

Ubiquitous diffraction resonances in positronium formation from fullerenes

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Due to the dominant electron capture by positrons from the molecular shell and the spatial dephasing across the shell width, a powerful diffraction effect universally underlies the positronium (Ps) formation from fullerenes. This results in trains of resonances in the Ps formation cross section as a function of the positron beam energy, producing structures in recoil momenta in analogy with classical single-slit diffraction fringes in the configuration space. This work opens a hitherto unknown avenue of Ps spectroscopy with nanomaterials and motivates level-differential measurements.

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I. INTRODUCTION

Following the impact of positrons with matter the formation of an exotic electron-positron bound pair, positronium (Ps), is a vital process in nature. This channel accounts for as large as half of the positron scattering cross section from simple atoms and molecules [1], as well as an even higher success rate of Ps formation on surfaces and thin films [2]. Other than probing the structure and reaction mechanisms of matter, the Ps formation is a unique pathway to the electron-positron annihilation process [3,4] with both astrophysical [5] and applied [6] interests. The possible production of a Bose-Einstein condensate of Ps has also been predicted [7,8], besides the importance of Ps in diagnosing porous materials [9] as well as in probing bound-state QED effects [10]. Moreover, efficient Ps formation is the precursor of the production of dipositronium molecules [11] and antihydrogen atoms [12,13] required to study the effect of gravitational force on antimatter [14,15].

Theoretical investigations to calculate Ps formation cross sections from atomic hydrogen [16–18], noble gases [19–21], and alkali metals [22,23] are aplenty. For some of these systems, *ab initio* close-coupling calculations, pioneered by Walters *et al.* [24], have been very successful [25]. Calculations with molecular targets, although relatively limited, include molecular hydrogen [25,26], polyatomic molecules [27], and the water molecule [28]. Simultaneously, precision experimental techniques to measure Ps formation signals have also been achieved by impinging positrons into varieties of materials, such as atomic and molecular gases [29,30], molecular solids [31], liquids and polymers [32], zeolites [33], metal surfaces and films [34], metal-organic frameworks [35,36], and embedded mesostructures [37]. Very recently high yields of laser-assisted production of low-energy excited Ps is achieved in the interaction of cold-trapped positrons with Rydberg excited Cs atoms [12].

However, in spite of such a broad landscape of Ps research, little attempt of Ps formation by implanting positrons in nanoparticles, in gas or solid phase, has so far been made, except for a single theoretical study using Na clusters [38].

On the other hand, straddling the line between atoms and condensed matters are clusters and nanostructures that not only have hybrid properties of the two extremes, but also exhibit outstanding behaviors with unusual spectroscopic effects [39]. Formation of a quasifree electron gas within a finite nanoscopic region of well-defined boundary, as opposed to a longer-range, highly diffused Coulomb-type boundary characteristic of atoms and molecules, is a property of nanosystems which ensures predominant electron capture from localized regions in space. This may lead to diffraction in the capture amplitude, particularly at positron energies that cannot excite plasmon modes. The Ps formation from fullerenes can be singularly attractive to access this diffraction phenomenon due to fullerene's eminent symmetry and stability, and its previous track record of success in spectroscopic experiments [40]. In this Rapid Communication, we show that the Ps formation amplitude from the positron colliding with C₆₀ does include a strong, observable diffraction effect, resulting in a system of peaks in the form of broad shape resonances, in the total ground and excited Ps formation cross section for state-selected captures.

II. A BRIEF DESCRIPTION OF THE METHOD

The C₆₀ molecule is modeled by smearing 60 C⁴⁺ ions in a spherical jellium shell, fixed in space, with an experimentally known C₆₀ mean radius $r_c = 6.7$ a.u. and a width determined *ab initio* [41]. Inclusion of molecular orientations will have a minimal effect on the result due to the C₆₀ symmetry [42]. The delocalized system of a total of 240 valence electrons from 60 carbon atoms constructs the ground state in the Kohn-Sham local-density approximation (LDA) [41] improved by the gradient-corrected Leeuwen and Baerends exchange-correlation functional (LB94) [43]. This produced bands of π (one radial node) and σ (nodeless) states with highest occupied molecular orbital (HOMO) and HOMO-1 to be of $7h$ ($\ell_i = 5$) and $6g$ ($\ell_i = 4$) π character, respectively—a result known from the quantum chemical calculations [44] supported by direct and inverse photoemission spectra [45], and from energy-resolved electron-momentum density measurements [46]. The LDA radial ground state potential and the radial HOMO wave function are shown in Fig. 1. Linear-response-type calculations using this ground state basis well

