Wave-packet analysis of multichannel resonances in positron scattering by a helium ion

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(Received 2 June 2004; published 1 December 2004)

We present the wave-packet analysis for two *S*-wave resonances in positron scattering by a helium ion whose existence was predicted by Bhatia and Drachman but has been controversial. The evolution of the wave packet is solved to exhibit temporary formation of the quasistationary state. For both the resonances, the position and width are determined through the resulting time delays in a consideration of a multichannel nature to agree with those by previous variational eigenenergy calculations. It is further found that the lower resonance dominantly forms from, and decays into, the $n=2$ states of the helium ion, while the higher one the $n=3$ states.

DOI: 10.1103/PhysRevA.70.062701 PACS number(s): 34.85.+x

I. INTRODUCTION

Resonances are the most striking phenomena in the whole range of scattering experiments in physics. In its simplest form, a resonance manifests itself in a sharp peak of a cross section as a function of energy. According to the time-dependent wave-packet description [1–4], the resonance is observed as temporary formation of a metastable state in a projectile-target complex, thus defined as a maximum of the *time delay* of a scattering wave packet.

The wave-packet formalism has been extensively applied to scattering calculations owing to recent increase of computer power. Mitnik, Griffin, and Pindzola [5] have applied the formalism to a doubly excited ($2s^2$) resonance in electron scattering by a helium ion (He^+). They have demonstrated rapid formation and exponential decay of the resonance when the temporal width T of a wave packet is much shorter than the resonance lifetime τ. For an actual wave packet in beam experiments, however, the opposite condition $T \gg \tau$ is realized so that the formation and the decay of a resonance are almost overlapped in the time domain. It leads to a well defined concept of the time delay because the wave packet retains its shape in the scattering. Thus, the nature of a resonance should be analyzed through observing the time delay when $T \gg \tau$.

In the positron-helium ion system (e^+, e^-, He^{2+}), many resonances have been found in previous theoretical studies [6–10]. Bhatia and Drachman [6] predicted two *S*-wave resonances in a variational eigenenergy calculation with the stabilization method. Their prediction was confirmed in complex eigenenergy calculations with the complex coordinate rotation method by Ho [7], by Ho and Yan [8], and by Toya, Kino, and Kudo [9]. The energy position ε_λ and the width Γ_λ of the two resonances, labeled by $\lambda=1$ and 2, were precisely determined to be $(\epsilon_1, \Gamma_1/2)=(-10.082, 1.761)$ and $(\epsilon_2, \Gamma_2/2)=(-5.050, 0.535)$ in eV [7]. They are multichannel resonances lying above the excited $n=2$ and 3 states of the helium ion (He^+), respectively, and both supported in spite of asymptotic Coulomb repulsion between the positron and the helium ion. However, the resonances were not reproduced in scattering calculations with the close-coupling method by Igarashi and Shimamura [10] and by Bransden, Noble, and Whitehead [11]. They observed no potential well supporting the resonances in hyperspherical adiabatic potential curves [10], and no increase of π in the eigenphase sum [11]. Hence, the existence of the resonances has been a question in controversy.

In the present paper, we present a wave-packet analysis for the two *S*-wave resonances in positron scattering upon a helium ion by solving time-dependent coupled-channel (TDCC) equations. The TDCC method is known to be successfully applied to electron and positron scattering by atoms (see Refs. [5,12–14] and references therein). We observe wave-packet behaviors characteristic of a resonance, and determine its position and widths (partial as well as total) through the time delays in a consideration of a multichannel nature. The values obtained for ϵ_λ and Γ_λ turn out to be in good agreement with those predicted in the previous eigenenergy calculations [6,7,9]. It is further found that the lower resonance dominantly forms from, and decays into, the $n=2$ states of the helium ion, while the higher one the $n=3$ states. Atomic units (a.u.) $e=m=\hbar=1$ are used unless otherwise stated.

