Vol 17 No 3, March 2008
1674-1056/2008/17(03)/0801-06
Chinese Physics B
© 2008 Chin. Phys. Soc.
and IOP Publishing Ltd

Short-ranged potential effects on the recurrence spectra of lithium $M = 1$ atoms in parallel electric and magnetic fields*

Wang Wen-Peng(王文鹏), Li Hong-Yun(李洪云),
Wang Shu-Bao(王树宝), and Lin Sheng-Lu(林圣路)†

College of Physics and Electronics, Shandong Normal University, Jinan 250014, China

(Received 11 July 2007; revised manuscript received 21 August 2007)

This paper presents recurrence spectra of highly excited lithium atoms with $M = 1$ state in parallel electric and magnetic fields at a fixed scaled energy $\varepsilon = -0.03$. Short-ranged potentials including ionic core potential and centrifugal barrier are taken into account. Their effects on the states and photo-absorption spectrum are analysed in detail. This demonstrates that the geometric features of classical orbits are of special importance for modulations of the spectral pattern. Thus the weak polarization as well as the reduction of correlation of electrons induced by short-ranged potentials give rise to the recurrence spectra of lithium $M = 1$ atoms more compact than that of the $M = 0$ one, which is in good agreement with the experimental prediction.

Keywords: closed-orbit theory, recurrence spectra, short-ranged potential, centrifugal barrier
PACC: 0365S, 3210W, 3290, 3150

1. Introduction

Closed-orbit theory has been testified to be the quantitative and perfect approach to calculate and interpret the recurrence spectra.[1−3] Taking intrinsic nonintegrable and irregular dynamics into account we find that a rigorous manipulation of highly excited multielectron atoms in strong external fields is still regarded as a theoretical challenge.[4] Studies on the effects of the ionic core during the last about ten years have significantly enhanced our understanding of the core-scattering. The modelling core potential method proposed by Bruno Hüpper *et al* opened a feasible way to deal with the nonhydrogen atoms in external fields.[5] Keller and Morgan have reported the first experimental observation of the manifestation of exchange effects in the Rydberg–Stark recurrence spectra of helium.[6] And Monteiro and Wunner revealed the puzzling structures in recurrence spectra of general Rydberg atoms in magnetic field based on exact quantum R-matrix method.[7]

Many investigations were performed restrictively to Rydberg atomic $M = 0$ state up to now.[4,8−10] No direct theoretical treatments of the multielectron atoms with $M = 1$ have been reported previously. The recent experiment on the Rydberg helium atoms in a static electric field by Annemieke Kips *et al* has suggested that the discrepancies between $M = 0$ and $M = 1$ states can be neglected in a certain sense.[11] However, according to our analysis in this paper the discrepancies between both arise from the centrifugal barrier and display a significant influence.

This paper is organized as follows. Firstly, we introduce the model potential and discuss the scaling behaviours of the Hamiltonian of the system. The corresponding recurrence spectra for lithium $M = 1$ atoms in parallel electric and magnetic fields at a constant scaled energy $\varepsilon = -0.03$ are calculated in extended closed-orbit theory framework. Finally these spectra are compared with hydrogen and lithium $M = 0$ atoms, respectively. The results demonstrate clearly that the short-ranged potential effects on the resonant structures of recurrence spectra are notable.

2. Theory and method

2.1. Hamiltonian

The lithium atom is highly excited to Rydberg state $M = 1$ by the absorption of a σ polarized pho-

*Project supported by the National Natural Science Foundation of China (Grant Nos 10774093 and 10374061).
†E-mail: sllin@sdnu.edu.cn

ton in continuous laser.[12,13]

The system can be substantially simplified to the movement of a single electron in an attractive Coulomb potential modified by a short-ranged model potential combined with the external parallel electric and magnetic fields along z axis. The Hamiltonian reads

$$H = \frac{1}{2}\left(p_\rho^2 + p_z^2 + \frac{p_\varphi^2}{\rho^2}\right) + \frac{\gamma}{2}L_z + \frac{1}{8}\gamma^2\rho^2 + fz + V(r), \quad (1)$$

where $\gamma = B/B_0$ is the magnetic field strength measured in the units of $B_0 \approx 2.35 \times 10^5$T and $f = F/F_0$ with $F_0 \approx 5.14 \times 10^9 \mathrm{V\cdot cm^{-1}}$. The component L_z of the orbital angular momentum is conserved.

