Vibrational cross sections for positron scattering by nitrogen molecules

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We present a systematic study of low-energy positron collision with nitrogen molecules. Vibrational elastic and excitation cross sections are calculated using the multichannel version of the continued fractions method in the close-coupling scheme for the positron incident energy up to 20 eV. The interaction potential is treated within the static-correlation-polarization approximation. The comparison of our calculated data with existing theoretical and experimental results is encouraging.

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I. INTRODUCTION

The collision process of a charged particle with an atom or molecule is a many-body problem. Quantum-mechanical treatment of such a process consists in the resolution of the time-independent Schrödinger equation of $N+1$ particles, which is in general very difficult. Therefore, the main goal of theoretical efforts objectives new methodology that solves this many-body equation in a most exact way as possible. In this sense, positron-molecule scattering constitutes a very interesting problem for such a purpose. Apparently, theoretical treatment for the positron-molecule interaction seems to be simpler than that for the electron, due to the distinguishability between the projectile and the target particles. Consequently, there is no need to account for the exchange effects in the collision dynamics. On the other hand, it is known that the static part (V_{st}) of the positron-molecule interaction is repulsive whereas the correlation-polarization potential (V_{cp}) is predominantly attractive. Therefore, the scattering parameters calculated using a static-polarization-correlation (SPC) approach are very sensitive to the delicate balance of the repulsive and attractive components of the interaction potential [1], due to the cancellation of the two parts during the computation. Small changes in V_{cp} may cause significant variation in the calculated cross sections. Particularly if the calculations are carried out using a model polarization potential, the accuracy of the calculation would depend directly on how realistic the proposed model can represent the correlation-polarization interaction between the projectile and the target. It is known that a complete description of the positron-molecule interaction dynamics should also account for the contributions due to the positron-annihilation and the positronium-formation mechanisms. Even at very low incident energies where the positronium-formation channel is closed, the contribution due to the virtual positronium formation has still to be accounted for. In this sense, the V_{cp} for positron-molecule scattering cannot be the same as that for electrons. The construction of a model that can provide reliable cross sections in a wide energy range for a variety of molecules is still an open problem. Therefore, the comparison of the theoretical scattering parameters with the measured values would provide an estimate of the accuracy of the polarization potential used [2–4].

The positron-molecule scattering calculations become even more complicated when nuclear degrees of freedom are also included into the scattering calculations. Especially in the low-energy region where the projectile spends a longer time with the target molecule, the coupling between the electronic and rovibrational motions is relevant and must be adequately treated. To tackle this situation, approaches with different coupling schemes, namely, the adiabatic nuclei (AN) model [5], the rotational laboratory-frame close-coupling (LFCC) approximation [6–9], the body-frame vibrational close-coupling (BFVCC) approximation [6–9], etc, can be employed in such studies. However, the applicability of the different theoretical methods depends on the energy of the incident particle.

Recently, our group has started theoretical investigation on low-energy positron-molecule collisions [3,4]. Within the SPC framework, the continued fractions method (MCF) [10] was applied to solve the fixed-nuclei scattering equations. The comparison of our results with the existing experimental and other calculated data is encouraging. Moreover, MCF was also successfully applied in cross-section calculations for electron-impact vibrational excitation of H_2 [11,12].

In the present work, we extend the application of the MCF to study the vibrational excitation of N_2 induced by low-energy positron impact. The SCP approximation is used to represent the dynamics of the interaction. State-to-state cross sections for vibrational $\nu = 0 \rightarrow \nu' = 0-4$ transitions are reported in the $0-10$ eV range.

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To date, there are relatively few theoretical investigations on vibrational excitation of molecules induced by positron impact. Among them, positron-impact vibrational excitation of H_2 is the most studied [2,13–15]. Particularly for N_2, the only theoretical study reported in the literature is that of Gianturco and Mukherjee [13]. In their work, cross sections for vibrational excitations from the $\nu = 0 \rightarrow \nu' = 1,2,3,4$ are calculated using the BFVCC approximation in the incident-energy range varying from the threshold to 8 eV. In addition, some theoretical studies of elastic positron collisions with this target were performed in past years using the Kohn variational method [16] and the multichannel Schwinger variational method (SMC) [1].

