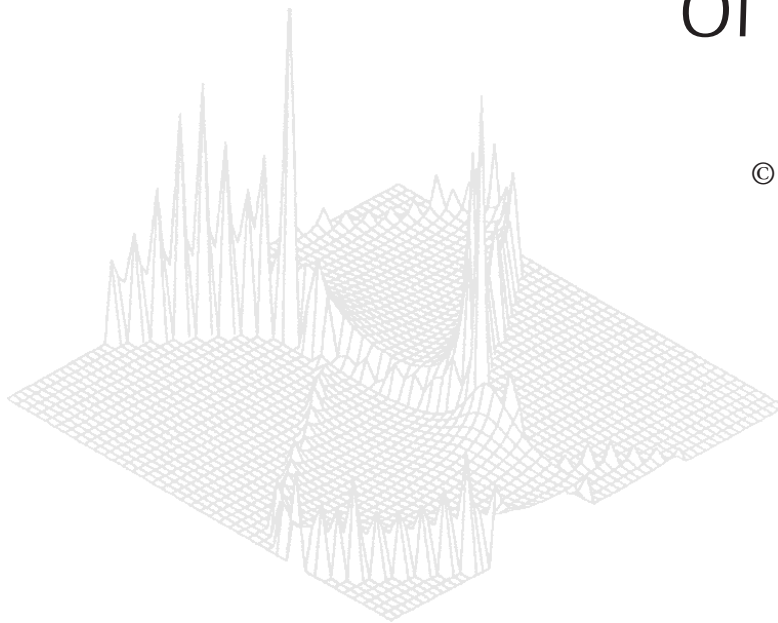

C S I R O P U B L I S H I N G

Australian Journal of Physics

Volume 52, 1999
© CSIRO Australia 1999



A journal for the publication of
original research in all branches of physics

www.publish.csiro.au/journals/ajp

All enquiries and manuscripts should be directed to

Australian Journal of Physics

CSIRO PUBLISHING

PO Box 1139 (150 Oxford St)

Collingwood

Vic. 3066

Australia

Telephone: 61 3 9662 7626

Facsimile: 61 3 9662 7611

Email: peter.robertson@publish.csiro.au



Published by **CSIRO PUBLISHING**
for CSIRO Australia and
the Australian Academy of Science



Time-dependent Approach to Positron–Hydrogen Scattering*

J. B. Wang,^{A,B} N. Riste,^B S. Midgley,^B A. T. Stelbovics^A and J. F. Williams^B

^ACentre for Atomic, Molecular and Surface Physics,
School of Mathematical and Physical Sciences, Murdoch University,
Perth, WA 6150, Australia.

^BDepartment of Physics, University of Western Australia,
Perth, WA 6907, Australia.

Abstract

This paper examines the positron–hydrogen scattering process by numerically solving the time-dependent Schrödinger equation in the s-wave model. The overall behaviour of the system wavefunction as it propagates through the collision region is studied above the positronium formation threshold and is found to match expectations qualitatively.

1. Introduction

Positron–hydrogen scattering involves four possible processes, i.e. elastic scattering, atomic excitation, atomic ionisation, and positronium formation. As a member of the class of three-body Coulomb problems, this study is of fundamental importance in atomic physics. It is also important because it involves interactions of matter with antimatter and thus has applications in cosmology and astrophysics.

Over the past decades, extensive studies have been conducted for a similar three-body Coulomb system, namely electron–hydrogen scattering, but much less work has been done for the positron–hydrogen system. Experimentally, this is mainly due to the difficulty of developing appropriate positron sources. However, substantial progress has been made in this direction in the past decade and useful cross section data are now available. The interested reader is referred to the review papers by Raith (1998) and Charlton (1998). Positron–hydrogen scattering is also a more challenging theoretical problem because of the extra reaction channel, i.e. positronium formation. Substantial progress has also been made in theoretical calculations but several questions remain to be resolved. One of the most important is that relating to the description of ionisation because the usual close-coupling equation formalism requires expansion in hydrogenic and positronium states. These over-complete expansions raise questions about double counting for ionisation and also have the potential to cause numerical instabilities.

