Volume 7, Number 8 ACTA PHYSICA SINICA August, 1998
1004-423X/98/07080561-06 (Overseas Edition) © 1998 Chin. Phys. Soc.

# ENERGY AND LIFETIME OF CORE-EXCITED $Be^+$ RESONANCES*

Gou Bing-cong(苟秉聪) and Deng Wen-sheng(邓文生)
*Beijing Institute of Technology, Beijing* 100081, *China*
Zhang Jian-ping(张建平)
*Institute of Applied Physics, Sichuan United University, Chengdu* 610065, *China*

(Received 5 February 1998)

The energies, shifts, widths, and radiative rates of double excited $Be^+$ resonances are calculated using the saddle point and saddle-point complex-rotation methods. A restricted variational method is used to extrapolate a better nonrelativistic energy. Relativistic effects are included using first-order perturbation theory. These results are used to make a better understanding of observed $Be^+$ spectra.

**PACC:** 3120T

## I. INTRODUCTION

The advances of the synchrotron radiation and computer technology have revived considerable experimental and theoretical interests in the study of doubly and triply excited lithium-like systems. The high resolution Auger spectra of lithium-like double and triply excited states were reported by R$\phi$dbro *et al.*[1] These resonances were calculated using the saddle-point variation method[2] three years later. Recently, Kiernan *et al.*[3] and Azuma *et al.*[4] reported the observation of many higher-lying $^2P^o$ resonances of hollow lithium using different experiment techniques. Journel *et al.*[5] made the first partial photoionization cross section measurement in the triply excited energy region. The Hartree-Fock configuration interaction(HF-CI), multi-configuration Dirac-Fock(MCDF), and $\boldsymbol{R}$-matrix methods were used to identify these resonances, respectively. In 1996, Diehl *et al.*[6] and Cubaynes *et al.*[7] made high-precision measurements for the energies and widths of $^2P^o$, $^2S$ and $^2P$.

The calculation of energy and lifetime of doubly and triply excited resonances are very challenging because there is a infinite number of open channels associated with those resonances. Recently, Chung and Gou[8−10] used the saddle-point complex-rotation method to calculate the energy and width of triply excited lithium-like ions. Piangos *et al.*[11] calculated the radiative lifetimes of triply excited states of the Li isoelectronic sequence using the state-specific theory method. In Ref.[2], the number of linear parameters is limited to about 100 terms, the energy was calculated with a more limited closed-channel wave function and the shift from its interaction with continua was not included. The widths and relativistic corrections were not considered. Recently, computational methods such as the restricted variation method[12] have been developed. Hence, the energies and widths of these reso-

* Project supported by the National Natural Science Foundation of China under Grant No. 19774012

nances can be calculated to a much higher precision than before. These results can be used to identify the observed Auger spectra of $Be^+$.

## Ⅱ. THEORETICAL METHOD

In LS coupling scheme, the non-relativistic Hamiltonian is

$$H = \sum_{i=1}^{3} \left( -\frac{1}{2}\nabla_i^2 - \frac{4}{r_i} \right) + \sum_{\substack{i,j=1 \\ i<j}}^{3} \frac{1}{r_{ij}} \ . \tag{1}$$

In general, the saddle-point wave function of core excited three-electron system[8] can be written as

$$\begin{aligned} \Psi_{\rm b} = A \sum C_{mnk}^{l_1 l_2 L_{12} l_3} & \left[1 - P(\boldsymbol{r}_1)\right] \left[1 - P(\boldsymbol{r}_2)\right] \left[1 - P(\boldsymbol{r}_3)\right] \\ & \times \phi_{mnk}(r_1, r_2, r_3) Y_{l_1 l_2 L_{12}}^{l_3 LM}(\widehat{r}_1, \widehat{r}_2, \widehat{r}_3)\, X(1,2,3) \ . \end{aligned} \tag{2}$$

The radial basis functions are Slater orbitals

$$\phi_{mnk}(r_1, r_2, r_3) = r_1^m r_2^n r_3^k \mathrm{e}^{-(\alpha_i r_1 + \beta_i r_2 + \gamma_i r_3)} \ . \tag{3}$$

In Eq.(2) the projection operator is given by

$$p(\boldsymbol{r}_i) = |\phi_0(\boldsymbol{r}_i) >< \phi_0(\boldsymbol{r}_i)| \ , \tag{4}$$

here the vacancy orbital is

$$\phi_0(r) = N \exp(-qr) \ . \tag{5}$$

Using saddle-point variational method, $q$ is a parameter determined in the energy maximization processes, the linear parameters $C$ and the nonlinear parameters $\alpha_i$, $\beta_i$ and $\gamma_i$ in Eqs.(2) and (3) are determined in the energy optimization processes. We obtain the basic wave function $\Psi_{\rm b}$ and the corresponding saddle-point energy $E_{\rm b}$.