Experimentally, there is no cross-section data for positron-impact vibrational excitation of N_2. As far as we know, there are some data of total cross sections (TCS) in absolute scale [17–20] and also vibrationally unresolved relative elastic differential cross sections (DCS) [21] available in the literature. Therefore, the comparison of our calculated results and the existing experimental and theoretical data may provide deeper information on positron-N_2 scattering.

This article is organized as follows. In Sec. 2, we briefly outline the theoretical method used; in Sec. 3, the calculated results are presented and compared with those available in the literature, and finally in Sec. 4, a short conclusion is presented.

II. THEORY

In our study, the dynamics of the interaction between the incident positron and N_2 molecule is described using the BFVCC approximation [22]. Within this formalism, the wave function of the inelastically scattered positron is the solution of a set of vibrationally coupled scattering equations,

$$\left(\nabla^2 + k_\nu^2\right) F_\nu = \sum_{\nu'} U_{\nu\nu'} F_{\nu'} \tag{1}$$

where F_ν is the positron scattered wave function, associated with the vibrational state ν of the target, $k_{\nu'}$ is the magnitude of linear momentum of the scattered positron, and $U_{\nu\nu'}$ is a matrix element of the potential operator and is given by

$$U_{\nu\nu'}(\vec{r}) = \iint \nu(R)^* \psi_0(\vec{r}_e, R)^* V_{\text{int}} \times (\vec{r}_e, \vec{r}, R) \nu(R) \psi_0(\vec{r}_e, R)\, dR\, d\vec{r}_e. \tag{2}$$

In the above equation, $\vec{r}_e$ represents collectively the position vector of target electrons, $\vec{r}$ is the position vector of the positron, R is the internuclear distance, $\nu(R)$ and $\psi_0(\vec{r}_e, R)$ are the vibrational part and electronic part of the molecular wave function, respectively, and

$$V_{\text{int}}(\vec{r}_e, \vec{r}, R) = -\sum_i \frac{1}{|\vec{r}_i - \vec{r}|} + \sum_j \frac{Z_j}{|\vec{R}_j - \vec{r}|} + V_{\text{cp}}(\vec{r}, R), \tag{3}$$

where $\vec{r}_i$ and $\vec{R}_j$ are position vectors of ith electron and jth nucleon of the target, respectively. The R-dependent V_{cp} has an asymptotic form,

$$V_{\text{pol}} = -\frac{1}{2}\left\{\frac{\alpha_0(R)}{r^4} + \frac{\alpha_2(R)}{r^4} P_2[\cos(\theta)]\right\} \tag{4}$$

at large r. In Eq. (4), α_0 and α_2 are the R-dependent spherical and nonspherical components of the dipole polarizability.

At small r, the V_{cp} is predominantly the positron-electron correlation. Its functional form is given as [23]

$$2V_{\text{cor}} = \begin{cases} -\frac{1.56}{\sqrt{r_s}} + (0.051 \ln r_s - 0.081) \ln r_s + 1.14, & r_s \leqslant 0.302, \\ -0.92305 - \frac{0.05459}{r_s^2}, & 0.302 \leqslant r_s \leqslant 0.56, \\ -\frac{13.15111}{(r_s+2.5)^2} + \frac{2.8655}{(r_s+2.5)} - 0.6298, & 0.56 \leqslant r_s \leqslant \infty, \end{cases} \tag{5}$$

where $r_s = [3\pi\rho(\vec{r}_e, R)/4]^{1/3}$ and $\rho(\vec{r}_e, R)$ is the electronic density.

The calculation starts with computation of ground-state molecular wave functions at the Hartree-Fock (HF) level, for 15 internuclear distances (R) ranging from 1.8 to 3.0 a.u. The basis functions used in the HF calculations are those of Huzinaga [24]. For each R, an interaction potential parametrically dependent on R,

$$U(\vec{r}; R) = \int \psi_0(\vec{r}_e, R)^* V_{\text{int}}(\vec{r}_e, \vec{r}, R) \psi_0(\vec{r}_e, R)\, d\vec{r}_e, \tag{6}$$

is calculated via integration over the coordinates of target electrons. In the above integration, the R-dependent polarizabilities used are those of Morrison and Saha [25]. In order to perform the integration over R in Eq. (3), for each $\vec{r}$, the obtained results from Eq. (6) are interpolated in a 1000-point R grid. The vibrational wave functions are obtained by solving the equation,

$$\left\{\frac{d^2}{dR^2} + 2\mu[\varepsilon_\nu - \varepsilon(R)]\right\} \nu(R) = 0, \tag{7}$$

where μ is the molecular reduced mass and $\varepsilon(R)$ is the potential curve of the ground-state target. In our calculation, the vibrational wave functions were calculated using the numerical method of Cooley [26] from the Rydberg-Klein-Rees (RKR) potential curve of the ground electronic state N_2 [27]. Finally, the integration over R in Eq. (2) is carried out for each $\vec{r}$ using a Gauss quadrature.

