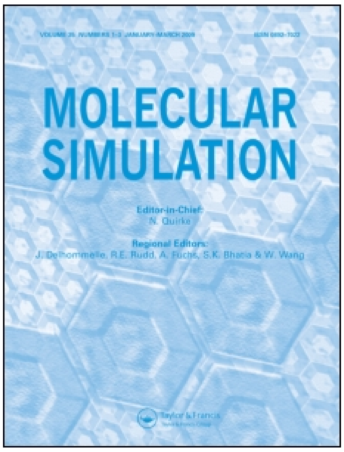

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# CALCULATION OF THE SCATTERING PSEUDOPOTENTIAL FOR THE HELIUM ATOM FREE THERMALIZED POSITRON USING QUANTUM PATH INTEGRAL MONTE CARLO METHOD

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A procedure for calculation of the nonlocal interaction of the helium atom with the positron in a mixed Gibbs state at temperature of several K is suggested and carried out. The integration over the positron variables is made numerically with the aid of PIMC random walk in the space of Feynman trajectories. Calculations indicate that the local approximation used in [2] if applied properly results in a wrong (positive) sign of the He-$e^+$ interaction. The negative nonlocal part exceeds twice the absolute value of the local part thus providing attractive character of the resulting interaction.

KEY WORDS: Helium, positron, cluster, Path Integral Monte Carlo.

## 1. INTRODUCTION

Experiments on the annihilation rate of thermalized free positrons in gaseous helium at temperature slightly higher than the helium critical point (5–7 K for $^4$He) [1] indicated helium clustering on positrons. Isothermal growth of the helium density is initially accompanied by linear increase of the annihilation rate, then at a certain point it jumps and remains constant in a definite interval of bulk density, then follows further linear increase. The jump of the annihilation rate could be only caused by the increase of the local density in the region of positron localization due to polarization of helium atoms by the Coulomb field of the positron. Until now there existed only semiphenomenological approaches in the theory of the phenomenon [2,3]. It is interesting to describe it on a microscopic level. Approaching the problem one should take into account that the thermal wave length for a free positron (or an electron) at temperatures of several Kelvins is about 200–300 Å and consequently the problem should be treated with the aid of quantum statistics.

An appropriate instrument of such treatment is the Path Integral Monte Carlo (PIMC) method [4–10] which enables one to calculate equilibrium properties of quantum systems at constant temperature. The procedure of the method is based on the isomorphism of the quantum statistical problem with the problem of classical statistics for a chain multiatomic "molecule", which directly follows from the expression of the canonical density matrix in terms of the Feynman path integral formalism [11,12].

The important feature of the method is its universality. In its initial formulation it requires no simplifying phenomenological assumptions. The idea of the essential sampling involved in the MC method provides the optimal distribution of the computation efforts according to contributions to the partition function. Being principally rigorous in nonrelativistic statistics the PIMC method enables us to develop on its basis certain approximate modifications to treat particularly complicated cases.

In this paper we construct an algorithm in which positron is being considered as a quantum particle, i.e. is represented by a closed trajectory with the charge distributed among the vertices. The field of these charges polarizes helium atoms, and the field of the induced dipoles is included in He-positron interaction. The positron trajectory can freely penetrate into He-atoms which physically corresponds to the distinguishability between electrons and positrons.

## 2. PATH INTEGRAL MONTE CARLO METHOD

The PIMC method is based on the representation of the statistical operator $\exp(-\beta\hat{H})$ as a product of high temperature operators:

$$\hat{G} = \left[\exp\left(-\frac{\beta\hat{H}}{N}\right)\right]^N, \text{ where } \hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}),$$

$$\beta = (kT)^{-1},\ V(\mathbf{r}) - \text{external field.} \tag{1}$$

In coordinate representation the canonical partition function being the trace of the operator (1) is expressed as a $3N$-dimensional integral of the product of high temperature density matrices:

$$Z = \int d\mathbf{r}_1 \ldots d\mathbf{r}_N \prod_{i=1}^{N} \langle \mathbf{r}_i | \exp(-\beta\hat{H}/N) | \mathbf{r}_{i+1} \rangle, \tag{2}$$

with condition $\mathbf{r}_{N+1} = \mathbf{r}_1$. In high temperature limit ($\beta/\text{N} \rightarrow \text{O}$) the density matrix could be represented in the form [7]:

$$\langle \mathbf{r}_i | \exp(-\beta\hat{H}/N) | \mathbf{r}_{i+1} \rangle = G_0(\mathbf{r}_i, \mathbf{r}_{i+1}\ ;\ \beta/N) \exp\left[-\frac{\beta}{N} V(r_{i+1})\right] \tag{3}$$

$G_0$ is the density matrix of a free particle at temperature TN:

$$G_0(\mathbf{r}, \mathbf{r}'\ ;\ \beta/N) = \left[\frac{N}{\Lambda^2}\right]^{3/2} \exp\left[\frac{\pi N(\mathbf{r} - \mathbf{r}')^2}{\Lambda^2}\right],\ \Lambda = \frac{h}{\sqrt{2\pi mkT}}, \tag{4}$$

where $\Lambda$ is the thermal de Broglie wave length of a particle with mass $m$ at temperature $T$.

For the partition function (2) (with the account of (3) and (4)) we obtain the finite dimensional approximation.

$$Z_N = \int d\mathbf{r}_1 \ldots d\mathbf{r}_N \left[\frac{N}{\Lambda^2}\right]^{3N/2} \exp\left[-\sum_{i=1}^{N} \frac{\pi N}{\Lambda^2}(\mathbf{r}_{i+1} - \mathbf{r}_i)^2 - \frac{\beta}{N}\sum_{i=1}^{N} V(\mathbf{r}_i)\right], \tag{5}$$

($Z_N$ tends to $Z$ as $N \rightarrow \infty$). So the partition function for a single quantum particle formally corresponds to the classical partition function (configurational integral) of a closed chain (trajectory) of $N$ vertices in external field, each vertex interacting with its nearest (along the chain) neighbours by means of a harmonic force with rigidity parameter $(Nm/\beta^2\hbar^2)$. This correspondence was classified as the quantum classical isomorphism [5]. The mean linear size of the trajectory corresponds to the quantum uncertainty of the particle position and in the absence of the external field has an order of $\Lambda$. In the limit $(N \to \infty)$ the multidimensional integral (5) tends to a continuous Wiener integral over all possible continuous closed trajectories.