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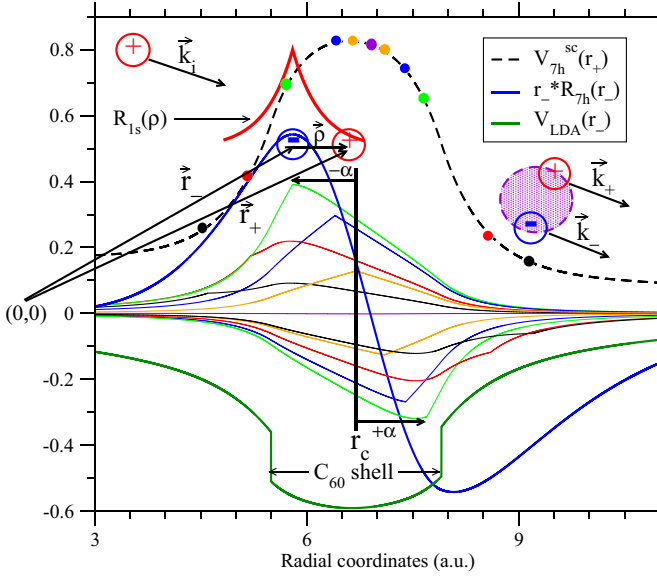


FIG. 1. The scattering potential V_{2h}^{sc} of the positron from C_{60}^+ after a $7h$ (HOMO) electron is captured, the radial HOMO wave function, and the free C_{60} ground state LDA radial potential identifying the shell width. The position vectors, from the C_{60} center $(0,0)$ roughly placed in the figure, and momentum vectors (for capture in the forward direction) are shown schematically. A bunch of curves peaking around the C_{60} radius r_c represents products of scattering potential, radial HOMO, and radial $Ps(1s)$ (shown) wave functions for the choices of electron positions marked by correspondingly color-coded dots. See the text for the description of α .

explained the measured photoemission response of C_{60} at the plasmon excitation energies [41,47]. Similar calculations at higher energies also supported an effective fullerene width accessed in the experiment [40]. Jellium-type modeling of multiwalled carbon nanotubes also had success in describing laser pump-probe measurements [48].

Consider an incoming positron of momentum \vec{k}_i which captures an electron from a C_{60} bound state $\phi_i(\vec{r}_-)$ to form a Ps state $\phi_f(\vec{\rho})$. As illustrated in Fig. 1, the positron and electron position vectors, \vec{r}_+ and \vec{r}_- , respectively, originate from the center of C_{60} so that $\vec{\rho} = \vec{r}_- - \vec{r}_+$ and $\vec{k}_{+(-)}$ denote positron (electron) outgoing momenta in Ps that are equal, resulting in $2\vec{k}_{+(-)}$ being the momentum of Ps itself. Since we access energies above C_{60} plasmon resonances, the many-body effect is not important, justifying the use of mean-field LDA wave functions and potentials in the framework of an independent particle model. Therefore, the *prior* form of the Ps formation amplitude can be given in the continuum distorted-wave final-state (CDW-FS) approximation [38,49] as

$$T(\vec{k}_i) \sim \int d\vec{r}_- F_{\vec{k}_-}^{(-)*}(\vec{r}_-) W(\vec{r}_-; \vec{k}_i) \phi_i(\vec{r}_-), \quad (1)$$

in which

$$W(\vec{r}_-; \vec{k}_i) = \int d\vec{r}_+ F_{\vec{k}_+}^{(-)*}(\vec{r}_+) \phi_f^*(\vec{\rho}) \times \left[V_i^{sc}(r_+) - \frac{1}{\rho} \right] F_{\vec{k}_i}^{(+)}(\vec{r}_+), \quad (2)$$