After the vibrational coupling potential operator $U_{\nu\nu'}(\vec{r})$ is calculated, we can now solve the BFVCC equations, given in Eq. (1). To do so, we first convert that equation [28] into a matrix form of integral equations, whose elements are

given as

$$\Psi_{\nu\nu'} = S_{\nu\nu'}\delta_{\nu\nu'} + G^0_{\nu\nu}\sum_{\nu''} U_{\nu\nu''}\Psi_{\nu''\nu'} \tag{8}$$

where $\Psi_{\nu\nu'}$ is the scattering positron wave function associated with the $\nu \to \nu'$ vibrational transition; $\delta_{\nu\nu'}$ is the Kronecker delta, $S_{\nu\nu}$ is the solution of the unperturbed Schrödinger equation, and $G^0_{\nu\nu}$ is the free-particle Green's operator, both associated with the vibrational state $|\nu\rangle$. The dimension of this is the number of the vibrational states included in the calculation. Five vibrational states are included in the present study.

The BFVCC integral equations are solved using the multichannel version of method of continued fractions (MCF-MC) [11,12,29]. The application of MCF consists in defining a weakened interaction potential, in nth order as

$$\widetilde{U}^{(n)} = \widetilde{U}^{(n-1)} - \widetilde{U}^{(n-1)}|\widetilde{S}^{(n-1)}\rangle(\widetilde{A}^{(n-1)})^{-1}\langle\widetilde{S}^{(n-1)}|\widetilde{U}^{(n-1)}, \tag{9}$$

and the nth order correction to the D matrix is defined through the relation,

$$\widetilde{D}^{(n)} = \langle\widetilde{S}^{(n-1)}|\widetilde{U}^{(n-1)}|\widetilde{S}^{(n-1)}\rangle + \widetilde{A}^{(n)}[\widetilde{A}^{(n)} - \widetilde{D}^{(n-1)}]^{-1}\widetilde{A}^{(n)}, \tag{10}$$

where

$$\widetilde{A}^{(n)} = \langle\widetilde{S}^{(n)}|\widetilde{U}^{(n)}|\widetilde{S}^{(n)}\rangle, \tag{11}$$

and

$$\widetilde{S}^{(n)} = \widetilde{G}^P\widetilde{U}^{(n-1)}\widetilde{S}^{(n-1)}. \tag{12}$$

The scattering matrix element associated with the $\nu \to \nu'$ vibrational transition, $K_{\nu\nu'}$, is related to the $D_{\nu\nu'}$ element as follows:

$$K_{\nu\nu'} = -D_{\nu\nu'}. \tag{13}$$

The iterative procedure in the MCF is interrupted when the previously selected convergence criterium is achieved. In the present study, the scattering matrix with their dominant elements converged better than 0.1% are obtained within five iterations. The converged scattering matrix represents the exact solution of the BFVCC scattering equation.

Next, the transition T-matrix element of the problem can be obtained as

$$T_{\nu\nu'} = -\frac{2K_{\nu\nu'}}{(1 - iK_{\nu\nu'})}. \tag{14}$$

In this study, a j_t-basis expansion [30] is used to calculate DCS, as follows:

$$\frac{d\sigma}{d\Omega}(\nu \to \nu') = \frac{k_f}{k_i}\sum_{j_t m_t m'_t}\frac{1}{2j_t+1}\left|B^{j_t}_{m_t m'_t}((\nu \to \nu'),k_0,k_f,\hat{r})\right|^2, \tag{15}$$

where $\vec{j}_t = \vec{l}' - \vec{l}$ is the momentum transfer during the collision, the m_t and m'_t are the projections of $\vec{j}_t$ in the LF and BF axes, respectively. The terms $B^{j_t}_{m_t m'_t}(\nu \to \nu')$ are the $\vec{j}_t$-expansion coefficients of the scattering amplitude, given by