The knowledge of the canonical partition function enables us to obtain the equilibrium properties by differentiation of free energy with respect to appropriate variables. In particular using (2) we obtain for the internal energy:

$$E = -\frac{\partial(\ln Z)}{\partial\beta} = \int d\mathbf{r}_1,\ldots,d\mathbf{r}_N P(\mathbf{r}_1,\ldots,\mathbf{r}_N;\,\beta)\cdot e_N(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \langle e_N\rangle\langle\ \rangle_{\mathrm{c}} \qquad (6)$$

where

$$P(\mathbf{r}_1,\ldots,\mathbf{r}_N;\,\beta) = \frac{1}{Z_N}\prod_{i=1}^{N}\left\langle \mathbf{r}_i\middle|\exp\left(-\frac{\beta\hat{H}}{N}\right)\middle|\mathbf{r}_{i+1}\right\rangle,$$

$$e_N(\mathbf{r}_1,\ldots,\mathbf{r}_N) = -\sum_{i=1}^{N}\frac{\partial}{\partial\beta}\left[\ln\left\langle \mathbf{r}_i\middle|\exp\left(-\frac{\beta\hat{H}}{N}\right)\middle|\mathbf{r}_{i+1}\right\rangle\right],$$

and $\langle\ \rangle_c$ is the canonical averaging. Here $P(\mathbf{r}_1,\ldots,\mathbf{r}_N;\,\beta)$ is the configurational weight function, $e_N$ is usually being called the estimator for the internal energy [7]. In principle any equilibrium average could be expressed similarly to (6) with an appropriate estimator.

For the energy (6) with (5) for $Z_N$ we obtain:

$$E = \frac{3N}{2\beta} - \frac{N\pi}{\Lambda^2\beta}\left\langle\sum_{i=1}^{N}(\mathbf{r}_i - \mathbf{r}_{i+1})^2\right\rangle_c + \frac{1}{N}\cdot\sum_{i=1}^{N}\langle V(\mathbf{r}_i)\rangle_c, \qquad (7)$$

where averaging is being done over the distribution $P(\mathbf{r}_1,\ldots,\mathbf{r}_N;\beta)$ (6). For the kinetic energy we get the following estimator [4]:

$$e_N^k = \frac{3N}{2\beta} - \frac{N\pi}{\Lambda^2\beta}\sum_{i=1}^{N}(\mathbf{r}_i - \mathbf{r}_{i+1})^2 \qquad (8)$$

For the potential energy the estimator $e_N^p = e_N - e_N^k$ corresponds to the last term in (7).

In [4,5,7,9,10] particular attention is payed to ways of construction of various estimators. Kinetic energy estimator (8) was discussed in [4]. Though formally rigorous in the limit $(N \to \infty)$, this estimator is not convenient for computational use being represented by difference of two values close to each other one of which fluctuates. In [7] it was pointed out that various (more than one) estimators could correspond to the same physical quantity having the same MC-average but different higher moments. Values of dispersion could also depend on the external field. The energy estimator (8) (used in [4]) not always yields to minimal dispersion. The relative dispersion in this case increases with $N$ as $N$.

One of the ways to decrease the dispersion was proposed in [7] where a new kinetic energy estimator was constructed. It was based on the virial theorem and was called a virial estimator:

$$e_N^{k(v)} = \frac{1}{2N}\sum_{i=1}^{N}\left[\mathbf{r}_i,\ \frac{dV(\mathbf{r}_i)}{d\mathbf{r}_i}\right]. \qquad (9)$$

Comparison of results for two types of estimators in calculations for harmonic oscillator with various trajectory lengths $N$ indicated that average for both of them are equal but standard deviations $[\langle(\delta e_N^k)^2\rangle]^{1/2}$ and $[\langle(\delta e_N^{k(v)})^2\rangle]^{1/2}$ considerably differ: the first increase as $N^{1/2}$ whereas the latter is insensitive to $N$. So for greater $N$ it is more convenient to use the virial estimator. However, it should be pointed out that dependence of the dispersion on temperature for these estimators is different. Our computational experience with other analogous atomic systems indicated that the dispersion of the first estimator ($e_N^k$) falls with cooling of the system faster than for the second estimator ($e_N^{k(v)}$) so that at considerably low temperatures the estimator $e_N^k$ becomes competitive with $e_N^{k(v)}$

## 3. MODEL HAMILTONIAN OF He–e$^+$ INTERACTION

To construct the model Hamiltonian the He atom is considered as a quantum system of two electrons in the Coulomb field of the nucleus with the charge 2e. The interaction energy of the positron with this system in a nondisturbed state is a sum of its interaction with the fixed nucleus ($2e/R$) and the electron distribution in the ground state of He in the absence of external fields determined by the wave function [13]:

$$\varphi_0(r_1, r_2) = \frac{1}{\pi}\left[\frac{Z'}{a}\right]^3 \exp\left[-\frac{Z'}{a}(r_1 + r_2)\right]$$

Here $Z' = 2\text{-}\sigma$-the screened nuclear charge ($\sigma = 5/16$-the screening coefficient accounting for the repulsion forces between electrons) $r_1$, $r_2$-distances of electrons from the nucleus, a-Bohr radius.

In the coordinate representation the operator of helium electrons' interactions with the positron is:

$$V(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}) = -\frac{e^2}{R_1} - \frac{e^2}{R_2}, \tag{10}$$

where $R_1 = |\mathbf{r}_1 - \mathbf{r}|$, $R_2 = |\mathbf{r}_2 - \mathbf{r}|$-distances between the positron and the 1-st and 2-nd electron respectively.