where the short-range positron- C_{60}^+ interaction, after the i th electron is captured, *plus* the long-range $1/r_+$ interaction between them gives the positron scattering potential, $V_i^{sc}(r_+)$, from the C_{60}^+ ion; the LDA version of this potential for a HOMO electron capture is given in Fig. 1. $1/\rho$ is the Coulomb interaction between the positron and the captured electron. For a given electron position, Eq. (2) embodies the *snapshot* amplitude for the transition of an incoming positron to a Ps-bound outgoing positron. $W(\vec{r}_-; \vec{k}_i)$ thus provides the perturbation in Eq. (1) for the capture of the bound electron into a moving Ps. The use of this perturbative model (CDW-FS) is fully justified, since we focus on impact energies well above the threshold for Ps formation.

III. RESULTS AND DISCUSSIONS

We use Eqs. (1) and (2) *exactly* to compute our numerical results, but consider some following *ad hoc* simplifications only to extract the underlying physics. Integrations over $1/\rho$ in Eq. (1) will produce a steady contribution $S(\vec{k}_i)$ to the amplitude in energy which we ignore temporarily. This steady behavior may be justified by the steady Ps formation cross section of atomic hydrogen $1s$ capture into $Ps(1s)$ [Fig. 2(a)] where V_i^{sc} in Eq. (2) is simply replaced by $1/r_+$. Also, to better explain our results, we approximate the three distorted Coulomb continuum waves, representable by confluent hypergeometric functions [38], in Eqs. (1) and (2) as

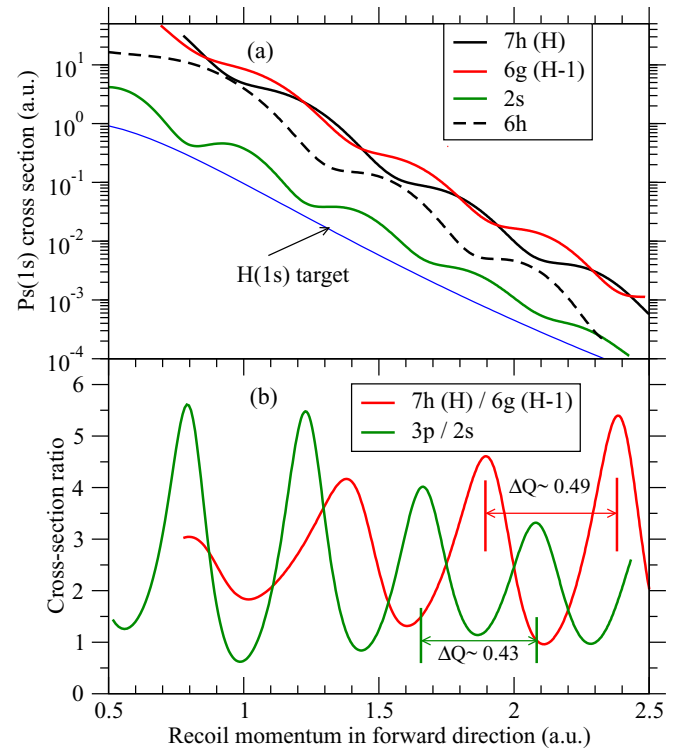


FIG. 2. (a) $Ps(1s)$ formation cross sections for captures from HOMO (H), HOMO-1 (H-1), $2s$ (bottommost π level), and $6h$ (a σ level) as a function of recoil momentum (Q) in the forward direction. The result of hydrogen $1s$ capture is also shown for comparison. (b) The ratios of two pairs of these cross sections illustrate strong resonances. Separations (ΔQ) between some resonances are marked.

plane waves of the form $F_{\vec{k}}^{(-)}(\vec{r}) \sim \exp(-i\vec{k} \cdot \vec{r})$. These plane waves can expand in spherical harmonics:

$$\exp(-i\vec{k} \cdot \vec{r}) \sim \sum_{\ell,m} i^\ell j_\ell(kr) Y_{\ell,m}(\hat{k}) Y_{\ell,m}^*(\hat{r}). \quad (3)$$

