Isotopic Effects in the Muon Transfer from $p\mu$ and $d\mu$ to Heavier Atoms

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The results of accurate hyperspherical calculations of the muon-transfer rates from muonic protium and deuterium atoms to nitrogen, oxygen, and neon are reported. Very good agreement with measured rates is obtained and, for the three systems, the isotopic effect is perfectly reproduced. The transfer rate is higher for deuterium in the cases of nitrogen and neon due to constructive interferences between two transfer paths. The lower transfer rate for deuterium in the case of oxygen results from a large resonant contribution.

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In the framework of muon catalyzed nuclear fusion, isotopic dependence of the muon-transfer rate from hydrogen isotopes ($x\mu$, $x = p$ or d) to a heavier atom A has been extensively studied from the experimental point of view [1–3]. The results at thermal energies and below have shown that the transfer rate λ^p from muonic protium differs significantly from the transfer rate λ^d from muonic deuterium. Moreover, the observed isotopic variation of this rate drastically depends on the atom studied. Since the muon transfer occurs at very small internucleus distances [4], the process can be described as

$$(x\mu)_{1s} + A^{Z+} \rightarrow x + (\mu\mathrm{A})^{(Z-1)+}. \quad (1)$$

Although there have been several full three-dimensional calculations of muon-transfer rates at low energies between muonic hydrogen and low-Z atoms (see Ref. [5] and references therein), quantum-mechanical treatment of this reaction involving heavier nuclei is a numerically challenging problem. Indeed, as the charge Z of the nuclei increases, both initial-state polarization of the muonic-hydrogen and Coulomb final-state interactions increase. Moreover, the number of open channels even at zero relative kinetic energy increases with Z. Thus, up to now only approximate calculations have been performed [4,6–9].

In this Letter we present the first exact three-dimensional quantum calculations of muon exchange for collision energies in the range 10^{-3}–10 eV from both muonic protium and deuterium atoms to nitrogen, oxygen, and neon. Very good agreement with available experimental data is obtained. Moreover, our results provide physical insight into the isotopic effects.

The calculations were performed as follows. We use a time-independent close-coupling method and hyperspherical elliptic coordinates [10] extended to nonzero total angular momentum [11]. At each hyperradius ρ, the wave function is expanded on a set of adiabatic states depending on the hyperspherical angles. We use the approximate separability of the Hamiltonian at fixed ρ for a three body Coulomb potential [12] to compute these states efficiently and accurately [11]. The matrix representation of the Hamiltonian operator is diagonalized in a basis of products of functions depending on only one hyperspherical angle. These one-dimensional functions are expanded on a basis of Legendre functions. For energies below 10^{-1} eV, the de Broglie wavelength of the system ($\lambda > 1$ Å) is much larger than the effective range of the potential interaction ($a \sim 0.1$ Å). Thus, even at thermal energies, the muon-transfer process is equivalent to an ultracold collision that requires high precision calculations. For the energies of the hyperspherical states (in particular, the one that corresponds to the entrance channel of reaction (1) for which convergence is worst), our method achieves an absolute accuracy of 5×10^{-7} eV. This is about a thousand times smaller than the lowest collision energy considered. To perform the propagation, we use a diabatic-by-sector representation [13]: in each sector, a locally diabatic hyperangular basis computed at the center of the sector is used. For a given total angular momentum J, the scattering S-matrix and transfer probabilities $P_J(E)$ are obtained by a standard matching analysis at large ρ, which makes it possible to switch from hyperspherical to Jacobi coordinates [14]. With a match at $\rho \sim 1$ Å, the convergence of the transfer probabilities is better than 0.1%. For the energy range considered here, we included 88 coupled channels [$(x\mu)_{1-2} + A^{Z+}$ and $(A\mu)^{(Z-1)+}_{4-13} + x$] for nitrogen and oxygen. For neon, because of the larger charge of the nucleus $Z = 10$, many more channels have to be included to obtain the convergence of the results. In this case, calculations have been made with 133 channels [$(x\mu)_{1-2} + \mathrm{Ne}^{10+}$ and $(\mathrm{Ne}\mu)^{9+}_{4-16} + x$]. The muon-transfer cross section is then given by

$$\sigma(E) = \frac{\pi\hbar^2}{2mE}\sum_J (2J+1)P_J(E), \quad (2)$$

where $m = m_A(m_x + m_\mu)/(m_A + m_x + m_\mu)$. Finally, the muon-transfer rate is calculated using

$$\lambda(E) = N\left(\frac{2E}{m}\right)^{1/2}\sigma(E), \quad (3)$$

N being the number density of liquid hydrogen (4.25×10^{22} cm^{-3}). Partial transfer rates $\lambda_J(E)$ obtained with a single J value instead of the sum in Eq. (2) can also be defined.

