp. Instead, we propose applying the following formula in the new coordinates (cf. ref. [16]):

$$g(\boldsymbol{r}) = \lim_{M\to\infty} \frac{1}{M} \sum_{j}^{M} \frac{\frac{1}{N}\sum_{i}^{N} |\Psi(\xi_1^j, \xi_2^j, ..., \xi_i^j = \boldsymbol{r}, ..., \xi_N^j)|^2}{|\Psi(\xi_1^j, \xi_2^j, ...\xi_N^j)|^2}, \tag{10}$$

that gives $g(r)$ with an accuracy depending only on the number M of sampled (according to Metropolis method) configurations of particles. The averaging in eq. (10) with respect to the number N of indistinguishable particles improves the statistics of the calculation. An example of the e-p correlation function obtained from the present calculations (eq. (10)) is shown in fig. 2 (circles). The scattered points visualise the results obtained conventionally. The equivalent formula for the e-p correlation function in conventional coordinates reads

$$g(\boldsymbol{r}) = \lim_{M\to\infty} \frac{1}{MN} \sum_{\substack{j<M \\ i<N}} \frac{|\Psi(\boldsymbol{x}_+, \boldsymbol{x}_1^j, .., \boldsymbol{x}_i^j = \boldsymbol{x}_+ + \boldsymbol{r}, .., \boldsymbol{x}_N^j)|^2}{|\Psi(\boldsymbol{x}_+, \boldsymbol{x}_1^j, ...\boldsymbol{x}_N^j)|^2}. \tag{11}$$

The electrons, according to their state, contribute in different ways to the value of the electron density on the positron. The knowledge of this effect is crucial for the interpretation of the experimental data (measurements of angular correlation of annihilation quanta). The 2γ

annihilation rate to the particular final state Φ_ν of $N-1$ electrons (with a hole of momentum k) and emitted gamma quanta with total momentum q can be defined as

$$\Lambda_\nu(\boldsymbol{q}) \sim \sum_{i=1}^{N} \left| \int \mathrm{d}\tau \Phi_\nu^*(\boldsymbol{x}_1, ..., \boldsymbol{x}_{i-1}, \boldsymbol{x}_{i+1}, ..., \boldsymbol{x}_N) \frac{e^{i\boldsymbol{q}\boldsymbol{x}_+}}{2\pi^{3/2}} \times O_i^s \delta(\boldsymbol{x}_i - \boldsymbol{x}_+) \Psi(\boldsymbol{x}_1, ..., \boldsymbol{x}_N, \boldsymbol{x}_+) \right|^2, \tag{12}$$

where O_i^s is the spin projection operator and $\delta(\boldsymbol{x}_i - \boldsymbol{x}_+)$ acts as the positron coordinate projection operator (see *e.g.*, [6,20]). If Φ_ν is given by a form similar to (2) (without $\varphi(\boldsymbol{x}_+)J_{ep}(X)$), then one of the determinants is of order $N-1$ (without i-th column and k-th row). Thus, the momentum-dependent enhancement factor ε can be defined by using eqs. (12) and (9), given the proper normalization value S (by utilizing the calculated value of the contact density). Defining $\Psi(\xi_1, \xi_2, \xi_i = 0, ..., \xi_N) \equiv \Psi^{\mathrm{o}}(R_i)$ and $\Phi_k(\xi_1, \xi_2, ..., \xi_{i-1}, \xi_{i+1} ..., \xi_N) \equiv \Phi_k(R_i)$, we get the following Monte Carlo formula [16]:

$$\varepsilon(\boldsymbol{k}) = S \frac{\displaystyle\sum_j^M \frac{\langle \Phi_k^*(R_i^j)\Psi^{\mathrm{o}}(R_i^j)\rangle_i}{|\Psi(R^j)|^2}}{\displaystyle\sum_j^M \frac{\langle |\Phi_k(R_i^j)|^2\rangle_i}{|\Psi(R^j)|^2}} \times \frac{\displaystyle\sum_j^M \frac{\langle \Phi_k(R_i^j)\Psi^{\mathrm{o}}(R_i^j)\rangle_i}{|\Psi(R^j)|^2}}{\displaystyle\sum_j^M \frac{\langle |\Psi^{\mathrm{o}}(R_i^j)|^2\rangle_i}{|\Psi(R^j)|^2}}, \tag{13}$$

where the expressions $|\Phi_k(R_i^j)|^2/|\Psi(R^j)|^2$ and $|\Psi^{\mathrm{o}}(R_i^j)|^2/|\Psi(R^j)|^2$ can be treated as weighting factors. The points ξ are distributed according to $|\Psi|^2$.

The calculations have been performed on a PC (the code has been written in Fortran90) for 227 particles in the fcc-type elementary cell (the rhombic dodecahedron). In these calculations the chosen electron densities corresponded to $r_s = 2, 3, 4, 5, 6, 8$ and 10. The minimization method used in this work bases on a combination of the analytical derivatives method [21] and the stochastic gradient method [19]. At first, in the minimization procedure the trial function parameters have been found only for the system of electrons without the positron. This function has been corrected in relation to the Ortiz method by using eq. (5) which, *e.g.*, lowers the energy only slightly (by $\sim 0.04\%$ for $r_s = 6$); however, the change in the function (the variance lowers by $\sim 7\%$) has noticeable later consequences for the positron parameters. The next step was to add the positron to the system and to find the appropriate parameters for the full e-p wave function, having the first set of parameters (corresponding only to the electrons) frozen. The whole number of the considered parameters was 24. Successively, the appropriate corrections (6) to the e-p Jastrow factor and 3-particle correlations (7) were taken into account. Several tens of thousands of iterations have been performed during the minimization procedure for each r_s value. In each iteration 12 new different configurations of the coordinates of all particles have been considered.