To further improve the calculation of energy, we expend the total wave function[12] as

$$\Psi(1,2,3) = D_0\, \Psi_{\rm b}(1,2,3) + \Psi_2(1,2,3) \ , \tag{6}$$

where

$$\Psi_2(1,2,3) = A \sum_{i=1}^{I} D_i\, \Psi_{n(i),\, l(i)}(1,2,3) \ . \tag{7}$$

$\Psi_2$ is a function to saturate the functional space. In practice, we will break up $\Psi_2$ into many parts. A secular equation will be constructed for each part. Each of the nonlinear parameters in the basis function of $\Psi_2$ is optimized in the restricted variational calculation.[12]

To obtain the width using the saddle-point complex-rotation method[13], we write the total wave function as

$$\Psi(1,2,3) = \Psi_{\rm b}(1,2,3) + \sum_i A \phi_i(1,2) U_i(3) \ , \tag{8}$$

where

$$U_i = \sum_n d_{i,n} r^n \exp(-\alpha_i r) \ , \tag{9}$$

$\phi_i(1,2)'$s are the target states of the open channels. $U_i$ represents the wave function of the outgoing electron, in $U_i$ the $r$ is complex scaled. The proper angular and spin coupling between $\phi_i$ and $U_i$ to obtain the correct total $L$ and $M$ is implicitly assumed in the above equation. In the calculation, the nonlinear parameters obtained from the saddle-point calculation in $\Psi_{\rm b}(1,\ 2,\ 3)$ are retained, but the linear parameters are recalculated to allow for full interaction between the closed-channel and the open-channel wave functions. The energy from $\Psi(1,2,3)$, $E - {\rm i}\Gamma/2$, gives the position and the width of the resonances. The difference, $E_{\rm s} = E - E_{\rm b}$, represents the shift from the saddle-point energy to the resonance energy.

The total energy is further improved by including the mass polarization effect and relativistic corrections. The explicit expressions of these perturbation operators are given in Ref.[13], they will not be repeated here.

## Ⅲ. RESULT AND DISCUSSION

The thirteen doubly excited states of $Be^+$ we studied are the lowest $^4P^o$, the lowest four $^2S^o$, five $^2P^o$ and three $^2D^e$ resonances. The non-relativistic energies of these states are given in Table 1. The autoionizing states of core-excited atomic system can be thought of as inner shell vacancy states that are quasi-bound. These states are degenerate with the continuum. If the continuum is not carefully removed from the variational wave function, in some cases this could lead to variational break down. In this work, $1s^2 + kL$ is open channels and need to be removed from the saddle-point wave functions. The optimized value of $q$ for all these states is close to 3.5, indicating that the 1s electron approximately half shields the 1s vacancy orbital. By the Pauli antisymmetry principle, there is no $q$ value quoted for the (1s2s2p) $^4P^o$ state. In the present work, the number of wave functions used is much larger than those in Ref.[2] and more angular-spin components are used. As a consequence, the improvement of $E_{\rm b}$ over that of Ref.[2] ranges from –0.002 a.u. for $1s2s2p\,^4P^o$ to –0.005 a.u. for $[(1s2s)^1S,\ 3p]\ ^2P^o$. These energies are further improved by the restricted variation method with $\Delta E_{\rm RV}$, the total improvement $\Delta E_{\rm RV}$ ranges from 18.7 to 99.6 $\mu$a.u.