A scattering event is clearly a time-dependent process. During such an event two particles approach each other, interact, and then separate. In the case where the event is on an atomic scale and is fully quantum mechanical in nature, the system wavefunction of the particles will evolve as the collision takes place in

* Refereed paper based on a contribution to the Australia–Germany Workshop on Electron Correlations held in Fremantle, Western Australia, on 1–6 October 1998.

accordance with the time-dependent Schrödinger equation. Nevertheless, nearly all reported theoretical studies of electron/positron scattering from atoms utilise a time-independent approach. For example, the convergent-close-coupling method (Bray and Stelbovics 1995, 1997; Ryzhikh and Mitroy 1997), the distorted-wave Born approximation method (Madison *et al.* 1995; Wang *et al.* 1995), the convergent R -matrix method (Bartschat *et al.* 1996), the intermediate energy R -matrix method (Scott *et al.* 1997), the hyperspherical-coordinates method (Yang *et al.* 1996), the converged J -matrix method (Konovalov and McCarthy 1996), and the Faddeev method (Faddeev and Merkuriev 1993; Kvitsinski and Hu 1996) are all time-independent theories.

The kernel of these methods is built around a set of stationary scattering states that are independent of time. Over the past half a century, considerable and continuous progress has been made in developing these very sophisticated time-independent methods, which can now describe a wide range of experimental findings. However, there are many mathematical difficulties inherent in the time-independent approaches, for example, the difficulty in handling the boundary conditions of continuum states in electron-atom collisions due to the long-range Coulomb interactions. These difficulties are of such magnitude that formal time-independent scattering theory has not yet led to a universally-valid computational method for the ionisation problem (McCarthy 1996; Bray 1997). Moreover, the time-independent approach provides little information on the transient state of the system during the scattering process.

On the other hand, the time-dependent approach has a more natural correspondence to reality, i.e. starting from an initial state of the system and following the events through time. It gives a direct solution of the quantum equations of motion and consequently has many distinct advantages over the traditional time-independent methods. For example, it provides information on transient behaviours and allows direct visualisation of the collision process, where one can ‘watch’ the electron and atom wavepacket evolving in time and in space. It handles continuum states, ionisation, resonance and post-collision interaction in the most natural way and is thus free of the difficulties encountered by the time-independent approaches. As an initial value problem, it is also comparatively easy to implement, flexible, and versatile in treating a large variety of quantum many-body problems. It is therefore expected to resolve some serious discrepancies between existing theories and experiments.

In this paper we examine the time-dependent approach for a simplified model of s-wave positron-hydrogen scattering by numerically propagating the positron-hydrogen system wavefunction in time through the collision region. Preliminary results are reported.

2. Theory

The general time-dependent theory of wavepacket propagation has been available for many years (see e.g. Goldberger and Watson 1964; Taylor 1972), but computational techniques have been slow to develop and practical calculations have had to await the arrival of powerful computers. The formal solution of the time-dependent Schrödinger equation is $\psi(\mathbf{r}, t + \Delta t) = \exp(-iH\Delta t)\psi(\mathbf{r}, t)$, where $H = -\nabla^2/2 + V(\mathbf{r})$ is the system Hamiltonian, $V(\mathbf{r})$ is the interaction potential, and \mathbf{r} denotes collectively the spatial coordinates. It is the method of

approximating the exponential time propagator $\exp(-iH\Delta t)$ that distinguishes different time-dependent schemes.

In an earlier publication (Wang and Scholz 1998) we discussed several approaches including the Euler expansion, the first (FOD) and second (SOD) order difference schemes, the Taylor expansions, the split operator scheme, and the Chebyshev scheme. We applied the Chebyshev scheme to one-dimensional potential scattering and our results were in excellent agreement with exact solutions. This paper extends our previous work to study s-wave positron–hydrogen scattering. A comprehensive discussion on the time-dependent approaches especially related to quantum chemistry can be found in the review article written by Balakrishnan *et al.* (1997).