$$B^{j_t}_{m_t m'_t}(\nu \to \nu';\Omega) = \sum_{l'lm'm}(-1)^m a_{ll'mm'}(ll'0m_t|j_t m_t) \times (ll'mm'|j_t m'_t)Y_{lm_t}(\Omega'), \tag{16}$$

and $a_{ll'mm'}$ are the partial-wave dynamics coefficients associated with the $\nu \to \nu'$ vibrational transition and are related to the partial-wave components of the matrix elements $T_{\nu\nu'}$ via

$$a_{ll'mm'}(\nu \to \nu') = -\tfrac{1}{2}\pi[4\pi(2l'+1)]^{1/2}i^{l'-1}\langle k_f lm|T_{\nu\nu'}|k_0 l'm'\rangle. \tag{17}$$

Moreover, in order to compare our calculated results with the vibrationally unresolved experimental and theoretical data available in the literature, we define the vibrationally summed (VS) DCS for the initial vibrational state $\nu = 0$, as

$$\left[\frac{d\sigma}{d\Omega}\right]_{\rm VS} = \sum_{\nu'}\frac{d\sigma(0 \to \nu')}{d\Omega}. \tag{18}$$

Finally, the vibrational excitation integral cross section (ICS) is given by

$$\sigma(\nu \to \nu') = \int\frac{d\sigma(\nu \to \nu')}{d\Omega}d\Omega. \tag{19}$$

III. RESULTS AND DISCUSSION

In Fig. 1, we present our results of VS DCS at positron incident energies of 5.25, 6.75, 10.0, and 20.0 eV, in comparison with the vibrationally unresolved (VU) DCS calculated by de Carvalho *et al.* [1] using the SMC and the experimental VU DCS, in relative scale, of Przybyla *et al.* [21], normalized to our data at the scattering angle of 60°. In general, our VS DCS are in good qualitative agreement with the experimental data, particularly for energies of 10.0 and 20.0 eV. At lower energies, although the main features in the experimental data such as the minimum and maximum are reproduced by our calculation, the position of these features in calculated data are shifted to small scattering angles. This discrepancy may be attributed to the accuracy of the model $V_{\rm cp}$ used in our calculation since the disagreement is more pronounced at lower incident energies where the influence of the correlation-polarization effects is expected to be more relevant. Furthermore, the $V_{\rm st}$ component in our calculation was calculated exactly. Comparison with the calculated data of de Carvalho *et al.* [1] also show better agreement at 10 eV. At lower incident energies, although the first minimum appears at about the same position, their data exhibit a second minimum located at about 90° which is neither seen in our data nor in the experimental results. The disagreement observed between the results obtained using the two theoretical methods may reflect the different way of treating the correlation-polarization effects. Nevertheless, both methodologies were unable to reproduce the correct position of the minimum and maximum features seen in the experimental data. The fact that these two very different methodologies lead to similar position of the first minimum is both interesting and intriguing. More experimental investigations are certainly welcome to help clarify the discrepancies between the theoretical and experimental data.