II. NUMERICAL METHOD

The time-dependent wave function for an *S* wave is expanded over the coupled spherical harmonics $\mathcal{Y}_{Ll}^{00}(\hat{\mathbf{R}}, \hat{\mathbf{r}}) = [Y_L(\hat{\mathbf{R}}) \otimes Y_l(\hat{\mathbf{r}})]_0^0$ as

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$$\Psi(\mathbf{R},\mathbf{r},t)=\frac{1}{Rr}\sum_{Ll}\psi_{Ll}(R,r,t)\mathcal{Y}_{Ll}^{00}(\hat{\mathbf{R}},\hat{\mathbf{r}}), \tag{1}$$

where $\mathbf{R}$ and $\mathbf{r}$ are the position vectors of the positron and the electron relative to the helium nucleus, L and l being the angular momenta associated with $\hat{\mathbf{R}}$ and $\hat{\mathbf{r}}$. The TDCC equations for the radial function $\psi_{Ll}(R,r,t)$ are derived [14] to be

$$i\frac{\partial}{\partial t}\psi_{Ll}(R,r,t)=\left[T_{Ll,Ll}^{00}+\sum_{L'l'}V_{LlL'l'}^{00}\right]\psi_{L'l'}(R,r,t), \tag{2}$$

where $A_{Ll,L'l'}^{00}=\langle\mathcal{Y}_{Ll}^{00}|A|\mathcal{Y}_{L'l'}^{00}\rangle$ for operators $A=T$ and V. The operator T represents the kinetic energy including the centrifugal potential, while V is the Coulomb interaction among the three charged particles. The initial condition is taken as

$$\psi_{Ll}(R,r,t=0)=g_{kL}(R)\phi_{nl}(r)\delta_{Ll} \tag{3}$$

with the target nl state $\phi_{nl}(r)$ and an incoming wave packet. The latter is given by

$$g_{kL}(R)=\frac{1}{(w^2\pi)^{1/4}}\exp\left[-\frac{(R-R_0)^2}{2w^2}\right]\Phi_{kL}(R), \tag{4}$$

where w and R_0 are the width and the position of the initial Gaussian envelope, and $\Phi_{kL}(R)$ an asymptotic form of the Coulomb wave function at a collision energy $E=k^2/2$. The energy spread of the incident wave packet is taken to be $\Delta E/E=2/(kw)\sim 20\%$. The calculation is carried out for initial target states of $nl=1s$, $2s$, $2p$, $3s$, $3p$, and $3d$. The expansions over L and l in Eq. (1) are truncated by 9. The TDCC equation (2) is stably solved with numerical techniques developed in Ref. [13]. Numerical accuracy has been demonstrated in previous work [13,14].

III. RESULTS AND DISCUSSION

Figure 1 shows the time evolution of probability density $|\psi_{Ll}(R,r,t)|^2$, for the incoming S wave ($L=0$) at $E=3.5$ eV with the target $2s$ state. This energy corresponds to the predicted position of the lower $\lambda=1$ resonance. The first row $(a_1)-(a_4)$ in the figure shows free propagation taking the asymptotic Coulomb potential R^{-1}; only the initial channel $(L,l)=(0,0)$ is populated. The wave packet comes from the right in panel (a_1), reflects at the origin in (a_2) and (a_3), and goes out to the right in (a_4). In (a_2) and (a_3) are seen interference fringes of incoming and outgoing waves. In (a_4), the packet retains the incident Gaussian shape, though the spread gets wider.

The other three rows in Fig. 1 show the propagation with full collision interaction $2R^{-1}-|\mathbf{R}-\mathbf{r}|^{-1}$. Panels $(b_1)-(b_4)$ and $(c_1)-(c_4)$ indicate population in two open channels $(L,l)=(0,0)$ and (1, 1), respectively, while $(d_1)-(d_4)$ in a closed channel (2, 2). In the entrance channel, the interference fringes appear in (b_2) and (b_3) the same as in (a_2) and (a_3), though affected by the interaction in an internal region $R<30$. The outgoing packet is split into two parts as shown in (b_4). In another open channel (1, 1), on the other hand, a packet is generated in the interaction region [see (c_1)] and