The saddle-point energy is calculated from the closed channel part of the wave function. It differs from the resonance position by a shift ($E_{\rm s}$), which comes from the interaction of the closed-and open-channel wave functions. The energy levels of doubly excited $Be^+$ lying below the $Be^{2+}$ (1s2s) $^3S$ threshold can autoionize through only one decay channel,

$$(1s2l\ nl')^2L \rightarrow (1s^2)^1S + kL, \tag{10}$$

where $kL$ represents the Auger electron with angular momentum $L$. The convergence of the resonance width and the shift is excellent for all of the states investigated. This convergence is checked with respect to the angle of complex scaling (0.3-0.6 rad) and the variation of parameter $\alpha_i$. Many of the widths are stable to five digits. The number of terms used in each $U_i$ ranges from 14 to 16. The total nonrelativistic term energy is obtained by adding the $\Delta E_{\rm RV}$, the shift $\Delta E_{\rm s}$, and the energy upper bound $E_{\rm b}$.

**Table 1.** Nonrelativistic energies (in $\mu$a.u.) of doubly excited states of lithium-like beryllium. $q$ is the nonlinear parameter in the vacancy orbital, $N_{\rm L}$ is the number of angular-spin components in the wave function, and $N$ is the number of linear parameters in the basic wave function.

| Resonances | $q$ | $N_l$ | $N$ | $-E_{\rm b}$ | $-\Delta E_{\rm RV}$ | $\Delta E_{\rm S}$ | $-E_{\rm nonrel}$ |
|---|---|---|---|---|---|---|---|
| $(1s2s2s)^2S$ | 3.478 | 25 | 684 | 10123471.3 | 27.4 | 242.0 | 10123257 |
| $(1s2s2p)^4P^o$ | | 20 | 384 | 10066587.5 | 25.3 | | 10066613 |
| $[1s,(2s2p)^3p]^2P^o$ | 3.468 | 32 | 612 | 9960721.3 | 66.9 | 364.4 | 9960424 |
| $[1s,(2s2p)^1p]^2P^o$ | 3.536 | 30 | 694 | 9879096.1 | 99.6 | −47.8 | 9879244 |
| $(1s2p2p)^2D$ | 3.179 | 25 | 641 | 9825839.2 | 37.7 | 155.1 | 9825722 |
| $(1s2p2p)^2S$ | 3.775 | 27 | 679 | 9700731.7 | 61.2 | 569.8 | 9700223 |
| $[(1s2s)^3s, 3s]^2S$ | 3.526 | 25 | 677 | 9585404.5 | 35.6 | −7.7 | 9585448 |
| $[(1s2s)^3s, 3p]^2P^o$ | 3.478 | 27 | 562 | 9566009.7 | 44.6 | 8.5 | 9566046 |
| $[(1s2s)^3s, 3d]^2D$ | 3.484 | 35 | 605 | 9525340.2 | 30.6 | 21.7 | 9525349 |
| $[(1s2s)^1s, 3s]^2S$ | 3.546 | 25 | 820 | 9502294.3 | 34.0 | 44.0 | 9502284 |
| $[(1s2s)^1s, 3p]^2P^o$ | 3.548 | 36 | 502 | 9473155.2 | 18.7 | 66.2 | 9473108 |
| $[(1s2p)^3p, 3s]^2P^o$ | 3.531 | 22 | 668 | 9446592.7 | 52.6 | 150.1 | 9446495 |
| $[(1s2s)^1s, 3d]^2D$ | 3.547 | 36 | 757 | 9433924.8 | 76.6 | 7.8 | 9433994 |

In addition to the shift $E_{\rm s}$ and $E_{\rm RV}$, the energy of these resonances is further corrected by the mass polarization and relativistic perturbations. The relativistic perturbation operators considered in this work are: correction to the kinetic energy($P^4$), the Darwin term, the electron-electron contact term and the orbit-orbit interaction. The relativistic corrections are calculated using first-order perturbation theory. The mass polarization perturbation operator is accurate to all orders. Using the $(1s^22s^2)^1S$ ground state energy $E_{\rm BeI}$=−14.669675 a.u., the term energy of these resonances can be calculated. These results are given in Tables 2.