The obtained parameters were used then to determine, according to eqs. (10) and (8), the e-p annihilation rates, estimating the error as less than 1%. The results for total energies and annihilation rates are given in table I and plotted in fig. 1. The importance of the different modifications of the Jastrow factor is shown by using different symbols in fig. 1. For $r_s < 5$ the annihilation rates are slightly lower than those resulting from ref. [10] (Lantto, ref. [9]). Thus, after taking into account other effects, *e.g.* the annihilation with core electrons in metals, they would fit better the corresponding experimental results (cf. ref. [4] and references therein). In general, building Friedel-type oscillations into the e-p Jastrow factor and adding the 3-particle interactions to the e-e Jastrow factor make it possible to achieve the correct e-p contact densities. At $r_s = 6$ they, however, locally rise up and then for $r_s > 6$ go down,

TABLE I – *Total energies (in atomic units) and annihilation rates for different densities of the EG. The numbers in the second row correspond to energies E_0 of the system noninteracting with the positron. The energies E_1 in the third row correspond to the case when the formula (6) was taken into account. The numbers E_T presented in the next row were obtained when all the corrections (5), (6), (7) to the Jastrow factors were taken into account. σ is the variance in calculations in the last case. The last row presents the annihilation rates for the last case.*

r_s	2	3	4	5	6	8	10
E_0	0.0024	−0.0685	−0.0784	−0.0765	−0.0719	−0.0634	−0.0550
E_1	0.0015	−0.0693	−0.0791	−0.0769	−0.0726	−0.0639	−0.0556
E_T	0.0010	−0.0698	−0.0797	−0.0776	−0.0728	−0.0643	−0.0561
σ	1.1×10^{-5}	2.7×10^{-6}	1.6×10^{-6}	1.1×10^{-6}	5.8×10^{-7}	4.1×10^{-7}	3.3×10^{-7}
λ ($10^9\,\mathrm{s}^{-1}$)	6.03	3.14	2.42	2.26	2.32	2.17	2.15

being slightly higher than the values corresponding to refs. [5] and [6]. This effect is clearer if formula (7) is not applied. The effect may be connected with the appearance of the a precursor of the positronium state (cf. Apaja *et al.* [8], see also [22]), that, unfortunately, cannot be properly described by our trial function consisting of Slater determinants (plane waves).

The parameters corresponding to $r_s = 2$ have also been used to calculate the MDEF that are shown in fig. 2. In general, fig. 2 resembles the corresponding figure of Kahana [23] (or Arponen *et al.* [24]), exhibiting an increase of $\varepsilon(k)$ with the momentum k. It means that the electron states of higher momenta are preferred in building up the screening cloud around the positron. The dependence of $\varepsilon(k)$ on k is weaker if the reference system is the interacting EG (Arponen's case). Unfortunately, in this first calculations, since the number of considered electrons is limited, only few k points in the momentum space are available.

The example comparison of our distribution of $\rho_0 4\pi r^2[g(r) - 1]$ to the PHNC figure is given in fig. 3. The similarity of our function to the one based on the perturbation theory is very good. Moreover, the figures corresponding to $4\pi r^2 \int [g(r) - 1]\mathrm{d}r$ (the example in inset of fig. 3, solid line) are close to the diffusion Monte Carlo (DMC) results of Gilgien (fig. 4.14 in ref. [13]), so we can consider the present trial function as a good importance function for the DMC, accelerating seriously the convergence of this method. Notice, however, that, because of the finite size of the simulation cell, the screening charge is shifted towards the positron from the remote part of the cell. Therefore the situation corresponds to that if there currently were $N - 1$ electrons far away from the positron (compare the dashed line in the inset of fig. 3). This polarization of electrons, absent in the infinite system, means that the value of λ obtained corresponds actually to a value of r_s greater by $\approx 0.2\%$, which is fortunately a negligible correction. This effect may have, however, more serious consequences when calculating the correlation energies. It appears also for a homogeneous EG and was not considered in refs. [12–14]. The studies of e-p correlation energies remain a separate important problem which cannot be considered seriously without DMC calculations. It would go beyond the scope of this article, however, it will be performed in the nearest future.

In conclusion, it has been shown that it is worth to come back to QMC in positron physics, since this method is able to yield correct values of important quantities in positron physics such as annihilation rates and MDEF. Hopefully, it may soon verify the existing many-body theories in this area. The annihilation rates can be calculated with arbitrary accuracy under given theoretical assumptions. The basic drawbacks of hitherto existing VQMC approaches to positron in a homogeneous EG, such as much too low values of the contact densities of the e-p correlation function for $r_s > 4$, have been removed. Thus, the main achievement of this paper is that our calculated values of λ lie above the corresponding rate for the positronium within a wide range of r_s and are the first reliable ones found for the simplest model of a metal

within the MC. These values can be applied to the real (and defected) materials through the LDA or other approximations (cf. [1–4]).

Moreover, the behaviour of the annihilation rates at $r_s = 6$ indicate the possible effect of the creation of the e-p quasi-bound state. This, however, requires further detailed studies of this region. The new trial function seems to become an excellent guiding function in the DMC method which is expected to produce the useful benchmark values for DFT theories. Some formulae (eqs. (10), (11) and (7)) and proposals (eq. (13)) may find applications in other systems of inhomogeneous electron density (*e.g.* systems with ions). The proposed transformation to the new coordinate system could be also applied to studies of systems containing, *e.g.*, muons. The first results for MDEF create possibilities for some new investigations in this subject, *e.g.*, there are still unanswered (although important for the experiment) questions about the behaviour of MDEF near the k_F point for different electron densities.

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