The results of our calculations are presented in Figs. 1–3 for nitrogen, oxygen, and neon, respectively.

For each system, total and partial transfer rates versus collision energy from $p\mu$ and $d\mu$ are reported separately in the top panels. In perfect agreement with standard analytical threshold behavior [15], we find that each partial transfer rate is proportional to E^J.

In the lower panel of Figs. 1–3 we present the total transfer rates for the two isotopes (λ^d, λ^p), together with the available experimental data. At thermal energy, the transfer rate from muonic deuterium is about 3 times higher than the one from muonic protium (see Fig. 1) for nitrogen and higher by a factor of 15 for neon (Fig. 2). For oxygen (Fig. 3) we observe an opposite trend: λ^d is about 0.8 times smaller than λ^p. The agreement between theory and experiments is very good for the three systems, and the right trend of the isotope effects is perfectly reproduced. The completely different isotope ratios can be understood in terms of partial wave contributions. The partial rate for $J = 0$ is systematically higher for $d\mu$ than for $p\mu$. Thus, at the lowest energies considered the total transfer rate is always higher for $d\mu$. At higher energies, the trend may be modified by resonant contributions of higher partial waves. For instance, in the case of oxygen, there is a strong $J = 1$ resonance that significantly increases the transfer from $p\mu$ at thermal energy.

In order to understand the systematic higher value of the transfer rate from $d\mu$ at low energies, we performed a two-state quantum calculation. Indeed, for all the systems considered, exact calculations have shown that one exit channel is predominantly populated, in particular, at low energies: $x + (\mathrm{N}\mu)^{6+}_{n=5}$ for nitrogen, $x + (\mathrm{O}\mu)^{7+}_{n=5}$ for oxygen, and $x + (\mathrm{Ne}\mu)^{9+}_{n=6}$ for neon. We use the analytic asymptotic forms for both entrance and exit channels with a Gaussian coupling to fit the quasicrossing of the hyperspherical adiabatic states for $J = 0$. The results for nitrogen are reported in Fig. 4. Similar results have been obtained for the other systems considered. The oscillatory pattern that appears on the exact results also shows up in the two-state model calculations. This pattern is typical of Stuckelberg oscillations [16], which are due to interferences between the two dominant paths for charge transfer, one corresponding to a charge exchange while particles are approaching and the other one while they are moving away. The phase shift between these two paths is given in a semiclassical picture by the difference between the corresponding action integrals and is thus proportional to $\sqrt{m}$. It turns out that at low energies, the phase shift produces constructive interferences for $d\mu$ and destructive interferences for $p\mu$. Transfer rates are thus higher for $p\mu$.

Actually, the experiments have been performed at a given temperature (mostly at room temperature [1–3], but data at $T = 20$ K are also available for neon). In such experiments, muons are stopped in a mixture of protium, deuterium, and a heavier element A at lower concentration. Muons are predominantly captured by protium and deuterium, but can subsequantly transfer to heavier elements through reaction (1). Deexcitation of the product complex (μA) induces x-ray cascades and provides time

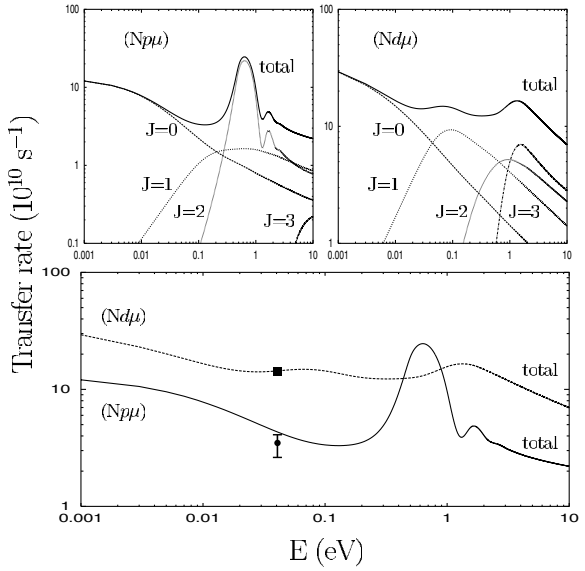

FIG. 1. Partial and total transfer rates versus collision energy for nitrogen. The circle (square) indicates the experimental results for N$p\mu$ (N$d\mu$).