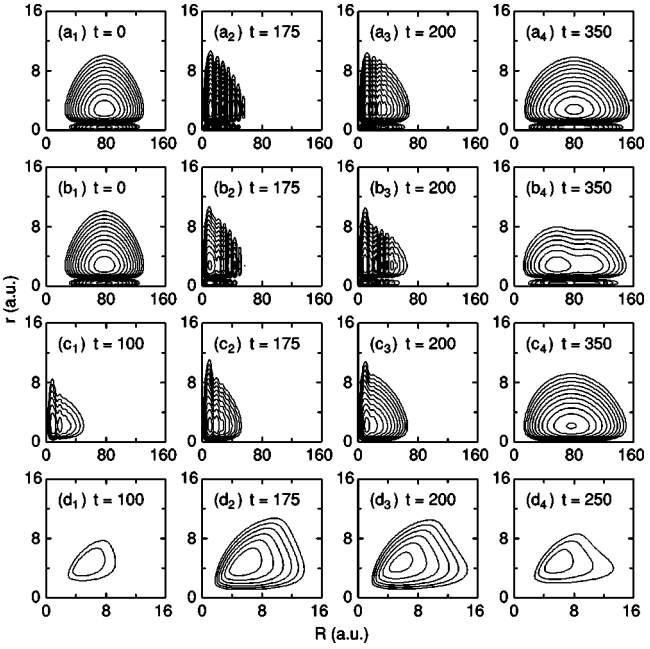

FIG. 1. Time evolution of wave-packet density $|\psi_{Ll}(R,r,t)|^2$ for the scattering of an S-wave positron with $E=3.5$ eV by a helium ion in the $2s$ state. The first row (a) shows $(L,l)=(0,0)$ channel when propagating with the asymptotic Coulomb potential; the other rows (b), (c), and (d), respectively, show (0, 0), (1, 1), and (2, 2) channels when propagating with the full collision interaction. The density profiles are plotted by contours in a logarithmic scale.

grows with time [see $(c_2)-(c_4)$]. This represents an angular momentum transfer process, $e^+ + \mathrm{He}^+(2s)\rightarrow e^+ + \mathrm{He}^+(2p)$. It is found from the comparison of (c_4) with (a_4) at a common time $t=350$ that the peak position is slightly shifted toward the left, which means a time delay due to the collision.

In the closed channel (2, 2), a hump is temporarily formed, retaining its shape as it appears, grows, decays, and disappears with time [see $(d_1)-(d_4)$]. This is a manifestation of a quasistationary state associated with a resonance. The extent of the hump is consistent with averaged distances among the three particles calculated in Ref. [9]. The hump has two ridges along $r\sim 4$ and $R=r$; the former comes from virtual excitation of the helium ion, while the latter from virtual formation of positronium. The positronium channel supports an attractive potential well due to the polarization force.

Figure 2 shows the time profile of a flux

$$A_f(t)=\left|\langle\phi_{n'l'}(r)|\psi_{l'l'}(R_\infty,r,t)\rangle_r\right|^2, \tag{5}$$

passing through a surface at a distance of $R_\infty\sim 80$ into the two open channels $f=n'l'=2s$ and $2p$. The time delay found in Figs. $1(c_4)$ and $1(a_4)$ for the (1, 1) channel is clearly confirmed in Fig. 2 as a peak shift between A_{2p} and A_{2s}(free). It is also found that the flux A_{2p} is comparable in magnitude to A_{2s}(free) of free propagation, while A_{2s}, having two humps, is smaller than A_{2s}(free) by one order. Note that the flux A_{1s} is several orders of magnitude smaller than A_{2s}(free).

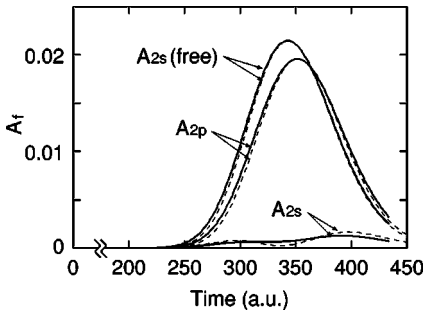

FIG. 2. Time profiles of a wave packet at $E=3.5$ eV. Solid lines represent $A_f(t)$ obtained from the TDCC calculation with Eq. (5), while broken lines give $A_f^r(t)$ constructed from the S matrix (7) with Eq. (10).

A time delay $\langle\tau\rangle_i$ for an incident channel $i=nl$ is calculated from the difference of mean distance $\langle\Psi(t)|R|\Psi(t)\rangle$ at sufficiently large t with full interaction and that with the asymptotic Coulomb potential. Figure 3 shows the time delays obtained for $n=1$ to 3 in the total energy ϵ region covering the two resonances predicted. The total energy is given by $\epsilon=E_n+E$, where E_n is the internal energy of the nl-state helium ion, i.e., $E_1=-54.423$, $E_2=-13.606$, and $E_3=-6.047$ eV. For the target $1s$ state, the delay indicates no sign of a resonance, almost zero and constant with the energy. For the target states of $2s$ and $2p$, however, the time delay has a maximum around $\epsilon=-10$ eV ($E\sim3.5$ eV), close to the position $\epsilon_1=-10.082$ eV predicted for the lower resonance. As the energy further increases, the delay decreases and turns negative; no sign of a resonance is seen around $\epsilon_2=-5.050$ eV predicted for the higher resonance. For the target states of $3s$, $3p$, and $3d$, however, the time delay clearly indicates a peak around ϵ_2.