**Table 2.** Relativistic energies (in $\mu$a.u.) of doubly excited resonances of lithium-like beryllium. Here $H_{\rm rel}$ is relativistic correction: the $p^4$ and Darwin term, the electron-electron contact term, and the orbit-orbit interaction. $H_{\rm mp}$ is the mass polarization. $T$ is the term energy above the $ls^22s^2$ ground state in meV.

| Resonances | $E_{\rm nonrel}$ | Perturbation corr. | | $E_{\rm total}$ | This work | Experiment[1] |
|---|---|---|---|---|---|---|
| | | $< H_{\rm rel} >$ | $< H_{\rm mp} >$ | | $T$ | $T$ |
| $(1s2s2s)^2S$ | −10123257 | −2020.2 | 0.6 | −10125276 | 123.660 | 123.63 |
| $(1s2s2p)^4P^o$ | −10066613 | −1972.6 | −32.4 | −10068618 | 125.196 | 125.20 |
| $[1s,(2s2p)^3p]^2P^o$ | −9960424 | −1954.6 | 24.0 | −9962354 | 128.094 | 128.11 |
| $[1s,(2s2p)^1p]^2P^o$ | −9879244 | −1890.9 | −23.5 | −9881158 | 130.304 | 130.32 |
| $(1s2p2p)^2D$ | −9825722 | −1782.5 | −36.0 | −9827540 | 131.763 | 131.79 |
| $(1s2p2p)^2S$ | −9700223 | −1783.5 | −18.9 | −9702026 | 135.178 | 135.10 |
| $[(1s2s)^3s, 3s]^2S$ | −9585448 | −1996.9 | −3.1 | −9587448 | 138.282 | 138.10 |
| $[(1s2s)^3s, 3p]^2P^o$ | −9566046 | −1987.5 | 2.4 | −9568031 | 138.924 | 138.70 |
| $[(1s2s)^3s, 3d]^2D$ | −9525349 | −1990.6 | 2.2 | −9527338 | 139.932 | 139.90 |
| $[(1s2s)^1s, 3s]^2S$ | −9502284 | −1881.0 | 6.6 | −9504159 | 140.550 | 140.50 |
| $[(1s2s)^1s, 3p]^2P^o$ | −9473108 | −1864.3 | −7.5 | −9474980 | 141.350 | |
| $[(1s2p)^3p, 3s]^2P^o$ | −9446495 | −1871.2 | −11.7 | −9448378 | 142.067 | |
| $[(1s2s)^1s, 3d]^2D$ | −9433994 | −1860.8 | 8.8 | −9435846 | 142.428 | |

To compare with other theoretical calculations and experiments, the Auger electron energies are calculated and presented in Table 3. The twelve calculated Auger energies lie within the quoted experimental uncertainty of of R$\phi$dbro *et al.*[1] and the term energies are lower than those of Bhatia.[14] In Refs.[1] and [2] the No.2 line was identified for $(1s2s2p)^4P^o$, but we note that the $(1s^2)^1S + kL$ can't be open channel for the lowest quartet state.

**Table 3.** Comparision between theoretical and experimental Auger channel energy (in eV) for doubly excited resonances of $Be^+$.

| Resonances | This work | Bhatia *et al.*[14] | Rϕdbro *et al.*[1] | |
|---|---|---|---|---|
| | | | Observed line No. | Position (in eV) |
| $(1s2s2s)^2S$ | 96.124 | 96.129 | 1 | 96.10±0.10 |
| $(1s2s2p)^4P^o$ | | | 2 | 97.59±0.10 |
| $[1s,(2s2p)^3p]^2P^o$ | 100.559 | 100.647 | 3 | 100.58±0.10 |
| $[1s,(2s2p)^1p]^2P^o$ | 102.767 | 102.976 | 6 | 102.79±0.1 |
| $(1s2p2p)^2D$ | 104.226 | 104.459 | 7 | 104.26±0.20 |
| $(1s2p2p)^2S$ | 107.641 | 107.929 | 12 | 107.57±0.20 |
| $[(1s2s)^3s, 3s]^2S$ | 110.751 | 110.913 | 16 | 110.61±0.20 |
| $[(1s2s)^3s, 3p]^2P^o$ | 111.288 | 111.447 | 17 | 111.19±0.20 |
| $[(1s2s)^3s, 3d]^2D$ | 112.394 | 112.621 | 18 | 112.36±0.20 |
| $[(1s2s)^1s, 3s]^2S$ | 113.017 | | 19 | 113.01±0.20 |
| $[(1s2s)^1s, 3p]^2P^o$ | 113.814 | | 20 | 113.77±0.20 |
| $[(1s2p)^3p, 3s]^2P^o$ | 114.531 | | 21 | 114.60±0.30 |
| $[(1s2s)^1s, 3d]^2D$ | 114.885 | 115.143 | 22 | 114.91[a] |

[a] Line position estimated from figure in Ref.[1].