Briefly, the Chebyshev scheme approximates the exponential time propagator by a Chebyshev polynomial expansion:

$$\psi(x, y, t) = \exp[-i(E_{\max} + E_{\min})t/2] \sum_{n=0}^N a_n(\alpha) \phi_n(-i\tilde{H}) \psi(x, y, t=0), \quad (1)$$

where E_{\max} and E_{\min} are the upper and lower bounds on the energies sampled by the wavepacket, $\alpha = (E_{\max} - E_{\min})t/2$, $a_n(\alpha) = 2J_n(\alpha)$ except for $a_0(\alpha) = J_0(\alpha)$, $J_n(\alpha)$ are the Bessel functions of the first kind, ϕ_n are the Chebyshev polynomials, and the normalised Hamiltonian is defined as

$$\tilde{H} = \frac{1}{E_{\max} - E_{\min}} [2H - (E_{\max} + E_{\min})]. \quad (2)$$

The above normalisation ensures that the expansion of Chebyshev polynomials is convergent. Since the Bessel functions fall to zero exponentially as n increases beyond α , it follows that terminating the expansion at $N > \alpha$ would yield accurate results. Note that α is proportional to the time step t and so is the number of terms required in the expansion. Since the time step t can be arbitrarily large, this scheme is often used as a one-step propagator to cover the complete interaction.

Although the Chebyshev scheme is mathematically more involved and in some cases computationally more expensive in comparison with other schemes, it is the most accurate time-dependent method to date (Mohan and Sathyamurthy 1988; Leforestier *et al.* 1991; Wang and Scholz 1998). This scheme has been employed in the field of quantum chemistry with considerable success (see e.g. Kosloff 1988; Cerjan and Kulander 1991; Mowrey 1993; Huang *et al.* 1993; Kroes and Neuhauser 1996; Gögtas *et al.* 1996; Balakrishnan *et al.* 1997), but it has yet to be utilised in the atomic physics community.

Some progress has been made in developing and applying the simpler schemes to problems in the field of atomic physics, including the calculation of electron impact ionisation of hydrogen (Bottcher 1985, FOD), Stark shift and lifetime of hydrogen (Hermann and Fleck 1988, split operator scheme), two-electron atom energies (Zhang *et al.* 1994, split operator scheme), atomic autoionisation (Schultz *et al.* 1994, FOD), photoionisation (Dehnen and Engel 1995, split operator scheme), s-wave electron scattering from hydrogen (Ihra *et al.* 1995,

split operator scheme), electron detachment from H^- (Kazansky and Taulbjerg 1996, split operator scheme), and e-H scattering (Pindzola and Schultz 1996, Taylor expansion; Pindzola and Robicheaux 1996, SOD method).

Very recently Larkin *et al.* (1998) studied the positron-hydrogen system using the split operator scheme. Their study was based on a linear one-dimensional model (i.e. the only scattering directions possible are forwards or backwards). This one-dimensional model is not the same as the well known s-wave model, or the Temkin-Poet model (Temkin 1962; Poet 1978), where only the first term in the partial wave expansion is retained. The s-wave model can be readily expanded to include the other partial waves systematically until convergence is achieved, while the linear one-dimensional model cannot be extended to obtain a full solution of the system unless all six dimensions are included in the calculation.

It is very encouraging that the above calculations were found to be in fairly good agreement with results from time-independent models and/or experimental data. Nevertheless, there is a general deep concern about the accuracy of the final system wavefunction obtained by the time-dependent schemes, since errors accumulated over the many time steps may cause severe distortion of the wavepackets. This prompted us to adopt the most accurate scheme to date, i.e. the Chebyshev scheme, for our investigation on the s-wave positron-hydrogen scattering.

3. Calculations and Results

In the s-wave Temkin-Poet model, all angular dependence is neglected and the time-dependent Schrödinger equation of the S-partial wave is given by

$$i \frac{\partial}{\partial t} \psi^S(r_1, r_2, t) = \left(-\frac{1}{2} \frac{\partial^2}{\partial r_1^2} - \frac{1}{2} \frac{\partial^2}{\partial r_2^2} + \frac{1}{r_1} - \frac{1}{r_2} - \frac{1}{r_>} \right) \psi^S(r_1, r_2, t), \quad (3)$$

where r_1 and r_2 are the distances of the positron and the electron relative to the nucleus respectively, $r_>$ refers to the greater of r_1 and r_2 , $\psi^S(r_1, r_2, t)$ is the s-wave wavefunction and the system Hamiltonian is

$$H = -\frac{1}{2} \frac{\partial^2}{\partial r_1^2} - \frac{1}{2} \frac{\partial^2}{\partial r_2^2} + \frac{1}{r_1} - \frac{1}{r_2} - \frac{1}{r_>}. \quad (4)$$