We determine the resonance parameters from the time delays $\langle\tau\rangle_i$ calculated. For a wave packet injected in channel i and ejected in channel f, the time delay can be represented as

$$\tau_{if}=\mathrm{Re}\left(-iS_{if}^{-1}\frac{dS_{if}}{d\epsilon}\right) \tag{6}$$

with the S-matrix element S_{if}. Its average over final channels leads to an expression $\langle\tau\rangle_i=\Sigma_f|S_{if}|^2\tau_{if}$, which is identical to a

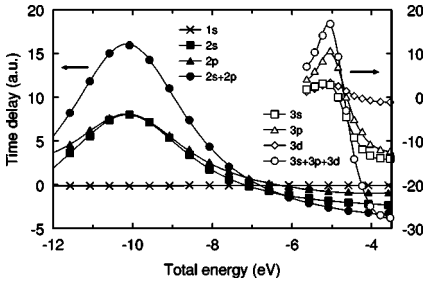

FIG. 3. Time delay of wave packets for positron scattering by nl-state helium ions. Symbols "$2s+2p$" and "$3s+3p+3d$" indicate the sums of the delays over the two and three states, respectively. Solid lines represent fittings to the formula (9). The left vertical axis corresponds to the $n=1$ and 2 states, while the right axis to the $n=3$ states.

diagonal element of the "lifetime matrix" $\mathbf{Q}=-i(\mathbf{S}^\dagger d\mathbf{S}/d\epsilon)$ given by Smith [15]. Taking the Breit-Wigner resonance formula for the S-matrix elements [16],

$$S_{if}^r(\epsilon)=e^{i(\Omega_i+\Omega_f)}\left(\delta_{if}+\frac{i\sqrt{\Gamma_{\lambda i}\Gamma_{\lambda f}}}{\epsilon_\lambda-\epsilon-i\Gamma_\lambda/2}\right), \tag{7}$$

we obtain a resonance formula for the time delay,

$$\langle\tau\rangle_i=\frac{\Gamma_{\lambda i}}{(\epsilon_\lambda-\epsilon)^2+(\Gamma_\lambda/2)^2}+2\frac{d\Omega_i}{d\epsilon}, \tag{8}$$

where $\Gamma_{\lambda i}$ is the partial width for channel i, with a total width given by $\Gamma_\lambda=\Sigma_i\Gamma_{\lambda i}$, and Ω_i is the background phase shift. As shown in Ref. [17], if Ω_i varies rapidly around ϵ_λ, its effect may appear to enhance and suppress the first term as if it gave rise to a resonance behavior. For the convenience of incorporating such a background contribution, we employ in the present analysis an effective formula with an additional parameter α,

$$\langle\tau\rangle_i=\frac{\alpha\Gamma_{\lambda i}}{(\epsilon_\lambda-\epsilon)^2+(\Gamma_\lambda/2)^2}+2\frac{d\Omega_i'}{d\epsilon}. \tag{9}$$

This expression is associated with the definition of resonance as the maximum of the time delay. The formula (9) is derived [1] from a Taylor expansion of the reciprocal of time delay around its peak position ϵ_λ, $\langle\tau\rangle^{-1}=a_0+a_2(\epsilon-\epsilon_\lambda)^2+O((\epsilon-\epsilon_\lambda)^3)$. The zeroth and second order terms in the expansion are converted into the resonance term of Eq. (9), while $O((\epsilon-\epsilon_\lambda)^3)$ into the background term. The condition of integer α would be further derived by imposing analyticity properties for the S-matrix elements.

The analysis of the time delay is justified when the shape of a wave packet is retained in the scattering, or equivalently when the energy spread ΔE of a wave packet is smaller than the resonance width Γ_λ. This condition is realized in our treatment as seen in Fig. 2, where the time profile of $A_{2s}+A_{2p}$ is similar to that of A_{2s}(free). The parameters ε_λ, Γ_λ, $\Gamma_{\lambda i}$, and α are determined by fitting the time delays in Fig. 3 with Eq. (9). The background contributions $d\Omega_i'/d\epsilon$ are given by a polynomial of $\epsilon-\epsilon_\lambda$ up to the first and second orders for the lower and higher resonances, respectively. Accuracies in the fitting are obtained to be better than 10%. The background obtained is almost flat in the lower resonance and slanting in the higher resonance.