Considering the polarization of the nucleus and correlation of the electrons, we find that $V(r)$ is the model potential with the analytical form

$$V(r) = V_{\mathrm{Coulomb}}(r) + V_{\mathrm{core}}(r), \quad (2)$$

where $V_{\mathrm{Coulomb}}(r)$ is the Coulomb potential, $V_{\mathrm{core}}(r)$ is the core potential.

$$V_{\mathrm{Coulomb}}(r) = -\frac{1}{r}, \quad (3)$$

$$V_{\mathrm{core}}(r) = -\frac{Z-1}{r}\left(1 + \frac{r}{a}\right)\mathrm{e}^{-r/a}, \quad (4)$$

where $a = 0.46948$ is the free length parameter determining the range of the core of lithium[4] and $V_{\mathrm{core}}(r)$ is assumed to be spherically symmetric with the asymptotic form $V_{\mathrm{core}}(r) \xrightarrow{r\to 0} -(Z-1)/r$ and $V_{\mathrm{core}}(r) \xrightarrow{r\to\infty} 0$. This kind of potential has also been used in studies of other nonhydrogen atoms.[10,11] Compared with previous works, we find that the classical trajectories are modified by the short-ranged potential including the centrifugal barrier $\dfrac{p_\varphi^2}{2\rho^2}$ and model potential $V_{\mathrm{core}}(r)$ at the moment. In the vicinity of ionic core, the core-scattered orbits will then be deflected by the short-ranged potential.

2.2. Scaled rule

One of the most significant techniques in the study of atoms in external electric and magnetic fields is the use of so-called scaled variables. The scaled variables are defined by the relations

$$\tilde{r} = r\gamma^{2/3}, \quad \tilde{p} = p\gamma^{-1/3}, \quad \tilde{t} = t\gamma,$$
$$\tilde{f} = f\gamma^{-4/3}, \quad \tilde{l}_z = L_z\gamma^{1/3}, \quad \hbar_{\mathrm{eff}} = \gamma^{1/3}, \quad (5)$$

here the letters with tilde describe the scaled variables and $\hbar_{\mathrm{eff}}$ is the effective Planck constant. The Hamiltonian of the system is rewritten as[14]

$$\varepsilon = E\gamma^{-2/3} = \frac{1}{2}\tilde{p}^2 + \frac{\tilde{l}_z}{2} + \frac{1}{8}\tilde{\rho}^2 + \tilde{f}\tilde{z} + V(\tilde{r}) \quad (6)$$

with

$$\tilde{p}^2 = \tilde{p}_\rho^2 + \tilde{p}_z^2 + \frac{\tilde{p}_\varphi^2}{\tilde{\rho}^2}. \quad (7)$$

The action of jth closed orbit is $S_j = 2\pi\tilde{S}_j\gamma^{-1/3}$ and $\tilde{S}_j$ can be evaluated

$$\tilde{S} = \frac{1}{2\pi}\oint_L (\tilde{P}_{\tilde{\rho}}\mathrm{d}\tilde{\rho} + \tilde{P}_{\tilde{z}}\mathrm{d}\tilde{z} + \tilde{P}_\varphi \mathrm{d}\varphi) = n_\varepsilon\gamma^{1/3} = n_\varepsilon\hbar_{\mathrm{eff}}, \quad (8)$$

where n_ε is principal quantum number and the integration follows the classical closed orbit L. Equation (8) can be regarded as the quantization condition for the scaled action. Making $\hbar_{\mathrm{eff}}(\gamma^{1/3})$ small enough and keeping $\tilde{S}_j$ finite for large n_ε, we find that the theoretical results are able to compare with those of experiments when changing E and B simultaneously to remain ε as a constant.

In general, because the core scattering is not pure Coulomb, the scaling behaviour is essentially violated for nonhydrogenic atoms. Once we pay attention to the predominant long-range classical dynamics of Rydberg atoms, however without particular consideration of the small region near the nucleus, luckily the scaled property is approximately shown to be still valid. Moreover for a strong magnetic field (2.7T–6T), the corresponding effective Planck constant $\hbar_{\mathrm{eff}}^{-1} = \gamma^{-1/3}$ varying from 33.9 to 44.3 satisfies the classical limited condition ($\hbar_{\mathrm{eff}} = \gamma^{1/3} \to 0$) and ensures the centrifugal barrier and Zeeman terms in Eq.(6) scaled perfectly. This situation will be seen in Table 1.