In calculations of the nonperturbed part of the He–e$^+$ Coulomb energy $U_{\text{Coul}}(\mathbf{r})$ we do not take into account the electron–positron correlation effects as far as these effects are accounted for later in the polarization part of the energy. In this case the complete He–e$^+$ wave function is represented by a product of the known electron wave function and the unknown positron wave function. The integration over the coordinates of the former is performed analytically thus yielding for $U_{\text{Coul}}(\mathbf{r})$:

$$\begin{aligned} U_{\text{Coul}}(\mathbf{r}) &= \frac{2e^2}{r} + \int \varphi_0(r_1, r_2)\left[-\frac{e^2}{R_1} - \frac{e^2}{R_2}\right]\varphi_0(r_1, r_2)\, d\mathbf{r}_1 d\mathbf{r}_2 \\ &= \frac{2e^2}{r}\exp\left[-2\frac{Z'}{a}r\right]\cdot\left[\frac{Z'}{a}r + 1\right], \end{aligned} \tag{11}$$

The integration over coordinates of the positron which is weakly coupled to the helium atoms should be carried out taking into account the thermally excited quantum states of the positron and will be made numerically by Markov random walk over a portion of Feynman trajectories (see sections 4, 5).

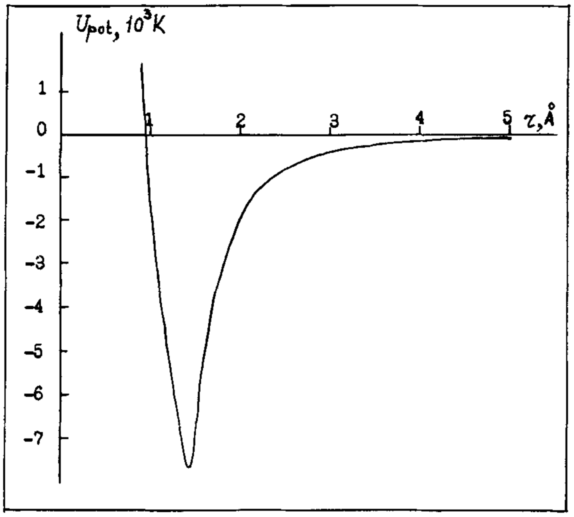

**Figure 1** Model potential of He–e$^+$ interaction (15).

Now let us consider the polarization of He atoms by the field of the positron. For a positron at a distance $r$ from the atomic centre exceeding the atom's radius $R_{He}$ (half of the Lennard-Jones parameter of He) the polarizable atom is considered as a point dipole and the contribution to the dipole moment of the atom from such a far positron is:

$$-\alpha\cdot e\cdot\frac{\mathbf{r}}{|\mathbf{r}|^3}, \tag{12}$$

where the polarizability of the He atom $\alpha = 0.201\,\text{Å}^3$ (see [14]), $\mathbf{r}$-radius vector starting at the atomic centre.

For the positron penetrating inside an atom the simplest model of a uniformly polarizable sphere is used. The dipole moment induced by the charge $e$ is calculated according to the evident expression:

$$\frac{\alpha}{V_{He}}\cdot e\cdot\int\frac{(\mathbf{r}'-\mathbf{r})}{|\mathbf{r}'-\mathbf{r}|^3}d\mathbf{r}', \tag{13}$$

$V_{He}$-volume of the atom. As a result of the integration of (13) we obtain:

$$-\alpha\cdot e\cdot(\mathbf{r}/R_{He}^3), \tag{14}$$

So on the account of (11), (12), (14) we obtain for the He-e$^+$ model potential:

$$U_{pot}(r) = U_{Coul}(r) - \alpha\cdot e^2\cdot\begin{cases}(1/r^4), & r \geqslant R_{He}\\ (r^2/R_{He}^6), & r < R_{He}\end{cases} \tag{15}$$

It is presented in Fig. 1. First term in (15) dominates at small and the second at great distances.

The estimator corresponding to this model potential is expressed as follow:

$$U_{\text{pot}} = \frac{1}{N}\left[\sum_{k=1}^{N} U_{\text{Coul}}(r_k) - \alpha \cdot e^2 \left(\sum_i \frac{r_i^2}{R_{\text{He}}^6} + \sum_j \frac{1}{r_j^4}\right)\right] \tag{16}$$

Here $N$ is the number of positron vertices and indices $i$ and $j$ ennumberate vertices located inside and outside the sphere of radius $R_{\text{He}}$ respectively.

## 4. COMPUTATIONAL DIFFICULTIES AND THE ALGORITHM

An attempt to simulate directly the system including a positron represented by a closed Feynman trajectory with sufficient number of vertices and a necessary number of He atom with the considered above He–e$^+$ interactions (16) by MC procedure is confronted by two problems, caused mainly by a very low temperature range (5–10 K) for which the thermal wave length of the positron lies in the range of 250–300 Å.

1. The number of He atoms which should be contained in this region in order to attain the experimentally observed densities $n = (0, 1\text{–}2, 0)\cdot 10^{22}\,\text{cm}^{-3}$ [1] is very large – $(3\text{–}70)\cdot 10^4$.
2. The potential He–e$^+$ has a very deep (8000 K) and narrow (with the half width 0.5 Å) located at a distance 1.43 Å from the atom centre (see Figure 1). To account correctly for this interaction the positron should be represented by a trajectory with the number of vertices sufficient to make the mean length of the harmonical link so small that at least several neighbouring vertices simultaneously get into the potential well. As the mean length of the link is $L = \Lambda/\sqrt{N}$ one should consider a trajectory of $(1\text{–}2)\,10^6$ vertices to provide a link length – 0.1 Å in appropriate range of temperatures. It is evident that realisation of a MC procedure with such a number of vertices and atoms is unimaginable. To overcome this obstacle we propose the following algorithm.