Table I shows the resonance parameters determined in this way. The present result is in good agreement with the previous results obtained in variational eigenenergy calculations by Bhatia and Drachman [6], by Ho [7], and by Toya, Kino, and Kudo [9]. Note that the parameter values determined may involve errors due to ambiguity in describing the background and due to the finite energy spread in the wave packet. They are expected to be at most comparable to the error accompanying by the parameter fitting. In the present calculation, the sum of partial widths $\Gamma_{1,2s}$ and $\Gamma_{1,2p}$ accounts for the total width Γ_1, and similarly, the sum of $\Gamma_{2,3s}$, $\Gamma_{2,3p}$, and $\Gamma_{2,3d}$ for Γ_2. All the other partial widths $\Gamma_{1,1s}$, $\Gamma_{2,1s}$, Γ_{2p}, and $\Gamma_{2,\mathrm{Ps}:1s}$ (with respect to the positronium $1s$ channel) are negligibly small. Hence, it is found that the lower and higher

TABLE I. Resonance parameters: position ϵ_λ, total width Γ_λ, and partial width $\Gamma_{\lambda,nl}$ for the nl channel in eV.

	ϵ_1	$\Gamma_1/2$	ϵ_2	$\Gamma_2/2$
Bhatia and Drachman [6]	−9.93		−5.31	
Ho [7]	−10.082	1.761	−5.050	0.535
Toya, Kino, and Kudo [9]	−10.080	1.760	−5.050	0.536
Present work	−10.14	1.85[a]	−5.01	0.52[b]

[a] $\alpha=0.72$, $\Gamma_{1,1s}/2=0.00$, $\Gamma_{1,2s}/2=0.92$, $\Gamma_{1,2p}/2=0.92$.
[b] $\alpha=0.40$, $\Gamma_{2,1s}/2=\Gamma_{2,2s}/2=\Gamma_{2,2p}/2=\Gamma_{2,\mathrm{Ps:1}s}/2=0.00$, $\Gamma_{2,3s}/2=0.16$, $\Gamma_{2,3p}/2=0.29$, $\Gamma_{2,3d}/2=0.06$.

resonances are dominantly coupled with the $n=2$ and 3 channels, respectively. The coupling with the 1s channel is negligible. This result is consistent with a previous study [14] for elastic scattering by the helium ion in the ground state; no resonancelike behavior was discerned in the phase shift. The parameter α obtained is considerably smaller than unity for both the resonances. If we fix $\alpha=1$ in the fitting procedure, we fail in reproducing the time delays within the polynomial expansion of $d\Omega_i'/d\epsilon$. Therefore, we consider that the maximum of the time delay is suppressed by a background contribution $d\Omega_i/d\epsilon$ in Eq. (8) which seemingly takes a minimum near the resonance position.

For confirmation, we construct the time profiles at the resonance position ϵ_1 shown in Fig. 2 from the Breit-Wigner formula (7) as

$$A_f^r(t) = |g_{k'l'}^r(R_\infty,t)|^2 \tag{10}$$

with the asymptotic form of the outgoing wave

$$g_{k'L}^r(R,t) = \int d\epsilon\, a(\epsilon)\frac{S_{if}^r(\epsilon)}{\sqrt{kk'}}\Phi_{kL}^*(R)e^{-i\epsilon t}, \tag{11}$$

where $\epsilon=E_n+E=E_{n'}+E'$ and $k'=\sqrt{2E'}$. The coefficient $a(\epsilon)$ is determined from the initial wave packet (3) as $a(\epsilon)=\langle u_{kL}(R)\phi_{nl}(r)|\psi_{Ll}(R,r,t=0)\rangle$ with the energy normalized scattering function $u_{kL}(R)$. The S-matrix elements in Eq. (11) are calculated with the formula (7) using the resonance parameters shown in Table I. The background phase shifts Ω_i are calculated with Eqs. (8) and (9). As seen from Fig. 2, the profiles A_f^r obtained with Eq. (10) reproduce the curves of A_{2s}(free), A_{2s}, and A_{2p} obtained from the present TDCC calculation with Eq. (5). The remarkable asymmetry in size found between amplitudes A_{2s} and A_{2p} is explained also with Eq. (7); $|S_{2s,2s}^r(\epsilon_1)|^2\simeq 0$ and $|S_{2s,2p}^r(\epsilon_1)|^2\simeq 1$, since $\Gamma_{1,2s}\simeq\Gamma_{1,2p}\simeq\Gamma_1/2$ and $\Gamma_{1,1s}\simeq 0$. Thus, the time profiles at the resonance position are explained as a multichannel resonance described by Eq. (7).