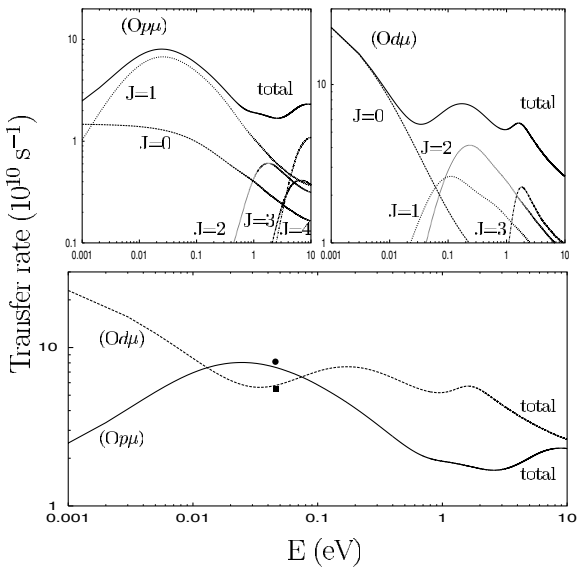

FIG. 2. Partial and total transfer rates versus collision energy for oxygen. The circle (square) indicates the experimental results for O$p\mu$ (O$d\mu$).

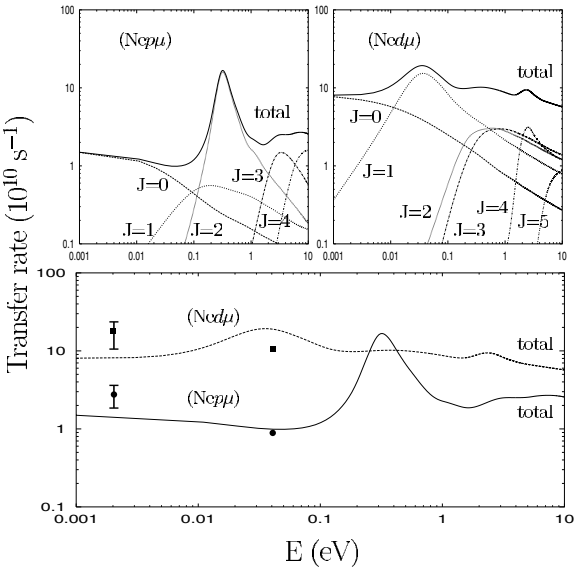

FIG. 3. Partial and total transfer rates versus collision energy for neon. Circles (squares) indicate the experimental results for Ne$p\mu$ (Ne$d\mu$).

spectra. The transfer rate is then obtained in fitting these time spectra with a single exponential function. This method assumes that the kinetic energy distribution of hydrogen isotopes at the considered temperatures is known. In order to compare the experimental results with our predictions, we need to calculate a temperature dependent muon-transfer rate $\lambda(T)$ defined as the average value of $\lambda(E)$ obtained with a Maxwellian kinetic energy distribution at temperature T. The values of these average transfer rates are reported in Table I. One noteworthy feature is the very good agreement with the available experimentals results. The quality of the agreement is lower for neon at $T = 20$ K. However, the error bar of the experimental results is larger in this case. Also, the

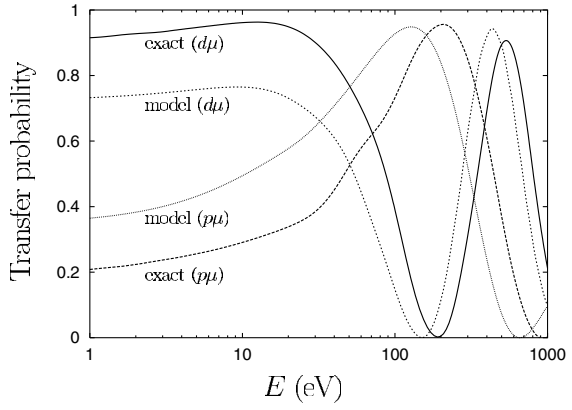

FIG. 4. Comparison between exact transfer probabilities from muonic protium and deuterium to nitrogen and the two-extracted-states model.

TABLE I. Total average transfer rates obtained with a Maxwellian distribution at the indicated energies. For comparison available experimental results taken from [1–3] are also reported. The used unit is 10^{10} s^{-1}.