In our model the mixed quantum state of the free positron at fixed temperature is described by a radial distribution function of the charge density in the positron cloud $\rho(R)$ ($R$-distance from the cloud mass centre). $\rho(R)$ is obtained by MC-simulation of a closed trajectory with comparatively small $(10^2\text{–}10^3)$ number of vertices at fixed temperature and in the absence of external field (the cloud mass centre being fixed). As far as the fluctuations of the centre of mass estimator: $\mathbf{R} = (1/N)\Sigma_i^N \mathbf{r}_i$ of a spatially localized positron in the limit of $N \to \infty$ tend to zero, the condition of fixed centre of mass for a trajectory with finite N coincides with the condition on the centre of mass for the Feynman trajectory limit $(N \to \infty)$.

Insertion of a helium atom into the region occupied by the positron cloud would result in deformation of the trajectory and consequently the density of the positron charge in the vicinity of the atom. For large distances the influence of the He atom on the positron cloud density vanishes due to exponential dependence of the local density deformation on the interaction energy in the Gibbs ensemble. So it becomes possible to divide the interaction energy into two terms:

1. first accounts for the contribution to the He–e$^+$ interaction from the deformation of the positron wave function in the vicinity of the He atom - local term.
2. the second - interaction of the induced He dipole with the nondisturbed part of the positron density - nonlocal term.

First term contains the potential and kinetic part, the second – only the potential contribution.

*Local Contribution*

We begin with the kinetic part of the first term, $E_k^1$. The virial estimator of the kinetic energy (9) corresponds to the operator:

$$\hat{K}^v = \frac{1}{2}\left[\mathbf{r}, \frac{dU_{\text{pot}}}{d\mathbf{r}}\right], \text{ which contrary to the operator } \hat{K} = -\frac{\hbar^2}{2m}\frac{d^2}{(d\mathbf{x})^2},$$

is diagonal in coordinate representation. Therefore

$$E_k^{\text{loc}} = \frac{1}{Z}\int \langle \mathbf{r}|\hat{K}^v \exp(-\beta\hat{H})|\mathbf{r}\rangle d\mathbf{r} = -\frac{1}{2}\int (\mathbf{r}, dU_{\text{pot}}/d\mathbf{r})\,\rho(\mathbf{r})d\mathbf{r},$$

where $Z$ is the partition function and $\rho(\mathbf{r}) = 1/Z\langle \mathbf{r}|\exp(-\beta\hat{H})|\mathbf{r}\rangle$ – the occupation numbers of the coordinate representation which could be considered as canonical averages of the density operator $\hat{\rho}(\mathbf{r}) = \delta(\mathbf{x} - \mathbf{r})$:

$$\begin{aligned}\rho(\mathbf{r}) = {} & \frac{1}{Z}\int \langle \mathbf{r}_i, \ldots, \mathbf{r}_{k-1}, \mathbf{r}, \mathbf{r}_{k+1}, \ldots, \mathbf{r}_N\rangle|\exp(-\beta\hat{H})|\mathbf{r}_1, \ldots, \mathbf{r}_{k-1}, \mathbf{r}, \mathbf{r}_{k+1}, \ldots, \mathbf{r}_N\rangle \\ & \times d\mathbf{r}_1, \ldots, d\mathbf{r}_{k-1}\, d\mathbf{r}_{k+1}, \ldots, d\mathbf{r}_N = \lim_{\omega\to 0}\frac{1}{\omega Z}\int \langle \mathbf{r}_1, \ldots, \mathbf{r}_N|\theta(\mathbf{r}_k - \mathbf{r}) \\ & \times \exp(-\beta\hat{H})|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle d\mathbf{r}_1, \ldots, d\mathbf{r}_N \equiv \lim_{\omega\to 0}\frac{1}{Z}\operatorname{Tr}(\hat{\rho}_\omega(\mathbf{r})\cdot\exp(-\beta\hat{H}))\end{aligned} \tag{17}$$

The operator $\hat{\rho}_\omega(\mathbf{r})$ is the unit step $\theta$-function localized in the $\omega$-vicintiy of $\mathbf{r}$ multiplied by the normalizing coefficient $\omega^{-1}$. Strictly speaking the density distribution operator $\hat{\rho}(\mathbf{r})$ should be defined as a limit (in certain sense) – $\lim_{\omega\to 0}\hat{\rho}_\omega(\mathbf{r})$; however, we put aside discussion of the question whether such limit transfer is correct, since in our calculations we always use the sublimit approximation operator $\hat{\rho}_\omega(\mathbf{r})$. The estimator corresponding to the density distribution operator $\hat{\rho}_\omega(\mathbf{r})$ (analogous to $e_N(\mathbf{r}_1 - \mathbf{r}_N)$ in expression (6)) is

$$\frac{1}{N\omega}\cdot\sum_i^N \theta(\mathbf{r}_i - \mathbf{r}),$$

here $\theta(\mathbf{R})$ – equals to 1 in small $\omega$-vicinity of the point $\mathbf{R} = 0$ and to zero in the rest space. So calculation of (17) is reduced to counting the number of vertices occuring in the $\omega$-vicinity of the point $\mathbf{r}$ in the Markov random walk over possible trajectories.

The calculation of the kinetic energy variation for the positron in the atomic field can be made now by integration:

$$\langle \Delta E_k^1\rangle = \frac{1}{2}\int (\mathbf{r}, dU_{\text{pot}}/d\mathbf{r})\,\Delta\rho(\mathbf{r})\,d\mathbf{r} = \frac{4\pi}{2}\int_0^\infty r\frac{dU_{\text{pot}}}{dr}\Delta\rho(r)\,r^2 dr, \tag{18}$$

where $\Delta\rho(r) = \rho'(r) - \rho_0$–deformation of the local density of the positron cloud $\rho$ in the helium atom field ($\Delta\rho(r) \to 0$, $r \to \infty$). The expression (18) represents in fact the difference between the two integrals, including deformed and nondeformed density of the positron distribution. The surface contributions (which are dropped aside in the standard expression of the virial estimator) in our case are absent due to the mutual subtraction which should occur outside the region of the local deformation of the positron cloud. As $\Delta\rho(r)$ falls quickly with distance from an atom, the upper integration limit in (18) can be substituted by $R_{loc}$ (several atomic radii). Since unperturbed local density $\rho_0$ is the normalizing constant with respect to $\rho'(r)$ ($\rho'(r \to R_{loc}) \to \rho_0$)-$\Delta\rho(r)$ is a linear function of $\rho_0$ and $g(r) = \Delta_\rho(r)/\rho_0$ does not depend on $\rho_0$.