Assuming that the hydrogen atom is initially in the ground state, its wavefunction is then given by

$$\psi_H(r_2) = r_2 e^{-r_2}. \quad (5)$$

The positron is assumed to be sufficiently far away from the hydrogen atom initially that it can be represented by a wavepacket for a free particle, i.e.

$$\psi_{e^+}(r_1) = e^{-(r_1-a)^2/4\sigma} e^{ikr_1}, \quad (6)$$

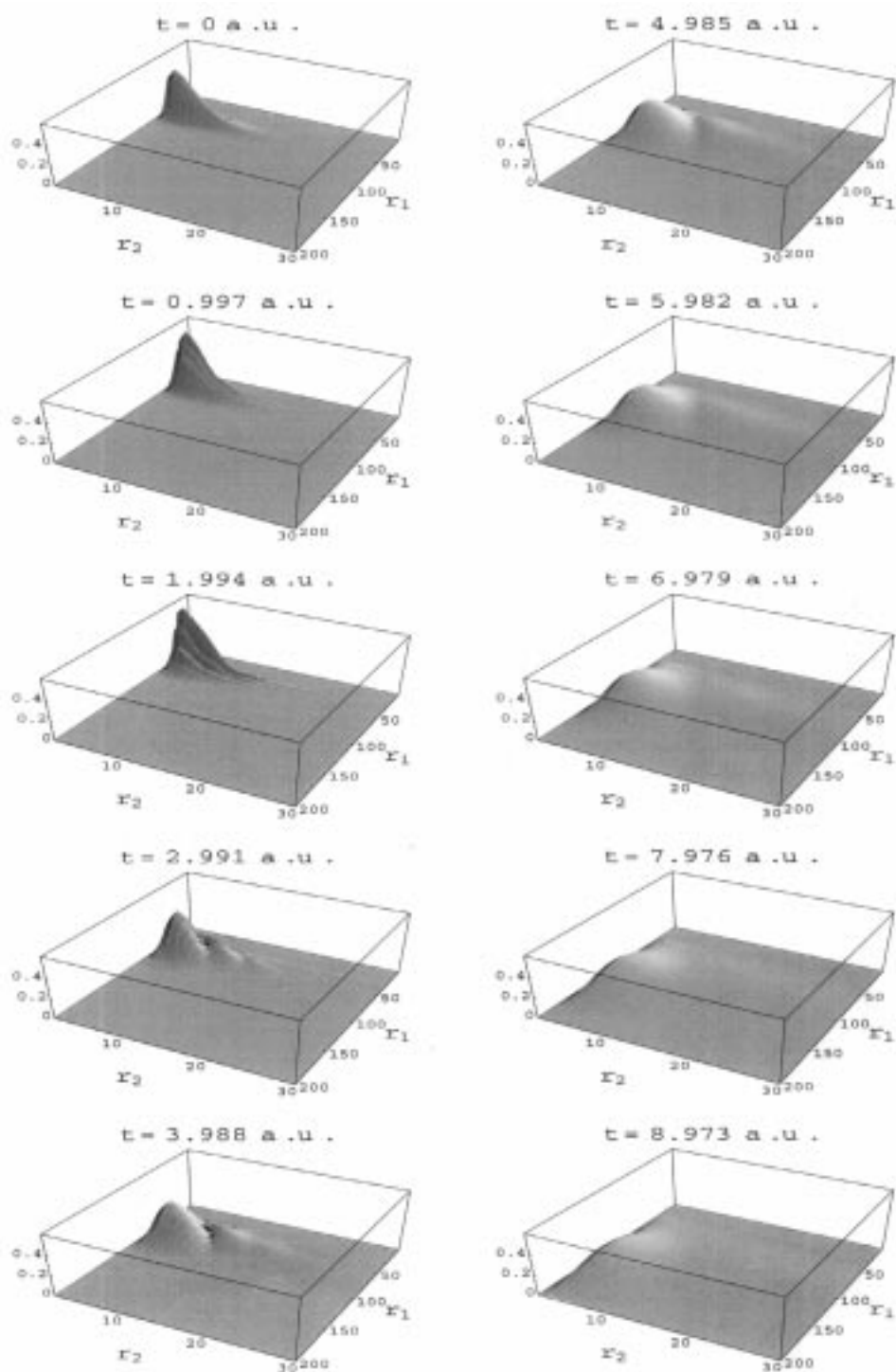


Fig. 1. Time evolution of the positron-hydrogen system wavefunction through the collision interaction. The dominant energy of the incident positron is 3.4 a.u.