2.3. Expression of averaged recurrence spectra

Following the familiar calculating process, the averaged oscillator strength density consists of a smooth background term and a sum of oscillating terms. The oscillating part is expressed as

$$f(z) = \sum_j C_j \sin(2\pi\tilde{S}_j z - \alpha_j\pi/2 - \varphi_j + 2\pi\mu_l), \quad (9)$$

where $z = \gamma^{-1/3}$, $\tilde{S}_j$ and α_j are the classical scaled action and Maslov index of jth closed orbit, respectively. We choose $\varphi_j = 3\pi/4$ in our calculations, accounting

for the centrifugal barrier leads to the result that all orbits along the fields are neglected.

In quantum mechanics the ionic core is entirely characterized by quantum defects $\mu_l(E<0)$, or for energies $E>0$ the translation of these short-range effects outside the core amounts to the radial phase shift δ_l. At the vicinity of the ionization threshold, these quantities are connected by Seaton's theorem $\delta_l=\pi\mu_l$. The quantum defects μ_l can be computed by

$$\mu_l = \frac{\sqrt{2}}{\pi}\lim_{R\to\infty}\left[\int_{r_{0,\mathrm{c}}}^{R}\sqrt{-V(r)-\frac{(l+1/2)^2}{2r^2}}\mathrm{d}r - \int_{r_0}^{R}\sqrt{\frac{1}{r}-\frac{(l+1/2)^2}{2r^2}}\mathrm{d}r\right], \quad (10)$$

where $r_{0,\mathrm{c}}$ and r_0 are the classical turning points for short-ranged potential and pure Coulomb potential respectively, and the relevant quantum defects are μ_0=0.411, μ_1=0.053.[15] Obviously, the short-ranged potential, particularly the centrifugal barrier, plays an important role in the quantum defects. As l increases the quantum defect might be dropped rapidly due to the screen effect for large l and generally $\mu_{l\geq 2}$ can be ignored.

In order to yield the recurrence spectra, we carry out Fourier transform for the photoabsorption recurrence spectra $f(E)$ in a finite interval $[z_1,z_2]$ with $\bar{z}=1/2\,(z_1+z_2)$ and $\Delta z=z_2-z_1$.

$$F(\tilde{S}) = \frac{1}{\Delta z}\int_{z_1}^{z_2} f(z)\exp\left[2\pi\mathrm{i}\tilde{S}(z-\bar{z})\right]\mathrm{d}z = \sum_j C_j \frac{\sin\left[\pi(\tilde{S}-\tilde{S}_j)\Delta z\right]}{2\pi(\tilde{S}-\tilde{S}_j)\Delta z} \times \exp[\mathrm{i}(-2\pi\mathrm{i}\tilde{S}_j\bar{z}+\alpha_j\pi/2+\varphi_j-2\pi\mu_l)], \quad (11)$$

where C_j is the amplitude related to the trajectory stability, and the classical scaled action $\tilde{S}_j$ can be specified by Eq.(8).

3. Results and discussion

3.1. Closed orbits

We obtain 32 stable orbits which contribute mostly to the spectra at fixed scaled energy $\varepsilon=-0.03$ and scaled electric field $\tilde{f}=0.01$. Figure 1 shows some closed orbits in the $\rho-z$ coordinate system. For sake of clarity, we assume that whenever the electron passes through z axis, the sign of ρ is changed. It is clearly that the strong centrifugal barrier obstructs the Rydberg electron from approaching to the z axis. Moreover these trajectories in the diagram deviate significantly from those of $M=0$ case where the excited electron can pass through the z axis.