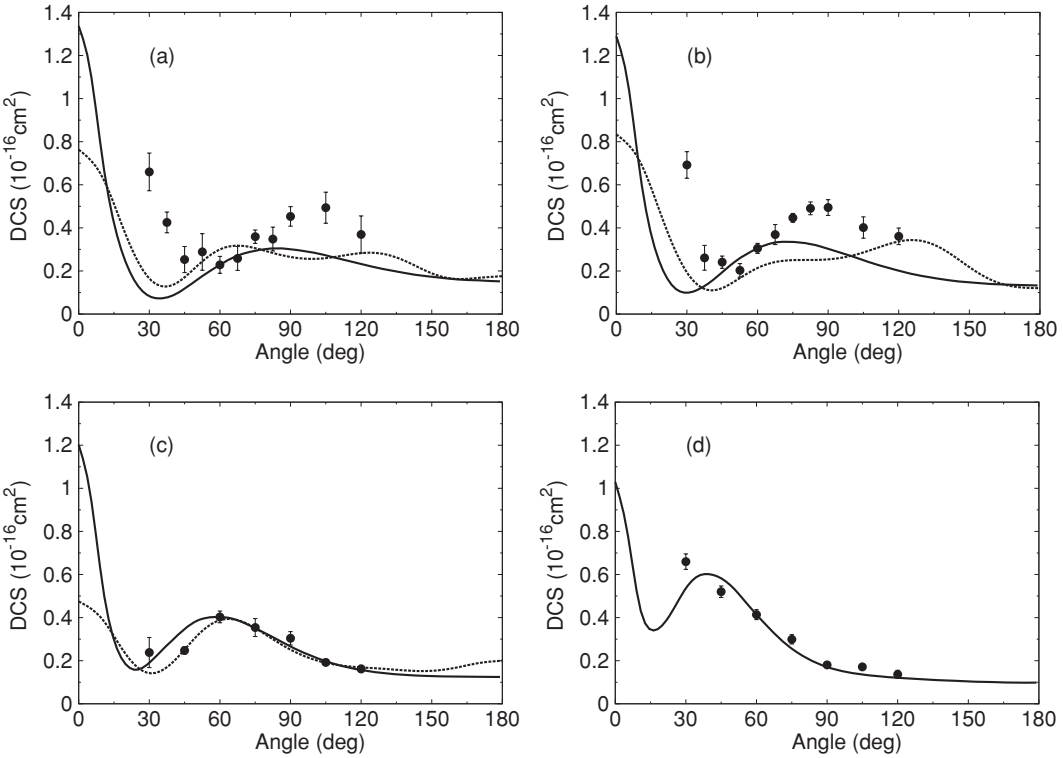

FIG. 1. Elastic DCS for the e^+-N_2 at (a) 5.25 eV, (b) 6.75 eV, (c) 10 eV, and (d) 20 eV. Solid line, present VS data using the MCF; dashed line, VU data of [1] calculated using the SMC; solid circles, experimental VU DCS of [21] in relative scale, normalized to our data at the scattering angle of 60°.

Moreover, the fact that our results do not show a second minimum structure at about 90° as seen in de Carvalho *et al.* [1] combined with the fact that our DCS are systematically larger than theirs at low angles may indicate the lack of higher partial-wave components in their calculations. In our methodology, the convergence in partial-wave expansion is easily verified by the inclusion of more terms, whereas in the SMC calculations, the inclusion of higher partial waves depends strongly on the basis set used.

In Fig. 2, we show our VS ICS in comparison with the VU theoretical results of de Carvalho *et al.* [1] and with the total cross sections (TCS) measured by Hoffmann [17] and Sueoka [19]. The vibrational elastic ($\nu = 0 \rightarrow \nu' = 0$) ICS calculated by Gianturco and Mukherjee [13] were also shown for comparison. Strictly speaking, the comparison with the experimental data should be made only for incident energies up to approximately 7.0 eV, in which only rovibrationally elastic and inelastic scattering channels are open. Moreover, the comparison of our VS results with the vibrationally elastic data of Gianturco and Mukherjee [13] is meaningful due to the fact that the contribution of this channel is dominant (more than 95%). In general, our results agree qualitatively with the experimental data. Particularly in the 3–8 eV range, a quantitative agreement is also observed. In the same way, there is an excellent agreement between our VS results and the vibrational elastic ICS data of Gianturco and Mukherjee [13] in the entire energy region which reinforces the fact that the contributions due to the vibrational excitations to TCS are negligible. Again, the difference seen between our results and those calculated by de Carvalho *et al.* [1] using the SMC is attributed to the distinct way of handling the correlation-polarization effects. Apparently, the results of de Carvalho *et al.* [1] agree better with the experimental data, particularly at energies near the position of the minimum. Above 7.0 eV, there is a rapid increase of the experimental TCS probably due to the fact that the positronium formation channel becomes energetically accessible.

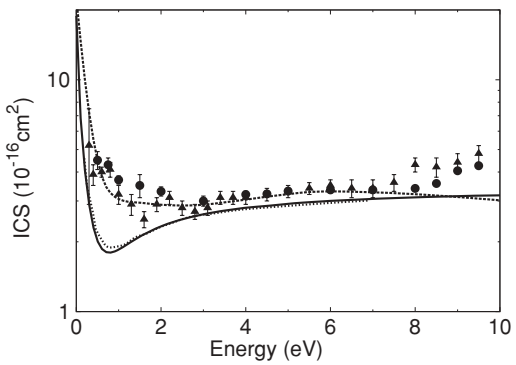

FIG. 2. Elastic ICS for e^+-N_2 scattering. Solid line, present VS data; dashed line, VU data of [1]; dotted line, vibrationally elastic data of [13]; solid circles, experimental TCS of [17]; solid triangles, experimental TCS of [19].