With these and assuming the capture in an n_{fs} Ps state $\phi_f(\vec{\rho}) \sim R_{n_{fs}}(\rho) Y_{0,0}(\hat{\rho})$, Eq. (2) simplifies to

$$W(\vec{r}_-; \vec{k}_i) \sim \int dr_+ r_+^2 j_0(qr_+) R_{n_{fs}}(\rho) V_i^{\text{sc}}(r_+) Y_{0,0}^*(\hat{q}), \quad (4)$$

where $\vec{q} = \vec{k}_+ - \vec{k}_i$ is the momentum transfer vector and Eq. (4) is isotropic in \vec{q} . [In writing Eq. (4), we assume Ps formations in the forward direction, which was found to be the most dominant direction in both earlier [50] and recent experiments [51], so that \hat{r}_- and \hat{r}_+ are identical and thus $\vec{\rho}$ is independent of \hat{r}_+ .] Adopting the same simplification for $F_{\vec{k}_-}^{(-)*}(\vec{r}_-)$ in Eq. (1) to apply in Eq. (3) and then combining with Eq. (4), we can rewrite the full amplitude (1) for a capture from the $C_{60} n_i \ell_i$ state as

$$\begin{aligned} T(\vec{k}_i) \sim & S(\vec{k}_i) + \frac{1}{k_- q} \iint dr_- dr_+ r_+ R_{n_{fs}}(\rho) V_i^{\text{sc}}(r_+) \\ & \times [r_- R_{n_i \ell_i}(r_-)] \sin(k_- r_- - \ell_i \pi/2) \sin(qr_+) \\ & \times Y_{0,0}^*(\hat{q}) Y_{\ell_i, m_i}^*(\hat{k}_-), \end{aligned} \quad (5)$$

where we used asymptotic forms of the spherical Bessel function $j_\ell(r) \sim \sin(r - \ell\pi/2)/r$. We will ignore the spherical harmonics in Eq. (5), since the forward direction is considered.

Before moving further let us note the following in the amplitude (5) in conjunction with Fig. 1: (i) Large values of V_i^{sc} only at the C_{60} shell indicates the shell to be the window of appreciable repulsive interactions of the positron with C_{60} . (ii) The shape of the Ps radial wave function $R_{n_{fs}}(\rho)$ identifies the region of success of Ps formation as a function of electron-positron separation $\rho = |\vec{r}_- - \vec{r}_+|$ where a Ps s state has the maximum probability density at $r_- = r_+$. (iii) The radial wave function of C_{60} i th level $r_- R_{n_i \ell_i}$ ensures that electrons must be available for the Ps to form. Considering Ps(1s) formation from the capture off C_{60} HOMO level, we took 11 electron positions in Fig. 1 within the interaction window around C_{60} radius (r_c) and plot the product $R_{1s}(\rho) V_{7h}^{\text{sc}}(r_+) [r_+ R_{7h}(r_+)]$ of the three quantities mentioned above; the r_- values considered are shown by dots in the same color as that of the curve it generates. Since Ps will have a propensity to successfully form toward $\rho = 0$, the curves show maxima and minima at various locations symmetrically on the left and right side, respectively, of r_c . This opposite orientation is because of the shape of the C_{60} $7h$ wave function which is asymmetric about its node. It is fair to approximate that the dominant behavior comes from the optimum positions at r_p . Thus, choosing $r_- = r_+ = r_p$ in Eq. (5) these contributions indicate trains of peaks given by $\sin(k_- r_- - \ell_i \pi/2) \sin(qr_+) \sim \sin(Qr_p - \ell_i \pi/2)$ where the recoil momentum $Q = k_i - 2k_\pm$ for the Ps formation in the forward direction. The amplitude $A(r_p)$ of the oscillation is proportional to the area (r_+ integral) under the corresponding bump. Hence, the remaining r_- integral in

Eq. (5) can approximate to a simpler form

$$T(\vec{k}_i) \sim S(\vec{k}_i) + \frac{1}{k_- q} \int dr_- A(r_p) \sin(Qr_p - \ell_i \pi/2). \quad (6)$$