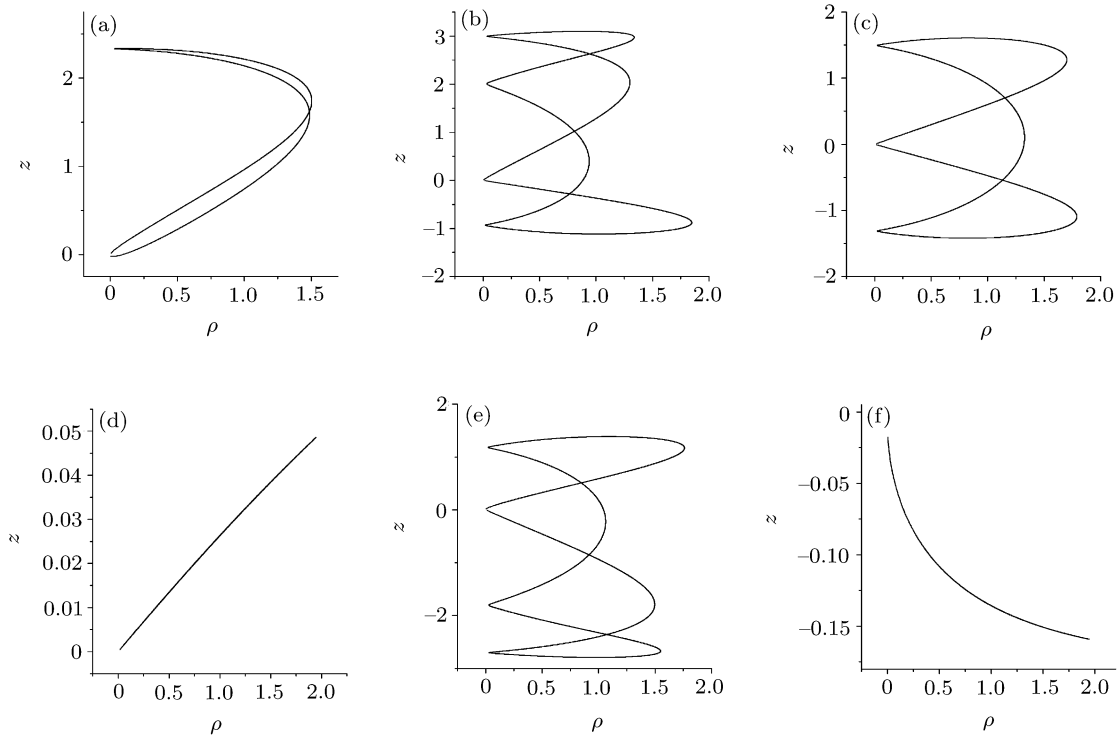


Fig.1. Some of the closed orbits of Li($M=1$) atoms in parallel electric and magnetic fields in (ρ,z) coordinate system. $\varepsilon=-0.03$, $\tilde{f}=0.01$, 2.7T< B <6T, $33.9<\hbar_{\mathrm{eff}}^{-1}<44.3$.

3.2. Recurrence spectra

In Fig.2, the recurrence spectrum of Li ($M = 1$) atoms is represented and compared with that of hydrogen atoms. It is evident that the novel structures of peaks in the spectra of Li atoms can be identified in terms of families of core-scattered classical orbits appearing in the positions where hydrogenic closed orbits do not exist. In spite of the fact that each new orbit has a low amplitude, the interference of all members of a family results in visible resonances in the recurrence spectra. The resonant peak labelled with (1,2) appearing at $\tilde{S}_{(1,2)} = \tilde{S}_1 + \tilde{S}_2 = 2.5264$ indicates the contributions of combination orbits 1 and 2 which undergo one time ionic core scattering. While the resonant peak at $\tilde{S}_{(2,3,4)} = \tilde{S}_2 + \tilde{S}_3 + \tilde{S}_4 = 5.164359$ is achieved by double ionic core scattering started from the closed orbit 2, consequently followed orbit 3 and then orbit 4. Indeed, from Table 1 it must be noted that the scaled actions of peaks in the recurrence spectra are mainly contributed by the first two terms in Eq.(8) and the last term is measured in order of 10^{-3} which can be neglected with respect to the total scaled actions. This implies that the scaled rule on Hamiltonian is feasible in this paper.