In Fig. 3, we show the vibrationally elastic (VE ICS) calculated for initial vibrational states $\nu = 0,1,2,3$, and 4. In general, the VE ICS increases with increasing ν. In fact, this increase of the ICS can be roughly related to the size of the

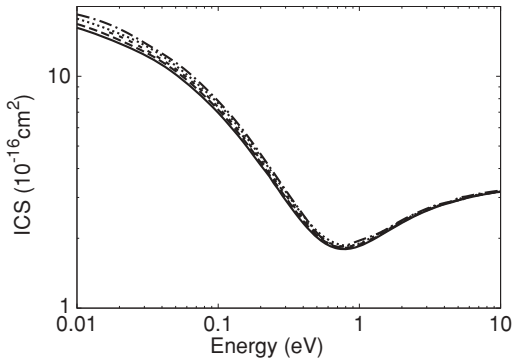

FIG. 3. Present vibrationally elastic ICS for the e^+-N_2 scattering. Solid line, for the $\nu = 0 \rightarrow \nu = 0$ transition; dashed line, for the $\nu = 1 \rightarrow \nu = 1$ transition; short dashed line, for the $\nu = 2 \rightarrow \nu = 2$ transition; dotted line, for the $\nu = 3 \rightarrow \nu = 3$ transition; dash-dotted line, for the $\nu = 4 \rightarrow \nu = 4$ transition.

target of a different vibrational level. Here, we consider that the molecular area of each vibrational level is proportional to the square of its mean internuclear distance (R_ν), which is taken as an average of the classical vibrational turning points ($R_{\min}$ and $R_{\max}$). The dependence of the ICS on ν can be seen in Fig. 4 where a plot of the ratio between the ICS from vibrational state ν and that from $\nu = 0$, calculated at 0.1 eV for $\Delta\nu = 0$ and near the peak for $\Delta\nu = 1$, versus $(R_\nu/R_0)^2$ is shown. A very good fitting of a linear function is seen. Nevertheless, it is verified that the size dependence of the ICS for N_2 is not sensitive in the sense that even for $\nu = 4$ the increase of ICS is only 13%. This verification strongly disagrees with that observed in similar studies for electron-H_2 scattering [31,32]. In those investigations, it was verified that the VE ICS are significantly dependent on the initial vibrational state of the molecule. The low R_ν dependence of the ICS observed here is probably due to the absence of shape resonances in positron-N_2 scattering. It is well known that the occurrence of shape resonances strongly enhances the vibrational couplings [22,31,33]. This difference may also be attributed partly to the lack of exchange effects in positron-molecule interaction. As shown by Mazon *et al.* [12],

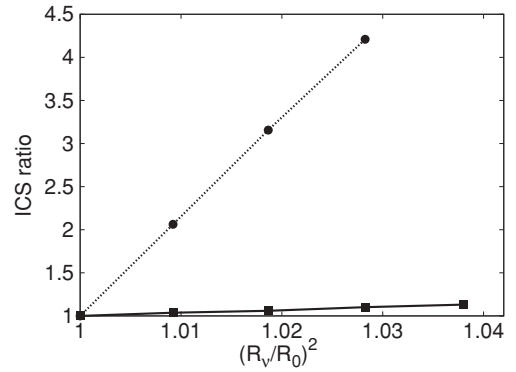

FIG. 4. Ratio of the ICS from vibrational state ν to that from $\nu = 0$ versus $[R_\nu/R_0]^2$. Solid line with solid square shows results for the $\Delta\nu = 0$ vibrational transitions; dotted line with solid circle shows results for the $\Delta\nu = 1$ vibrational transitions.