Nucleus	E (eV)	λ^p	Expt.	λ^d	Expt.
Nitrogen	0.04	5.2	3.4 ± 0.7	14.8	14.5 ± 0.2
Oxygen	0.04	7.77	8.5 ± 0.5	6.6	5.5 ± 0.5
Neon	2×10^{-3}	1.2	3 ± 1	10.5	18 ± 7
	0.04	1.02	0.849 ± 0.002	15.0	10.1 ± 0.3

Maxwellian distribution that we use to compute the average rate may not be realistic for liquid hydrogen.

These results are the first systematic theoretical analysis of the isotopic effects involved in the muon-transfer process and provide the best agreement with experimental data achieved up to now. For low energies, the predictions made by Gershtein [4] give a transfer rate from muonic protium 1.4 times higher than from muonic deuterium. These predictions are erroneous since, in their Landau-Zener–type treatment, they neglect the interference effects that we have shown to be crucial. For oxygen, approximate calculations performed by Sultanov and Adhikari are in good agreement with the experimental results [7]. These calculations consisted in a two-state integro-differential Fadeev-Hahn treatment with $J = 0$ partial wave. However, our present work shows that the $J = 1$ wave has to be taken into account in the calculations at thermal energy. Moreover, two states are not enough to achieve convergence. Thus, the apparent agreement of these calculations with experiments is most probably due to a cancellation of errors. Concerning the neon, the unexpected isotopic effects observed at low energy have been qualitatively described by Sayasov [9] using a uniform semiclassical treatment. For this system, calculations have been performed for protium by Romanov [8]. These results disagree with the experiments by at least a factor of 2, which we believe is due to their approximate treatment of the entrance channel. Our calculations give much better agreement with experiment (only 15% relative error).

In conclusion, we have performed accurate calculations of the muon-transfer rate from muonic protium and deuterium to nitrogen, oxygen, and neon using a hyperspherical elliptic close-coupling method. Very good agreement with experimental results has been obtained both for absolute values and isotopic ratios of the muon-transfer rates for the three systems. In particular, going from protium to deuterium, the higher rates for nitrogen and neon as well as the lower rate for oxygen are well reproduced. The low energy behavior of the ratio of the transfer rate from muonic protium and muonic deuterium is well understood in terms of quantum interferences involving different reaction paths. At higher energy resonances associated with nonzero total angular momentum, partial

waves can play a key role and, in particular, yield a higher rate from muonic protium than from muonic deuterium for oxygen at thermal energy.

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[1] L. Schellenberg, Muon Catal. Fusion **5/6**, 73 (1990/1991).
[2] R. Jacot-Guillarmod, Phys. Rev. A **51**, 2179 (1995).
[3] A. Werthmüller, A. Adamczak, R. Jacot-Guillarmod, L. S. F. Mulhauser, L. Schellenger, H. Schneuwly, Y. Thalmann, and S. Tresch, Hyperfine Interact. **116**, 1 (1998).
[4] S. S. Gershtein, Zh. Eksp. Teor. Fiz. **43**, 706 (1962) [Sov. Phys. JETP **16**, 501 (1963)].
[5] R. A. Sultanov and S. K. Adhikari, J. Phys. B **35**, 935 (2002).
[6] P. K. Haff, E. Rodrigo, and T. A. Tombrello, Ann. Phys. (N.Y.) **104**, 363 (1977).
[7] R. A. Sultanov and S. K. Adhikari, Phys. Rev. A **62**, 22509 (2000).
[8] S. V. Romanov, Eur. Phys. J. D **28**, 11 (2004).
[9] Yu. S. Sayasov, Helv. Phys. Acta **63**, 547 (1990).
[10] O. I. Tolstikhin, S. Watanabe, and M. Matsuzawa, Phys. Rev. Lett. **74**, 3573 (1995).
[11] A. Dupays, B. Lepetit, J. A. Beswick, C. Rizzo, and D. Bakalov, Phys. Rev. A (to be published).
[12] O. I. Tolstikhin and M. Matsuzawa, Phys. Rev. A **63**, 62705 (2001).
[13] B. Lepetit, J. M. Launay, and M. L. Dourneuf, Chem. Phys. **106**, 103 (1986).
[14] O. I. Tolstikhin and H. Nakamwa, J. Chem. Phys. **108**, 8899 (1998).
[15] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon, Oxford, 1977).
[16] E. C. G. Stuckelberg, Helv. Phys. Acta **5**, 369 (1932).