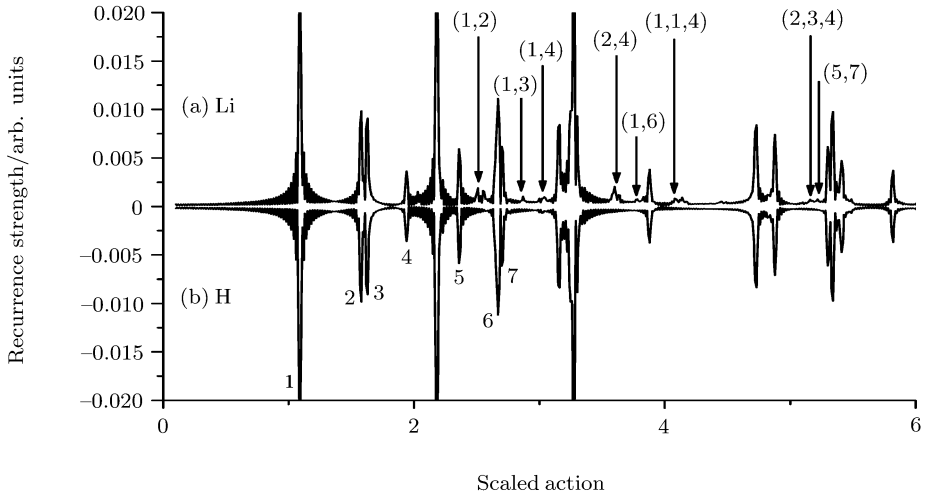


Fig.2. Comparison between the recurrence spectra of lithium atoms and hydrogen atoms in parallel electric and magnetic fields at $\varepsilon = -0.03$ and $\tilde{f} = 0.01$ with 2.7T< B <6T, $33.9 < \hbar_{\text{eff}}^{-1} < 44.3$. (a) The recurrence spectra of lithium atoms. (b) The recurrence spectra of hydrogen atoms.

Table 1. Dates of the closed orbits in Fig.1.

orbit	outgoing angle θ_i	total scaled action $\tilde{S}$	scaled action $\tilde{S}_\varphi\left(\int \tilde{P}_\varphi \mathrm{d}\varphi\right)$
a	18.004	1.5284569548933	$2.636575336679863\times10^{-3}$
b	26.589	2.5897648763785	$4.575564073216436\times10^{-3}$
c	58.131	2.2846867222629	$2.975460435664946\times10^{-3}$
d	88.410	1.0105484627160	$2.077674002037412\times10^{-4}$
e	135.051	2.6672932328215	$4.870965422811442\times10^{-3}$
f	169.760	1.0359514465742	$1.349330860904737\times10^{-3}$

Equation (8) shows that although the changes of the scaled action $\tilde{S}_j$ is small, the amplitudes C_j are sensitive to the geometric features of the closed orbits, therefore depend intimately on the short-ranged potential. Due to the high density of the states, the effects of the short-ranged potential are twofold. On the one hand, quantum mechanically, the repulsive centrifugal term $l(l+1)/\rho^2$ makes the electronic wave 'push out' with respect to the pure Coulomb radial wave. Consequently, the phase shift should be reduced by a positive $(-\delta_l/k)$ for $\delta_l < 0$. On the other hand, classical mechanically, the repulsive potential enables

the returning orbits not to arrive at z axis. The correlation and interference between electrons are reduced slightly. This seems in line with the physical intuition and leads to a lot of modifications in recurrence spectra.

In Fig.3, the positions of resonant peaks, such as $A-D$, move towards smaller scaled action in $M=1$ spectra. This is expected since the centrifugal barrier impedes the electron approaching z axis and leads to the closed orbits shorter slightly. This also induces a reduction of polarization and correlation of electrons for Li($M=1$) atoms. Consequently, the combination among primitive closed orbits are decreased, and some peaks that appear in the recurrence spectra of $M=0$ fade away. In brief, although centrifugal barrier contributes negligibly to the total scaled action, the variations in wave function turn out to be considerable. Therefore the recurrence structures are evidently modified. In addition, in the recurrence spectra of $M=0$ the peak marked by arrow E is related with the closed orbit that has an outgoing zero angle with respect to z axis, which does not present in the $M=1$ diagram. Because the amplitude of the jth closed orbit C_j is determined by terms $\cos(\theta_{\rm i})$ and $\cos(\theta_{\rm f})$, where $\theta_{\rm i}$ is the orbital outgoing angle and $\theta_{\rm f}$ is the orbital returning angle. The resonant peak labelled by the capitalized letter F in $M=0$ spectra is related with the closed orbit in the plane perpendicular to z axis, which has the ignorable spectral strength and is hard to see.