The previous scattering calculation by Bransden, Noble, and Whitehead [11] exhibits a marked increase of the eigenphase sum around the lower resonance in the form of an arctangent function, though the increase does not amount to π. These behaviors are consistent with the present result for the time delays. The condition of an eigenphase increase of π is too strict as an actual criterion of a resonance when the background phase varies rapidly with energy.

IV. SUMMARY

We have presented a multichannel wave-packet analysis for the two S-wave resonances in positron scattering by a helium ion. The time evolution of the wave packets shows behaviors characteristic of resonances. The time delays are calculated to determine the resonance positions as well as the total and partial widths. The position and total width are in good agreement with those obtained in the previous eigenenergy calculations. It is predicted that the two resonances can be observed in positron scatterings upon excited helium ions, the lower and higher resonances upon the $n=2$ and 3 states, respectively. The method of analyzing the time delays demonstrated in the present study would have extensive applications to resonances.

Note added in proof: A related work by Igarashi and Shimamura [18] was published. In this paper, they have calculated the eigenphase sum and derived a resonance formula (8) with the eigenphase theory.

ACKNOWLEDGMENTS

We are grateful to Dr. Y. Toya and Dr. M. Kamimura for helpful discussion. N.Y. appreciates support by the Special Postdoctoral Researchers Program of RIKEN. Y.K. wishes to acknowledge the Grant-in-Aid for Scientific Research, Ministry of Education and Culture, and the Inoue Foundation for Science for their generous financial support. The computation was partially carried out on the VPP5000 at JAERI and the VPP700E at RIKEN.

[1] M.L. Goldberger and K.M. Watson, *Collision Theory* (John Wiley & Sons, New York, 1964).
[2] R.G. Newton, *Scattering Theory of Waves and Particles* (Springer-Verlag, New York, 1966).
[3] J.R. Taylor, *Scattering Theory: The Quantum Theory of Nonrelativistic Collisions* (John Wiley & Sons, New York, 1972).
[4] S. Yoshida, Annu. Rev. Nucl. Sci. **24**, 1 (1974).
[5] D.M. Mitnik, D.C. Griffin, and M.S. Pindzola, Phys. Rev. Lett.

88, 173004 (2002).
[6] A.K. Bhatia and R.J. Drachman, Phys. Rev. A **42**, 5117 (1990).
[7] Y.K. Ho, Phys. Rev. A **53**, 3165 (1996).
[8] Y.K. Ho and Z.-C. Yan, Phys. Rev. A **66**, 062705 (2002).
[9] Y. Toya, Y. Kino, and H. Kudo, Mater. Sci. Forum, **445/446**, 446 (2004); Y. Toya, Ph.D. thesis, Tohoku University, 2003.
[10] A. Igarashi and I. Shimamura, Phys. Rev. A **56**, 4733 (1997).
[11] B.H. Bransden, C.J. Noble, and R.J. Whitehead, J. Phys. B **34**, 2267 (2001).
[12] M.S. Pindzola and D.R. Schultz, Phys. Rev. A **53**, 1525 (1996); M.S. Pindzola, D. Mitnik, and F. Robicheaux, *ibid.* **59**, 4390 (1999).
[13] N. Yamanaka and Y. Kino, Phys. Rev. A **64**, 042715 (2001); **65**, 062709 (2002); N. Yamanaka *et al.*, *ibid.* **67**, 052712 (2003).
[14] N. Yamanaka and Y. Kino, Phys. Rev. A **68**, 052715 (2003).
[15] F.T. Smith, Phys. Rev. **118**, 349 (1960).
[16] L.D. Landau and E.M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory*, 2nd ed. (Pergamon Press, London, 1958), Chaps. 17 and 18.
[17] L. Fonda, Fortschr. Phys. **20**, 135 (1972); A. Bohm, *Quantum Mechanics*, 3rd ed. (Springer-Verlag, New York, 1993), Chap. 18.
[18] A. Igarashi and I. Shimamura, Phys. Rev. A **70**, 012706 (2004).