Linear dependence of the functional (18) on $\Delta_\rho(r)$ results in linear dependence of $\langle \Delta E_k^l \rangle$ on the local nondisturbed density $\rho_0$ in the $R_{loc}$-vicinity of the helium atom:

$$\langle \Delta E_k^l \rangle = \rho_0 \cdot \left[ 2\pi \int_0^{R_{loc}} r \frac{\partial U_{pot}}{\partial r} g(r)\, r^2\, dr \right] \tag{19}$$

Linear dependence of the kinetic energy on $\rho_0$ is caused by the additive character of the virial estimator for the distant vertices the Feynman trajectory so that the increase, together with $\rho_0$ of the part of the Feynman trajectory inside the $R_{loc}$-vicinity results in linear growth of the kinetic energy.

Let us consider a helium atom at a distance $R_0$ from the centre of the positron cloud with a preliminary calculated radial density distribution $\rho_0(R)$ (represented by a table and normalized): $\Sigma\, 4\pi R_i^2\, \Delta R \cdot \rho_0(R_i) = 1$, where $\Delta R$-thickness of a spherical layer, $R_i$-radius of the $i$-th layer. In order to obtain the contribution to the interaction energy He-e$^+$ from the part of the trajectory located in the close vicinity of the atom we shall consider a spherical concentrical shell around the atom in order to exclude preferred directions. Let us also consider that a piece of trajectory containing $\Delta N$ successively linked vertices is located within this region. The linear dimension of the region occupied by the piece of trajectory containing $\Delta$N vertices is estimated as $L \cdot \sqrt{\Delta N}$ where $L$ is a mean length of the trajectory link. We put forward the following requirements to the small (local) system with a helium atom in the centre of a sphere of radius $R_{loc}$ and a piece of Feynman trajectory with $\Delta N$ vertices:

1. The diameter of the spherical region should be sufficiently large so that the local influence of He should not spread outside the region and at the same time sufficiently small in order that the density of the free positron cloud could be considered constant within the region.
2. Mean length of the trajectory link should be considerably (several times) shorter than the half width of the potential well.
3. At the same time $\Delta$N should not be too great so that the MC-procedure could be carried out on existing computers.

The calculation of $E_{kin}^l$ and $E_{pot}^l$ accounting for the helium interaction with the piece of trajectory of e$^+$ in the local system is carried out according to the following scheme.

A piece of trajectory containing $\Delta N$ vertices is simulated in the spherical shell of radius $R_{loc}$ (the total length of the trajectory is considered to be $N$): the deformation of the local positron density as a result of He atom insertion in the centre of the sphere in investigated. It is evident that the insertion of the atom would move the density maximum to the region of the minimum of the potential (Figure 1).

If we know the radial density distribution of the positron cloud $\tilde{\rho}'(r)$ and $\tilde{\rho}_0(r)$ in presence and absence of the atom correspondingly, we can study the behaviour of $\tilde{\rho}'(r)/\tilde{\rho}_0(r)$. It is evident that this ratio would be minimum in the centre of the sphere, maximum in the region of $\tilde{\rho}'(r)$ function maximum, far from the atom where its influence is already negligible, the ratio approaches a horizontal level. If we denote the limit

$$\lim_{r \to \infty} \frac{\tilde{\rho}'(r)}{\tilde{\rho}_0(r)} = \varepsilon, \tag{20}$$

it is possible to consider a relative change of the positron density caused by insertion of the He atom:

$$\frac{\tilde{\rho}'(r)}{\tilde{\rho}_0(r)} - \varepsilon = \tilde{g}(r) \tag{21}$$

The limit $r \rightarrow \infty$ in (20) should be treated as a transition to values outside the region of local deformation but inside the spherical cavity including this region.

Relative deformations of the positron density distribution caused by insertion of the helium atom weakly depend on presence or absence of the limiting shell if its walls are located sufficiently distant outside the region of local deformation of the positron cloud. So we identify $g(r)$ in the rigorous expression (19) with $\tilde{g}(r)$ determined by (21) and calculated in the local region around the helium atom. The adequacy of such substitution could be verified by calculations with successively increasing radii of the limiting shell which were actually carried out in our studies.

Integrations of the function $\tilde{g}(r)$ (calculated preliminary by PIMC method in the local system) with (15) for the potential energy over the spherical volume within radius $R_{loc}$ give us coefficients $C_{pot}$ and $C_{kin}$ which multiplied by the density of the free positron cloud in the point of localization of an atom $\rho(R_o)$ give values of local variation of the potential and kinetic energy of the trajectory correspondingly due to the presence of the atom. For $U_{pot}$ in (19) and similar expression for the potential part of local interaction we use formula (15). Hence:

$$\begin{aligned} r\frac{\partial U_{pot}(r)}{\partial r} &= -e^2 \exp\left[-\frac{Z'r}{a}\right]\cdot\left[2r\left(\frac{Z'}{a}\right)^2 + \frac{2Z'}{a} + \frac{1}{r}\right] \\ &\quad - \alpha \cdot e^2 \begin{cases} (-4/r^4), & r \geqslant R_{\mathrm{He}} \\ (2r^2/R_{\mathrm{He}}^6), & r < R_{\mathrm{He}} \end{cases} \end{aligned} \tag{22}$$

After integration over angles $\phi$ and $\theta$ expressions for coefficients $C_{pot}$ and $C_{kin}$ become:

$$C_{\mathrm{pot}} = 4\pi \int_0^{R_{loc}} dr\, r^2 \tilde{g}(r)\, U_{pot}(r) \tag{23}$$

$$C_{kin} = 4\pi \int_0^{R_{loc}} dr\, r^2 \tilde{g}(r)\, \frac{1}{2}\left[r\frac{dU_{pot}(r)}{dr}\right] \tag{24}$$