Table 4 gives the computed optical transition rates from the dipole-length ($R_l$), dipole-velocity ($R_v$) and dipole-acceleration ($R_a$) formulae. They are compared with those of Piangos and Nicolaides.[11] The results for one-photon-two-electron transition are not expected to be highly accurate, because these oscillator strengths are calculated with $\Psi_b$ only and the open channel part of the wave function is not included. Nevertheless, the transition rates in this work give reasonable agreement with the data of Piangos *et al.*[11] The results show that the optical emission rates are extremely small in comparison with the corresponding Auger rates of the core-excited states for systems considered in this work. The lifetime of the doubly excited states is about $10^{-13}$–$10^{-14}$ s. These results are given in Table 5. To compare with other theoretical calculation[14,16] and experiment[15], the Auger widths are also given in Table 5. These data for $Be^+$ should be useful in future experiments.

**Table 4.** Transition rate in $s^{-1}$ of doubly excited of $Be^+$. The number in brackets indicates the powers of 10.

| Transition | This work | | | | Pianges *et al.*[11] | | |
|---|---|---|---|---|---|---|---|
| | $R_l/s^{-1}$ | $R_v/s^{-1}$ | $R_a/s^{-1}$ | $\lambda$/nm | $R_l/s^{-1}$ | $R_v/s^{-1}$ | $\lambda$/nm |
| $(1s^22s)^2S \rightarrow$ | | | | | | | |
| $(1s^22p)^2P^o$ | 1.20[8] | 1.15[8] | 1.38[8] | 306.42 | | | |
| $[1s,(2s2p)^3p]^2P^o$ | 8.24[10] | 7.85[10] | 7.77[10] | 10.44 | 9.1[10] | 8.1[10] | 10.43 |
| $[1s,(2s2p)^1p]^2P^o$ | 6.82[9] | 7.53[9] | 7.72[9] | 10.25 | | | |
| $[(1s2s)^3s, 3p]^2P^o$ | 1.63[10] | 1.62[10] | 1.58[10] | 9.58 | | | |
| $[(1s2s)^1s, 3p]^2P^o$ | 1.00[9] | 1.16[9] | 1.14[9] | 9.39 | | | |
| $[(1s2p)^3p, 3s]^2P^o$ | 3.72[9] | 4.14[9] | 4.00[9] | 9.34 | | | |
| $(1s^22p)^2P^o \rightarrow$ | | | | | | | |
| $(1s2s2s)^2S$ | 5.97[9] | 4.30[9] | 4.15[9] | 11.24 | 9.2[9] | 1.7[9] | 11.238 |
| $(1s2p2p)^2D$ | 3.90[10] | 3.73[10] | 3.74[10] | 10.47 | 5.2[10] | 4.7[10] | 10.463 |
| $(1s2p2p)^2S$ | 3.46[10] | 3.27[10] | 3.16[10] | 10.18 | 5.4[10] | 4.2[10] | 10.146 |
| $[(1s2s)^3s, 3s]^2S$ | 4.83[7] | 3.93[6] | 2.87[6] | 9.93 | | | |
| $[(1s2s)^3s, 3d]^2D$ | 2.41[9] | 2.40[9] | 2.41[9] | 9.80 | | | |
| $[(1s2s)^1s, 3s]^2S$ | 3.96[9] | 3.33[9] | 3.38[9] | 9.75 | | | |
| $[(1s2s)^1s, 3s]^2D$ | 6.22[9] | 6.33[9] | 6.37[9] | 9.61 | | | |

**Table 5.** Width ($\Gamma_A$), radiative rate ($W_r$), Auger transition rat ($W_A$), and lifetime ($\tau$) of doubly excited states of $Be^+$.