Noticing that the bumps appear on either side of r_c at similar distances α (Fig. 1), Eq. (6) can be rewritten as

$$\begin{aligned} T(\vec{k}_i) \sim & S(\vec{k}_i) + \frac{1}{2k_- q} \int dr_- A(r_p) [\sin\{Q[r_c - \alpha(r_p)] \\ & - \ell_i \pi/2\} - \sin\{Q[r_c + \alpha(r_p)] - \ell_i \pi/2\}], \end{aligned} \quad (7)$$

where the negative sign between the two terms justifies the maxima and minima about r_c (Fig. 1). We finally obtain

$$\begin{aligned} T(\vec{k}_i) \sim & S(\vec{k}_i) - \frac{1}{k_- q} \cos(Qr_c - \ell_i \pi/2) \\ & \times \int dr_- A(r_p) \sin[Q\alpha(r_p)]. \end{aligned} \quad (8)$$

Obviously, the integrals in the above equation spatially dephase the $\sin(Q\alpha)$ modulation, since α varies with r_- , retaining peaks in the amplitude only via $\cos(Qr_c - \ell_i \pi/2)$. Here is the essence of what is going on. Within about the fullerene width region, a strong constructive and destructive interference takes place as a function of Q . When the odd integer multiple of the half-wavelength of *effective* continuum wave as a function of Q fits the distance r_p , systems of peaks (bright spots) in the energy domain are formed, which subsequently results in a single *centroid* fringe pattern via a dephasing mechanism in the integration over the electron position as described above.

Since these diffraction peaks appear in the energy (momentum) domain, we call them diffraction resonances which must also show up in the Ps formation cross section proportional to the squared modulus of Eq. (8). Further, this squaring operation modifies the functional form of the structures as $\cos(Qd_c - \ell_i \pi)$ in the cross section, where d_c is the C_{60} diameter. Broad resonances are seen in Fig. 2(a) for the numerical Ps(1s) formation cross section for the captures off four C_{60} levels as a function of the forward-emission recoil momentum Q corresponding to the electron excitation energy from roughly 50 eV (above the plasmon excitation) to 270 eV (below the K shell of atomic carbon). For a direct comparison, also presented in Fig. 2(a) is the steady result for the atomic hydrogen target showing no such resonances. The offsets between the peaks for the HOMO versus HOMO-1 versus $2s$ (the bottommost level of the C_{60} π band) results connect to the phase shift $\ell_i \pi/2$ in Eq. (8) that depends on the angular symmetry of the initial state. The shape and strength of these resonances are best illustrated by considering the cross-section ratios, shown in Fig. 2(b), which neutralizes the nonresonant background decays, and therefore can be accessed in experiments by the Ps formation spectroscopy with better accuracy much freer of the experimental noise. It is important to note that we used plane wave descriptions in our analysis to interpret the key results. But the actual character of the resonances is more diverse than this simple account, as seen in Fig. 2(b).

If the capture is from a C_{60} σ state, which has no radial node, we still also find Eq. (7) but with a positive sign between the two terms in the integration. This will produce a sine function