### *Nonlocal contribution*

Contribution to the variation of the positron energy due to interaction of the helium atom located at a distance $R_0$ from the centre of the positron cloud with the nondisturbed part of the positron cloud is calculated by integration of the expression (15) with the function $\rho_0(R)$:

$$E'_{\mathrm{pot}}(R_0) = \int_0^{2\pi} d\phi \int_0^{\infty} dR \cdot R^2 \rho(R) \int_0^{\pi} d\theta \sin(\theta) \cdot (U_{\mathrm{pot}}(r))$$

Here $r = |\mathbf{R}_0 - \mathbf{R}|$ – the distance between the centre of the atom and the point of integration. Taking into account the expression (15) we obtain:

$$E'_{\mathrm{pot}}(R_0) = 2\pi \cdot \int_0^{\infty} dR \cdot R^2 \rho(R) \cdot \left[ u_{\mathrm{Coul}}(R, R_0) + u_{\mathrm{pol}}(R, R_0) \right], \tag{25}$$

where integration over angle $\phi$ has been done and $u_{\mathrm{Coul}}(R, R_0)$ and $u_{\mathrm{pol}}(R, R_0)$ are Coulomb and polarization energies (15) integrated over $\theta$. The expression for $U_{\mathrm{pol}}(R, R_0)$ is obtained in the Appendix 1. For the $u_{\mathrm{Coul}}(R, R_0)$ we obtain analogous expression:

$$u_{\mathrm{Coul}}(R, R_0) = \frac{a \cdot e^2}{2R_0 RZ'} \left[ \left( \frac{2Z'}{a} |R - R_0| + 3 \right) \cdot \exp\left( -2\frac{Z'}{a} |R - R_0| \right) - \left( -\frac{2Z'}{a}(R + R_0) + 3 \right) \cdot \exp\left( -\frac{2Z'}{a}(R + R_0) \right) \right] \tag{26}$$

Integration (25) over $R$ with integrands (26), (A1), (A2), (A3) and tabulated $\rho_0(R)$ should be done numerically. As starting with a certain $R_M$ $\rho(R > R_M) = 0$, the upper limit of the integral (25) is made equal to $R_M$.

So the presence of the He atom at a distance $R_0$ from the centre of mass of the positron cloud changes the kinetic and potential energy of the positron with the distribution function $\rho_0(R)$ correspondingly by values:

$$\Delta E_{\mathrm{kin}} = C_{\mathrm{kin}} \rho(R_0) \text{ and } E_{\mathrm{pot}} = E'_{\mathrm{pot}}(R_0) + C_{\mathrm{pot}} \rho(R_0)$$

## 5. DETAILS OF COMPUTATION AND RESULTS

As a result of MC simulation of a free positron at temperature 5 K we obtained the distribution of the positron density presented in Figure 2. A closed trajectory with 100 vertices and fixed centre of mass was considered.

Applying estimation formulae of section 4 of this paper we chose the following parameters for simulation of the local system at 5 K:

mean distance between vertices $L = 0{,}1$ Å
total number of vertices of the trajectory $N = 10^6$
the piece of the trajectory in the local system $\Delta N = 10^3$
its linear dimension – 4,0 Å.

For $R_{\mathrm{loc}}$ we took a value slightly exceeding this figure in order to include the area where the influence of He is already small.

MC simulation of a random walk of the trajectory piece in the local system requires imposing of boundary conditions on its ends. One can consider the following possibilities: to leave the ends free or to fix them at some appropriately chosen points. In both cases there appear nonstandard vertices. It is evidently possible to neglect their influence by excluding from averaging some neighbouring vertices. In this case some "extra" vertices (which do not contribute to the calculated averages) should be included in MC process. Closing the ends of the considered piece of the trajectory seems to be most convenient. In this case we get rid of nonstandard and "extra" vertices in MC process all the vertices become equivalent. Of course there appear long range correlations but the correlated vertices are so distant along the trajectory

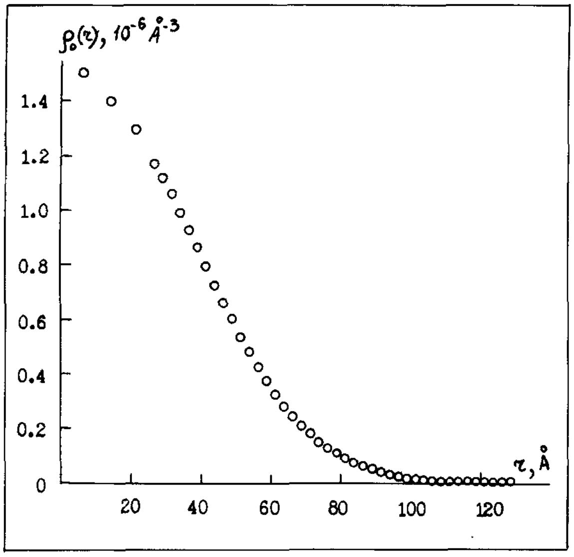

**Figure 2** Density distribution function for the positron cloud with the fixed centre of mass.

$(\Delta N - 10^3)$ that the effect seems to be non-essential. The closure of the ends can be considered as a kind of periodical boundary conditions.

When generating configurations of the local system we used the following types of MC steps.

1. Microscopic move – variation coordinates of a single ($i$-th) vertex:
   $\mathbf{r}_i \rightarrow \mathbf{r}_i + \Delta\mathbf{r}$
2. Macroscopic move of the first type – a parallel shift of the coordinates of all the vertices simultaneously:
   $\mathbf{r}_j \rightarrow \mathbf{r}_j + \Delta\mathbf{R} \quad j = 1, \dots N$
3. Macroscopic move of the second type – rotation of the whole trajectory around its centre of mass in coordinate planes XOY, YOZ, ZOX successively at random angles.

MC chains of $15 \cdot 10^3$ macrosteps have been generated. A macrostep contains $\Delta N$ attempts to make a micromove and one attempt to make a macromove of each type. If macromoves were excluded the convergence became considerably worse, especially for great $\Delta N$. The reason is that in each micromove only $1/\Delta N$ part of the trajectory is involved and after $\Delta$N microsteps in random directions, the macroscopic shift of the trajectory as a whole has an order of $\Delta \mathrm{r}/\sqrt{\Delta N}$.