| Resonances | $\Gamma_A$/meV | | $W_r/10^{13}\,s^{-1}$ | $W_A/10^{13}\,s^{-1}$ | $\tau/10^{-15}$ s |
|---|---|---|---|---|---|
| | This work | Others | | | |
| $(1s2s2s)^2S$ | 52.35 | 53.0[b]; 52.99[c]; | 0.0006 | 15.91 | 6.3 |
| $[1s,(2s2p)^3p]^2P^o$ | 3.80 | 4.58±0.13[a] | 0.0083 | 1.15 | 86.3 |
| $[1s,(2s2p)^1p]^2P^o$ | 20.81 | 17.0[b]; 21.0[c] | 0.0007 | 6.32 | 15.8 |
| $(1s2p2p)^2D$ | 27.25 | 30.3±1.1[a] | 0.0039 | 8.28 | 12.1 |
| $(1s2p2p)^2S$ | 5.66 | 8.0[b] | 0.0035 | 1.72 | 58.0 |
| $[(1s2s)^3s, 3s]^2S$ | 10.44 | 8.0[b] | 0.0000 | 3.05 | 28.6 |
| $[(1s2s)^3s, 3p]^2P^o$ | 0.33 | 0.02[b]; 0.32[c] | 0.0016 | 0.10 | 984.3 |
| $[(1s2s)^3s, 3d]^2D$ | 1.60 | 2.0[b] | 0.0002 | 0.49 | 204.0 |
| $[(1s2s)^1s, 3s]^2S$ | 6.07 | | 0.0004 | 1.84 | 54.3 |
| $[(1s2s)^1s, 3p]^2P^o$ | 0.37 | | 0.0001 | 0.11 | 908.3 |
| $[(1s2p)^3p, 3s]^2P^o$ | 4.78 | | 0.0004 | 1.45 | 68.9 |
| $[(1s2s)^1s, 3d]^2D$ | 0.07 | 0.18[b]; 0.08[c] | 0.0006 | 0.02 | 4854.4 |

[a] Bhatia, Ref.[14].

[b] Cederquist *et al.* Ref.[15].

[c] Davis and Chung, Ref.[16].

## REFERENCES


[1] M. Rødbro, R. Bruch and P. Bisgaard, *J. Phys.*, **B12**(1979), 2413.
[2] K. T. Chung, *Phys. Rev.*, **25**(1982), 1596.
[3] L. M. Kiernan, M. -K. Lee, B. F. Sonntag, P. Sladeczek, P. Zimmermann, E. T. Kennedy, J-P. Mosnier and J. T. Costello, *J. Phys.*, **B28**(1995), L161.
[4] Y. Azuma, S. Hasegawa, F. Koike, G. Kutluk, T. Nagata, E. Shigemasa, A. Yagishita and I. A. Sellin, *Phys. Rev. Lett.*, **74**(1995), 3770.
[5] L. Journel, D. Cubaynes, J. -M. Bizau, S. Al Moussalami, B. Rouvellou, F. J. Wuilleumier, L. Voky, P. Faucher and A Hibbert, *Phys. Rev. Lett.*, **76**(1996), 30.
[6] S. Diehl, D. Cubaynes, J. -M. Bizau, L. Journel *et al.*, *Phys. Rev. Lett.*, **76**(1996), 3915.
[7] D. Cubaynes, S. Diehl, L. Journel, B. Rouvellou *et al.*, *Phys. Rev. Lett.*, **77**(1996), 2194.
[8] K. T. Chung and B. C. Gou, *Phys. Rev.*, **A52**(1995), 3669.
[9] K. T. Chung and B. C. Gou, *Phys. Rev.*, **A53**(1996), 2189.
[10] B. C. Gou and K. T. Chung, *J. Phys.*, **B29**(1996), 6103.
[11] N. A. Piaongos and C. A. Nicolaides, *Phys. Rev.*, **A48**(1993), 4142.
[12] K. T. Chung and Zhu X-W, *Phys. Scr.*, **48**(1993), 292.
[13] K. T. Chung and B. F. Davis, *Phys. Rev.*, **A26**(1982), 3278.
[14] A. K. Bhatia, *Phys. Rev.*, **A18**(1978), 2524.
[15] H. Cederquist, M. Kisielinski, S. Mannervik and T. Andersen, *J. Phys.*, **B17**(1984), 1969.
[16] B. F. Davis and K. T. Chung, Phys. Rev., **A31**(1985), 3017.