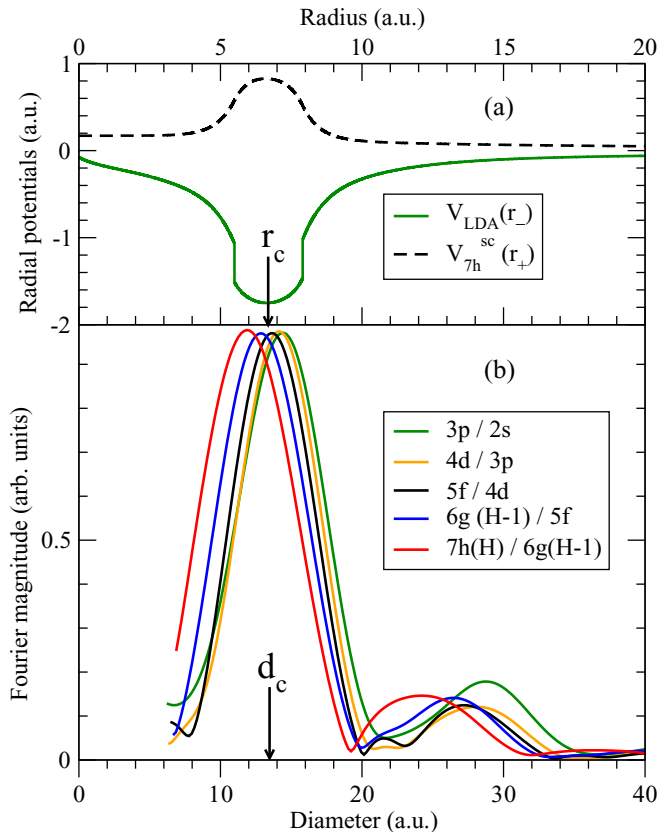


FIG. 3. (a) C_{60} LDA radial potential and the positron scattering potential for the HOMO capture. (b) The Fourier transform magnitudes of $\text{Ps}(1s)$ cross-section ratios for captures from various C_{60} π levels.

in Eq. (8) leading to $\cos(Qd_c - \ell_i\pi + \pi)$ structures in the cross section for a C_{60} σ electron capture. This suggests that for the same angular momentum the π electron capture cross section will produce 180° out-of-phase resonances compared to a σ electron capture, as clearly seen between the HOMO and $6h$ results in Fig. 2(a). This indicates that electronic structural information can also be accessed spectroscopically by Ps formation from fullerenes.

An elegant way to bring out the connection of diffraction resonances with the fullerene diameter is to evaluate the Fourier spectra of the cross sections as a function of Q . To generate the input signals with only the resonances on a flat, nondecaying background we considered ratios of the results of two consecutive angular levels of π electrons. Calculated Fourier magnitudes of these ratios in the reciprocal (radial) coordinate are displayed in Fig. 3(b). All the curves exhibit strong peaks located close to the diameter d_c , as expected. Note that the small, systematic offset of the peaks towards lower values with the increasing angular momentum is another signature of the fact that the continuum waves are Coulomb

distorted and so are more complicated than the simple plane waves used in the analysis. In fact, we anticipate this variation by noting in Fig. 2(b) the separations ΔQ of 0.49 and 0.43 a.u., respectively, for HOMO/HOMO-1 and $3p/2s$ ratio and then determining their reciprocal ($2\pi/\Delta Q$) values as 12.8 and 14.6 a.u. being somewhat different. In any case, these Fourier reciprocal spectra unequivocally support the theme that the host of broad resonances are indeed the fringe patterns in the energy domain for a Ps formation channel where the forward Ps emission diffracts in energy off the shell—a spherical slit. Furthermore, our calculations (not shown) for the formation of excited $\text{Ps}(2s)$ produced similar resonance structures. The $\text{Ps}(2p)$ channel is attractive too, since it can be monitored optically [52]. Also, using the C_{240} fullerene we found (not shown) the resonances to be more compact in energy than C_{60} , since C_{240} is a larger diffractor.

IV. FINAL COMMENTS

Fullerenes [40,47] and metallic nanoparticles [39,53] are nowadays available in gas phase. The challenge, however, is to probe the target-state differential Ps signals which current techniques cannot readily access [54]. But accessing this will be beneficial in general and, in particular, since the predicted resonances, having a target angular-state dependent shift [Eq. (8)], will wash out in the total Ps measurement. The technique to measure the recoil momentum of the cations can be improved by using a supersonic gas jet to increase the overlap with the positron beam. Resolving the Ps level is not so critical (although may still be done by laser spectroscopy of a dense Ps gas), since the $\text{Ps}(1s)$ signal should largely dominate. We believe that the current work will provide the much needed motivation to break the barrier to measure differential Ps production cross sections at least within an acute forward angle.

In conclusion, we calculate the Ps formation cross section in the CDW-FS method for electron captures from various C_{60} levels. The C_{60} ground state structure is modeled by a simple but successful LDA frame. Hosts of strong and broad shape resonances in the Ps formation are predicted. The resonances are engendered from a diffraction effect in the Ps formation process localized on the fullerene shell. The effect should be universal for Ps formation from nanosystems, including metal clusters, carbon nanotubes, or even quantum dots that confine finite-sized electron gas. This work ushers in a new research direction to apply Ps formation spectroscopy to gas-phase nanosystems which we hope can begin with fullerenes, since they currently enjoy significant attraction in precision measurements.

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