where a defines the starting position of the positron, k is the dominant momentum of the positron wavepacket, and σ is the inverse of the momentum spread in the initial positron wavepacket. Combining the two expressions gives the initial wavefunction for the positron–hydrogen system:

$$\psi(r_1, r_2, t = 0) = r_2 e^{-r_2 + ikr_1 - (r_1 - a)^2 / 4\sigma} . \quad (7)$$

Fig. 1 illustrates the time evolution of this wavefunction under the influence of positron–electron, positron–nucleus and electron–nucleus interactions. These time-dependent wavefunctions were obtained by propagating the wavefunction in time according to equation (1). The wavefunction is initially observed moving towards the nucleus of the hydrogen atom, then being scattered by the interaction potentials between the three particles, and finally moving away from the interaction region.

This simulation was carried out for a dominant incident energy of 3.4 a.u. with a 5% spread in momentum, which is well above the positronium formation threshold and also the ionisation energy of hydrogen. At this energy scattering flux into all channels should be significant. Therefore, we expect to see significant changes in the profile of the system wavefunction in the r_2 direction (i.e. the electron coordinate), representing a finite probability in finding the electron at greater distances from the nucleus. This is in accordance with the finite amplitudes of excitation (including direct excitation of the hydrogen atom and the rearrangement into the positronium atom excited states) and ionisation of the hydrogen atom at this energy. The enhancement of the larger distance amplitude along the $r_1 = r_2$ line can be interpreted as partially due to the formation of positronium and partially due to ionisation.

We cannot yet say with any certainty that positronium was formed at any particular stage just by looking at the s-wave wavefunctions, because the angular positions of the two particles are not known in this model. It was possible that even if the two particles were at the same radius, they could have been on opposite sides of the nucleus. Thus in contrast to the Temkin–Poet model of electron scattering from hydrogen, where the inelastic flux can be uniquely attributed to a discrete excitation or ionisation event, no such unique partitioning is possible because we need angular information beyond the scope of the s-wave model to resolve the combined flux into positronium-formation and ionisation channels. Further work involving more extended calculations including other partial waves will resolve the issue of how much of the amplitude along the $r_1 = r_2$ line refers to positronium formation and how much to ionisation.

4. Conclusions

We have examined the scattering of a positron from a hydrogen atom by numerically solving the time-dependent Schrödinger equation. Two approximations are used. The first is a Chebyshev polynomial expansion of the time evolution operator and the second a partial wave expansion of the initial wavefunction, of which only the s-wave term is retained. It was found that the time-dependent behaviour of the propagating wavefunction during and after the interaction matched expectations qualitatively. Thus the time-dependent method shows promise. It is worth noting that this method can be equally well applied over

a wide range of energies without affecting the numerical procedures. Further large-scale calculations including partial waves are needed to uniquely apportion the scattered flux and hence to obtain quantitative cross sections for inelastic, rearrangement and ionisation processes.

Acknowledgments

JBW would like to thank J. Pan, T. Scholtz and P. Abbott for helpful discussions. We would also like to acknowledge a grant of computer time from the Australian National University Supercomputing Facility for use of their VPP300, on which the reported calculations were performed.