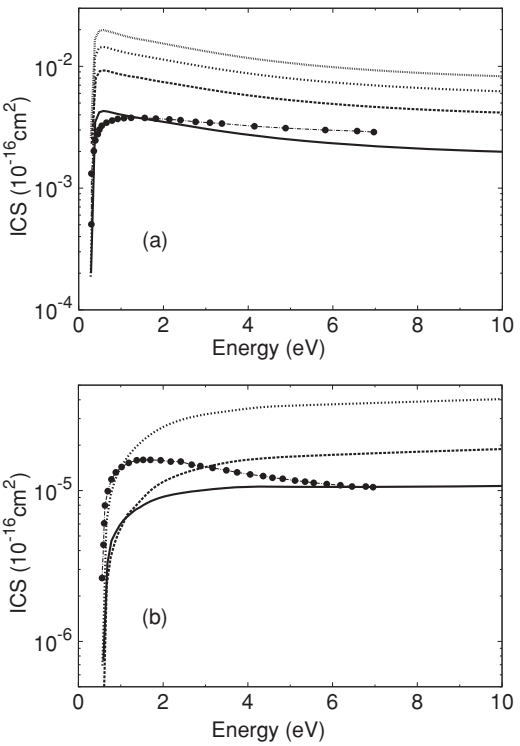

FIG. 5. ICS for vibrational excitation of N_2 induced by positron impact. (a) Transitions with $\Delta\nu = 1$: solid line, for the $\nu = 0 \rightarrow \nu = 1$ excitation; dashed line, for the $\nu = 1 \rightarrow \nu = 2$ excitation; short dashed line, for the $\nu = 2 \rightarrow \nu = 3$ excitation; dotted line, for the $\nu = 3 \rightarrow \nu = 4$ excitation; dash-dotted line with solid circles, ICS for the $\nu = 0 \rightarrow \nu = 1$ excitation from [13]. (b) Transitions with $\Delta\nu = 2$: solid line, for the $\nu = 0 \rightarrow \nu = 2$ excitation; dashed line, for the $\nu = 1 \rightarrow \nu = 3$ excitation; short dashed line, for the $\nu = 2 \rightarrow \nu = 4$ excitation; dash-dotted line with solid circles, ICS for the $\nu = 0 \rightarrow \nu = 2$ excitation from [13].

exchange effects play a very important role in low-energy electron-molecule interaction.

Finally, we present in Fig. 5 our calculated ICS for $\Delta\nu = 1$ and $\Delta\nu = 2$ vibrational transitions. The theoretical data of Gianturco and Mukherjee [13] for $\nu = 0 \rightarrow \nu = 1$ and $\nu = 0 \rightarrow \nu = 2$ excitations are also shown for comparison. For the $\nu = 0 \rightarrow \nu = 1$ transition, there is a generally good agreement between their ICS and our data. Nevertheless, significant discrepancies are seen in the ICS for the $\nu = 0 \rightarrow \nu = 2$ transition. The origin of this disagreement is not clear. However, since the difference between the two calculations increases with an increase in the quantum number of the excited vibrational state, we suspect that the potential curves used in the computation of vibrational wave functions might be different.

Unlike what happens on the VE scattering, the vibrational excitation ICS are highly dependent on the initial vibrational state. Such dependence is also shown in Fig. 4, where a plot of the ratio of the ICS from vibrational state ν to that from $\nu = 0$ versus $(R_\nu/R_0)^2$ for vibrational excitations with $\Delta\nu = 1$ is shown. Again, a very good fitting of a linear function is obtained, but with the slope much larger than that of VE scattering. The reasons behind this behavior change are also not clear. A possible interpretation is as follows.

For a vibrational transition to occur, a significant momentum transfer from projectile to the target is required. Intuitively, such a transfer would be more effective during a collinear collision. Thus, backward scattering would contribute more significantly to such processes. DCS at a large scattering angle are strongly dependent on the contribution of low partial-wave (small impact parameter) components. Therefore, the low-order multipolar interactions between the projectile and target are essential for such processes to happen. The fact that the magnitude of the quadrupole moment of N_2 depends strongly on the internuclear separation may partly explain the R_v dependence of the vibrational excitation cross sections.

In summary, this work presents a theoretical study on positron-impact vibrational excitation in N_2 using the BFVCC approach. Our calculated VS DCS agree qualitatively with the existing experimental data for VU elastic e^+–N_2 collisions, particularly at incident energy of 10 eV and above. The shift of the minimum and maximum features is attributed to the treatment of correlation-polarization effects. The ICS for vibrational elastic scattering are weakly dependent on the initial vibrational state, in contrast to what is observed for e^-–H_2 collisions. The absence of shape resonances in positron-molecule scattering may be the physical origin for this behavior. On the other hand, the vibrational excitation cross sections are highly R_v dependent. The physical origin of this dependence is not yet clear. A tentative explanation is given: The sensitive variation of the magnitude of the quadrupole of N_2 with bond length may be responsible for this dependence.

Moreover, the lack of experimental results of the vibrational excitation of molecules by positron impact seriously limited the discussion of the present study. Further experimental investigation on this area is certainly welcome in order to better understand the underlying physics involved in such processes.

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