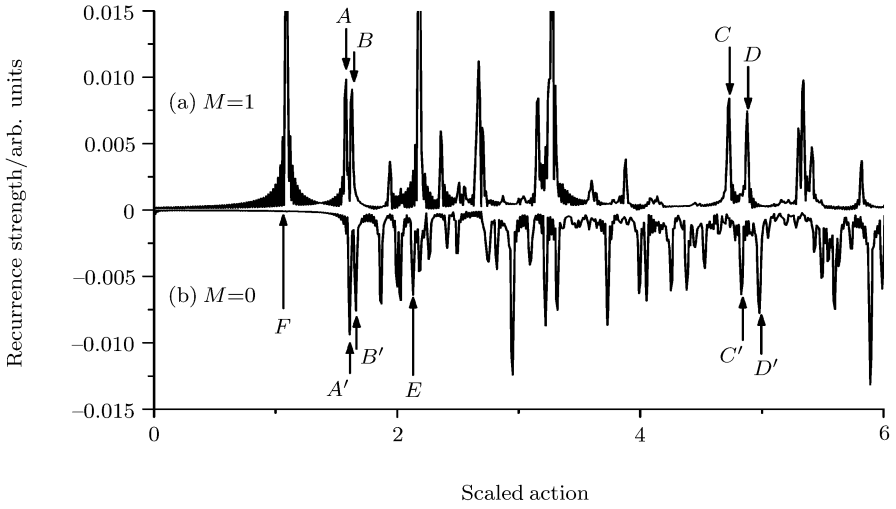


Fig.3. Comparison between the recurrence spectra of Li($M=1$) atoms and Li($M=0$) atoms in parallel electric and magnetic fields at $\varepsilon=-0.03$ and $\tilde{f}=0.01$ with 2.7T< B <6T, 33.9 < $\hbar_{\rm eff}^{-1}$ < 44.3. (a) The recurrence spectra of Li($M=1$) atoms. (b) The recurrence spectra of Li($M=0$) atoms.

4. Summary

We have extended the standard closed-orbit theory framework to approach the multielectron atoms with $M=1$ states in strong external fields. The scaled variables are applied in a semiclassical calculation. We have paid particular attention to the effects of short-ranged potential on the spectra. In comparison with $M=0$, the centrifugal barrier is an important contribution to the quantum defects, thus effects evidently the electronic state functions. Although the variations in the geometric features of the closed orbits lead to the positions of resonant peaks moved slightly only, the modulation of the recurrence spectra is substantially obvious. Indeed our intention is not to describe a particular atom but to study the general effects of short-ranged potential on the recurrence spectra. Perhaps this sensitive dependences of states are the general properties of the atomic or molecular system possessing nonintegrable dynamics or chaos.

References

[1] Du M L and Delos J B 1988 *Phys. Rev.* A **38** 1896

[2] Du M L and Delos J B 1988 *Phys. Rev.* A **38** 1913

[3] Zhang Y H, Zhang L Q, Xu X Y, Ge M H, Lin S L and Du M L 2006 *Chin. Phys.* **15** 502

[4] Lin S L, Zhang Q J, Zhao K, Song X H and Zhang Y H 2002 *Chin. Phys. Lett.* **19** 29

[5] Hüpper B, Main J and Wunner G 1996 *Phys. Rev.* A **53** 744

[6] Keeler M and Morgan T J 1998 *Phys .Rev. Lett.* **80** 5726

[7] Monteiro T S and Wunner G 1990 *Phys. Rev. Lett.* **65** 1100

[8] Song X H, Zhang Q L, Xue Y L, Zhao K, Li Y and Lin S L 2002 *Chin. Phys.* **11** 656

[9] Lin S L, Li H Y, Wang D H, Zhao W L and Gao F 2004 *Science in China Ser.* G **34** 141

[10] Wang D H and Ding S L 2003 *Phys. Rev.* A **68** 023405

[11] Kips A, Vassen W, Hogervorst W and Dando P A 1998 *Phys. Rev.* A **58** 3043

[12] Jensen R V, Flores-Rueda H, Wright J D, Keeler M L and Morgan T J 2000 *Phys. Rev.* A **62** 053410

[13] Kips A, Vassen W and Hogervorst W 2000 *J. Phys.* B **33** 109

[14] Holle A, Main J, Wiebusch G., Rottke H and Welge K H 1988 *Phys. Rev. Lett.* **61** 161

[15] Cacciani P, Liberman S, Luc-Koenig E, Pinard J and Thomas C 1988 *J. Phys.* B **21** 3523