References

- Balakrishnan, N., Kalyanaraman, C., and Sathyamurthy, N. (1997). *Phys. Rep.* **280**, 80–144.
- Bartschat, K., Hudson, E. T., Scott, M. P., Burke, P. G., and Burke, V. M. (1996). *Phys. Rev. A* **54**, R998–1001.
- Bottcher, C. (1985). *Adv. At. Mol. Phys.* **20**, 241–66.
- Bray, I. (1997). *Phys. Rev. Lett.* **78**, 4721–4.
- Bray, I., and Stelbovics, A. T. (1995). *Adv. At. Mol. Opt. Phys.* **35**, 209–54.
- Bray, I., and Stelbovics, A. T. (1997). *J. Phys. B* **30**, L493–7.
- Cerjan, C., and Kulander, K. C. (1991). *Comput. Phys. Commun.* **63**, 529–37.
- Charlton, M. (1998). In ‘Photonic, Electronic and Atomic Collisions’ (Eds F. Aumayr and H. Winter), pp. 361–71 (Word Scientific: Singapore).
- Dehnen, R., and Engel, V. (1995). *Phys. Rev. A* **52**, 2288–94.
- Faddeev, L. D., and Merkuriev, S. P. (1993). ‘Quantum Scattering Theory for Several Particle Systems’ (Kluwer: Boston).
- Gögtas, F., Balint-Kurti, G. G., and Offer, A. R. (1996). *J. Chem. Phys.* **104**, 7927–39.
- Goldberger, M. L., and Watson, K. M. (1964). ‘Collision Theory’ (Wiley: New York).
- Hermann, M. R., and Fleck, Jr, J. A. (1988). *Phys. Rev. A* **38**, 6000–12.
- Huang, Y. H., Zhu, W., Kouri, D. J., and Hoffman, D. K. (1993). *Chem. Phys. Lett.* **214**, 451–5.
- Ihra, W., Draeger, M., Handke, G., and Friedrich, H. (1995). *Phys. Rev. A* **52**, 3752–62.
- Kazansky, A. K., and Taulbjerg, K. (1996). *J. Phys. B* **29**, 4465–75.
- Konovalov, D. A., and McCarthy, I. E. (1995). *J. Phys. B* **28**, L39–45.
- Kosloff, R. (1988). *J. Phys. Chem.* **92**, 2087–100.
- Kroes, G. J., and Neuhauser, D. (1996). *J. Chem. Phys.* **105**, 8690–8.
- Kvitsinsky, A. A., and Hu, C. Y. (1996). *J. Phys. B* **29**, 2059–77.
- Larkin, J. M., Eberly, J. H., Lappas, D. G., and Grobe, R. (1998). *Phys. Rev. A* **57**, 2572–7.
- Leforestier, C., Bisseling, R. H., Cerjan, C., Feit, M. D., Friesner, R., Guldberg, A., Hammerich, A., Jolicard, G., Karrlein, W., Meyer, H. D., Lipkin, N., Roncero, O., and Kosloff, R. (1991). *J. Comput. Phys.* **94**, 59–80.
- McCarthy, I. E. (1996). *Aust. J. Phys.* **49**, 219–29.
- Madison, D. H., Schroeder, J., Bartschat, K., and McEachran, R. P. (1995). *J. Phys. B* **28**, 4841–51.
- Mohan, V., and Sathyamurthy, N. (1988). *Comput. Phys. Rep.* **7**, 213–58.
- Mowrey, R. C. (1993). *J. Chem. Phys.* **99**, 7049–55.
- Pindzola, M. S., and Robicheaux, F. (1996). *Phys. Rev. A* **54**, 2142–5.
- Pindzola, M. S., and Schultz, D. R. (1996). *Phys. Rev. A* **53**, 1525–36.
- Poet, R. (1978). *J. Phys. B* **11**, 3081–94.
- Raith, W. (1998). In ‘Photonic, Electronic and Atomic Collisions’ (Eds F. Aumayr and H. Winter), pp. 341–60 (Word Scientific: Singapore).
- Ryzhikh, G., and Mitroy, J. (1997). *J. Phys. B* **30**, 5545–65.
- Schultz, D. R., Bottcher, C., Madison, D. H., Peacher, J. L., Buffington, G., Pindzola, M. S., Gorczyca, T. W., Gavras, P., and Griffin, D. C. (1994). *Phys. Rev. A* **50**, 1348–58.
- Scott, M. P., Burke, P. G., Bartschat, K., and Bray, I. (1997). *J. Phys. B* **30**, L309–15.

- Taylor, J. R. (1972). 'Scattering Theory: Quantum Theory of Nonrelativistic Collisions' (Wiley: New York).
- Temkin, A. (1962). *Phys. Rev.* **126**, 130–42.
- Wang, J. B., and Scholz, T. T. (1998). *Phys. Rev. A*, in press.
- Wang, J. B., Williams, J. F., Stelbovics, A. T., Furst, J. E., and Madison, D. H. (1995). *Phys. Rev. A* **52**, 2885–900.
- Yang, X. Z., Bao, C. G., and Lin, C. D. (1996). *Phys. Rev. A* **53**, 3934–45.
- Zhang, L., Feagin, J. M., Engel, V., and Nakano, A. (1994). *Phys. Rev. A* **49**, 3457–62.

Manuscript received 30 November 1998, accepted 22 February 1999