The results of the MC study of the local density variation after insertion of the helium atom are represented in Figure 3. $\rho_0(r)$ has a "plateau" (with radius $\simeq$ 2,3 Å) in the centre of the considered area and slowly falls in the external region. Contrary to $\rho_0(r)$, $\rho'(r)$ has a maximum at a distance of 1,9 Å from the centre (with the half width $\simeq$ 2,3 Å), which corresponds to concentration of the trajectory in potential well of the He-e$^+$ interaction. The maximum of $\rho'(r)$ is slightly shifted from the minimum of the potential to greater distances.

Consider the ratio $\rho'(r)/\rho_0(r)$. It is:

- minimum ($\simeq$ 0,06) at small distances from the centre of the sphere where the helium atom is located,

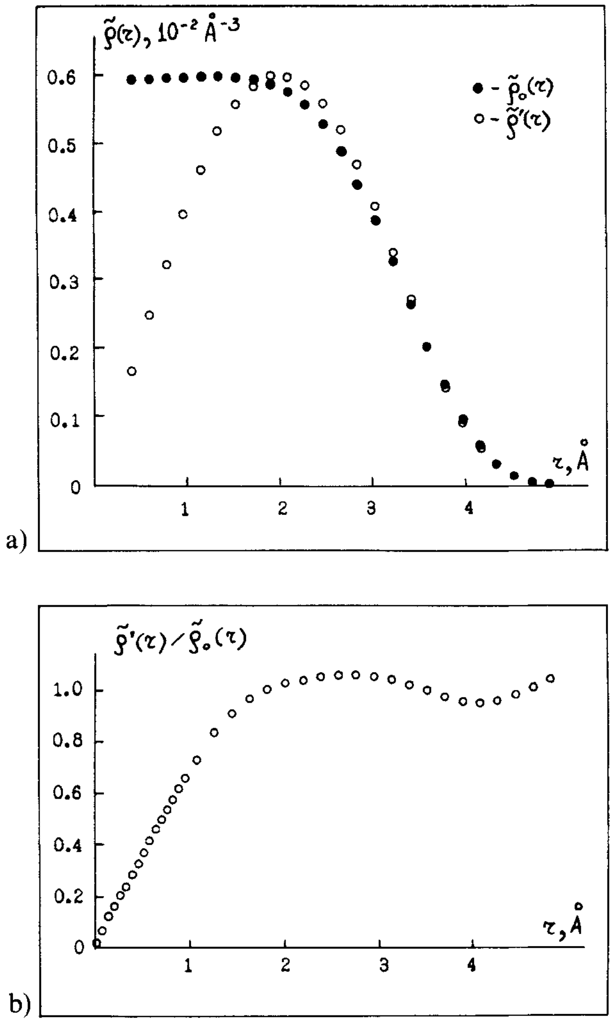

**Figure 3** Positron density distribution function in the local system in absence ($\rho_0(r)$) and presence ($\tilde{\rho}'(r)$) of the He atom (a); ratio of the densities $\tilde{\rho}'(r)/\rho_0(r)$ (b).

- maximum ($\simeq$ 1,06) in the region of the $\rho'(r)$ maximum,
- nearly horizontal ($\simeq$ 0,96) at far distances ($>$3,9 Å) from the centre,
- it has a considerable error in the vicinity of the boundary (with the width = 0,5 Å) which is excluded from further consideration.

For the ratio limit (20) we took the value 0,96; for the radius of the local region – $R_{loc}$ = 3,9 Å. Outside that radius we consider the positron density to be non-disturbed.

Using formulae (23) and (24) for the local coefficients we obtain the following values:

$$C_{kin} = 2{,}93 \cdot 10^{-35}\ \text{erg}\cdot\text{cm}^3 \qquad C_{pot} = -1{,}94 \cdot 10^{-35}\ \text{erg}\cdot\text{cm}^3$$

## 6. DISCUSSION AND CONCLUSION

We have formulated the procedure for computation of He-e$^+$ interaction and obtained the numerical results. Comparison of curves for (Figure 4)

$$\Delta E_{\text{kin}}(R_0) = C_{\text{kin}}\cdot\rho(R_0),\ E_{\text{pot}}^{\text{loc}}(R_0) = C_{\text{pot}}\cdot\rho(R_0) \text{ and } E'_{\text{pot}}(R_0)$$

indicates that all three contributions are comparable and neither of them could be neglected. Moreover the local part of the interaction $\Delta E_{\text{kin}}(R_0) + E_{\text{pot}}^{\text{loc}}(R_0)$ is positive that corresponds to repulsion of the He atom from the positron cloud. Such behaviour of the local part is caused by a narrow (compared with the size of the atom) and deep minimum of the He-e$^+$ potential curve (Figure 1). Strong deformation of the positron wave function in the region of the minimum results in considerable increase of the kinetical part $\Delta E_{\text{kin}}$ which is not completely compensated by the decrease of the potential energy $E_{\text{pot}}^{\text{loc}}$. Only the nonlocal part provides the attractive character of the resulting interaction.

Our result does not confirm the hypothesis suggested in [2]. In [2] a model potential He-e$^+$ is considered at $T = 0$ based on the assumption of local character of interaction:

$$E(\mathbf{r}) = 2\pi a_{+}|\Phi_{+}(\mathbf{r})|^2 \tag{27}$$

Here $E(\mathbf{r})$ - the potential to be determined, $a_+ < 0$ - scattering length of e$^+$ in helium for which the value averaged over the experimental data is used. $\Phi_+$ - the positron wave function in the Born-Oppenheimer approximation for which the Schroedinger equation is written:

$$-\tfrac{1}{2}\nabla^2\Phi_+ + 2\pi a_+(n(\mathbf{r}) - n_0)\Phi_+ = E_+\Phi_+ \tag{28}$$

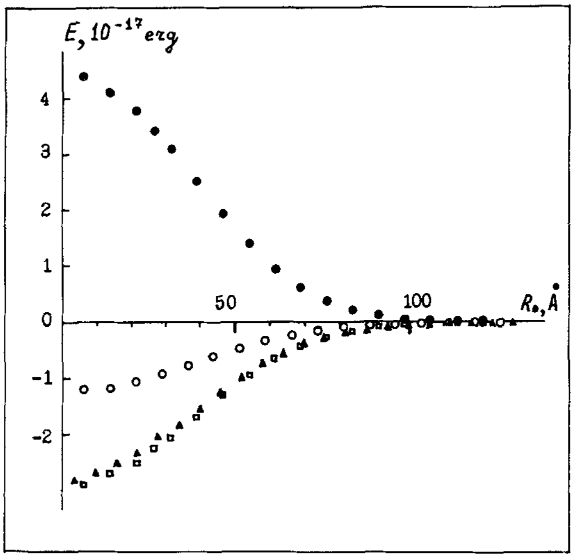

**Figure 4** Contributions to pseudopotential He-e$^+$ of local interaction (□ - $C_{\text{pot}}\cdot\rho(R_0)$ - potential part; ● - $C_{\text{kin}}\cdot\rho(R_0)$ - kinetic part) and nonlocal interaction (▲ - $E'_{\text{pot}}(R_0)$); ○ - resulting pseudopotential.

Distribution of the local density of He atoms $n(\mathbf{r})$ is made consistent with $\Phi_+(\mathbf{r})$ through the potential $E(\mathbf{r})$ by the extremum condition imposed on the potential $\Delta\Omega$ for the helium cluster on the background of the bulk density $n_0$:

$$\Delta\Omega = \int d\mathbf{r}\,(fn) - f(n_0) + (n - n_0)E - (n - n_0)\,\mu(n_0)), \tag{29}$$

where $f(n)$ – the reduced specific Helmholtz free energy. Functional differentiation of (29) $\delta\Delta\Omega/\delta n(\mathbf{r}) = 0$ yields to the local equation for the chemical potential:

$$\mu(n) - \mu(n_0) + E(\mathbf{r}) = 0 \tag{30}$$

The explicit dependence $\mu(n)$ for $^3$He and $^4$He is taken in the Van-der-Vaals approximation and (27)–(29) are solved together numerically with respect to $\Phi_+(\mathbf{r})$, $E(\mathbf{r})$, $n(\mathbf{r})$. The size of the cluster is determined by integration of the extra density profile

$$N = \int d\mathbf{r}\,(n(\mathbf{R}) - n_0) - 100 \div 200 \text{ atoms} \tag{31}$$

The temperature is inserted into the theory [2] only through the functional dependence $\mu(n)$ for helium, thermalization of positrons is not accounted. This could be valid if the area of the positron localization was comparable with the range of He–e$^+$ forces.

On the othe hand as it becomes evident from the present work, the explicit account for the Coulomb and polarization forces of interaction of the He atom with the point charge of e$^+$ results in a deep (8000 K) and narrow (0.5 Å) minimum at the distance of 1.5 Å from the helium centre. Even at temperatures of several Kelvins only a small part (0.01 %) of the positron cloud is localized in this narrow region and the state of the positron is mainly determined by its thermal wavelength ($\sim T^{-1/2}$) which constitutes several hundred angstroms. Such a state of the positron should be considered as an essentially mixed one and the purely quantum problem is transferred into quantum statistical one.

Repeated calculations with various sets of the local region radii $R_{\mathrm{loc}}$ as well as variation of $\rho_0$ (the systematic error of $\rho_0$ depends on the specific value of $R_{\mathrm{loc}}$ and the stochastic error – on MC chain length) indicate that values of the potential and of its parts are determined with the error of several per cent. The error could be decreased by the use of faster computers. We used a computer with a speed of $10^6$ op/sec and consumed several dozens of hours of CPU.

In future we plan to use the constructed pseudopotential in calculations of cluster formation of helium on thermalized positrons.

## APPENDIX 1

As far as in (15) the expression for the estimator of the polarizational interaction depends on the relation between $R$ and $R_0$, the calculation of $u_{\mathrm{pol}}(R, R_0)$ is carried out taking into account three possible situations:

1. The spherical surface of radius $R$, over which the integration is made is situated inside the He atom. In this case:

$$R_0 < R_{\mathrm{He}} \text{ and } 0 < R < R_{\mathrm{He}} - R_0$$

and in the integral over $\theta$ the estimator $(-\alpha r^2/R_{\mathrm{He}}^6)$ is used. As a result we obtain:

$$u_{\mathrm{pol}}(R, R_0) = -2\alpha\cdot e^2\cdot(R_0^2 + R^2)/R_{\mathrm{He}}^6 \tag{A1}$$

2. The spherical surface is outside the atom. Then:

$$R_0 > R_{He} \text{ and } R < R_0 - R_{He} \text{ or } R > R_0 + R_{He}$$

and the estimator $(-\alpha/r^4)$ is integrated. The result is:

$$u_{pol}(R, R_0) = -2\alpha{\cdot}e^2/(R_0^2 - R^2)^2 \tag{A2}$$

3. The spherical surface crosses the atom. Here

$$R_0 - R_{He} < R < R_0 + R_{He}$$

In that case the interval of integration over $\theta$: $[0; \pi]$ is separated into two: $[0; \theta]$ and $[\theta; \pi]$, where $\theta$ depends on relations of $R$, $R_0$ and $R_{He}$:

$$\cos(\theta_0) = \frac{R^2 + R_0^2 - R_{He}^2}{2R_0}$$

In the first interval the estimator $(-\alpha r^2/R_{He}^6)$ is used, in the second - $(-\alpha/r^4)$. In this case:

$$u_{pol}(R, R_0) = -\frac{\alpha{\cdot}e^2}{4RR_0}\left[\frac{3}{R_{He}^2} - \frac{(R_0 - R)^4}{R_{He}^6} - \frac{2}{(R_0 + R)^2}\right] \tag{A3}$$

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