Autoionization resonance states of two-electron atomic systems with finite spherical confinement

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(Received 27 January 2011; published 26 September 2011)

We investigate the lowest-lying S-wave resonant states of two-electron atoms confined by a spherical quantum cavity under the framework of the stabilization method. Hylleraas-type wave functions (basis length $N = 444$) taking the correlation effects between all the charged particles into account are used in the present paper. The finite oscillator potential is used to represent the confinement potential. We present the resonant parameters (energies and widths) of the quantum-confined two-electron atoms with different depths and various ranges of the potentials.

DOI: 10.1103/PhysRevA.84.032515 PACS number(s): 31.15.vj, 37.10.Gh, 32.80.Zb

I. INTRODUCTION

Quantum confinement of atomic and molecular systems [1] has drawn considerable attention due to its large applicability to several branches of physics and chemistry. For example, atoms trapped in nanocavities, such as in zeolite cages, endohedral capture of atoms in fullerenes, in nanobubbles formed around foreign objects in the environment of liquid helium, atoms under high pressure in the walls of nuclear reactors, molecular containers, storage of fuel cells, etc. [2–5], are all relevant for this field. Recently, considerable attention has also been paid to the study of quantum dots (artificial atoms) [6–11] and quantum-confined screened Coulomb impurities and natural atoms [12–23] as carriers, and impurities are often confined in low-dimensional semiconductor quantum well structures. Accurate knowledge of the electronic structure of compressed hydrogen and helium atoms is relevant as these two elements exist as the significant components of planets and stars. An atom confined within a cavity [12–22] behaves differently from a free atom in ways that provide insight into these various interesting problems. The influence of a spatial confinement on the physical properties of the trapped objects becomes significant if their effective sizes are of the same magnitude as the size of the cavity. We are concerned with the study of resonances of helium atoms confined by a spherical cavity.

The confined hydrogen atom has been widely studied with several techniques. In this case, the electron of the H atom experiences a constant potential in addition to the nuclear Coulomb potential. Various physical properties of the confined H atom, such as the modification of its atomic orbital, the binding energy, the energy levels and the level stability, and the density of impurity states have been reported in the literature [14]. Few attempts have also been made toward the quasibound or resonant states of a one-electron impurity atom in an isolated quantum dot and also in the presence of electric and magnetic fields [12,13]. It has been found that the resonance parameters are very sensitive to the cavity size as well as to the potential depth. The effect of low-dimensional quantum confinement on the resonance parameters is known only for a one-electron atom under external environment (for example, an external electric field [12,13]).

No calculation has been performed for the effect of quantum confinement on the autoionizing resonant states of two-electron atoms. Few attempts have been made to study the response of the ground and excited states of many-electron atoms confined by penetrable as well as impenetrable potential wells [15–22]. Very recently, Genkin and Lindroth [23] investigated screened Coulomb impurities on autoionizing two-electron resonances in spherical quantum dots. As helium is the simplest many-electron system, we are interested in studying the variations in the resonance parameters of the confined helium atom as a function of the confining potential in the present paper. For the case of a free helium atom, there are a series of resonance states associated with each He^+ threshold. In order to understand the resonance parameters for the confined helium atom, we focus our attention, first, upon the lowest doubly excited resonance state (the $2s^2\ ^1S^e$ state) of the He atom. In our present paper, we examine the quantum size effects on the doubly excited $2s^2\ ^1S^e$ state. As we have not found any earlier works for the size effect on doubly-excited resonance states of spherically confined helium atom, no comparison can be made here.

Here, we denote the lowest doubly excited resonance state as the $2s^2\ ^1S^e$ state. It is true that the notation for this doubly excited state is a simplified convention, and in fact, it is a combination of $2s^2$, $2p^2$, and other components, such as dd, ff, gg, and $(nl,n'l')$, etc., coupled to the final $^1S^e$ state, with nl and $n'l'$, respectively, being the principal and angular momentum quantum numbers for the two electrons. In the present paper, we use elaborate Hylleraas wave functions in which the odd and even powers of the interparticle coordinates r_1, r_2, and r_{12}, up to 15 are included. In the terminology of configuration interaction, the nl and $n'l'$, up to at least the 15th orbital and below, and even some higher orbitals, are implicitly included. As for the dominant configuration, in principle, one can project out various components from the wave functions and can examine the major contributions. However, no such projection was carried out in the present paper as in the free-atom case (without the confinement); the dominate configurations of the lowest doubly excited $^1S^e$ state have been well studied (see

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the references shown in Ref. [24]). Here, for the confinement cases, we just assume the dominate configuration of the wave functions for the lowest doubly excited $^1S^e$ state is still $2s^2$, with the understanding that the contributions from other one-electron higher angular momentum components are also included.

We perform our calculations under the framework of the stabilization method proposed by Mandelshtam *et al.* [25] as it is an effective and simple method for extracting resonance energies and widths. The computational procedure needs only the diagonalization of real matrix elements with different box sizes and is one of the most powerful tools for calculating resonance parameters. If a resonance exists in a given system and the employed wave functions are capable of representing the physics behind such a resonance, a stabilized or slowly varying eigenvalue would appear in the stabilization plot. This method was successfully employed by Kar and Ho [26] for calculations of resonant parameters below the $N = 2$ of the helium atom threshold in Debye plasma where the screened Coulomb potential is used to represent plasma effects. In the present paper, there is an extra constant potential in addition to the nuclear Coulomb potential due to the spherical confinement of the helium atom. In order to obtain accurate numerical results, here, we include electron-electron correlation effects using correlated Hylleraas-type wave functions. To achieve the converged results, we have used three different basis sets ($N = 308$, 372, and 444) of Hylleraas functions to calculate resonance parameters (energies and widths) and to examine convergence under the influence of quantum confinement. All of the present results were found to be well converged with the basis size $N = 444$. There is very good agreement between the present and the existing values of lowest autoionization states ($2s^2\ ^1S^e$) of the free helium atom [24,26–29].

II. THEORY AND CALCULATIONS

We have constructed the wave function for the $^1S^e$ state of a two-electron atomic system via the Hylleraas type,

$$\Psi_{klm} = \sum_{klm} C_{klm} \exp\left[-\alpha\left(r_1 + r_2\right)\right] r_{12}^k \left(r_1^l r_2^m + r_1^m r_2^l\right), \quad l \geqslant m, \tag{1}$$

with $+1 + m \leqslant \omega$ and where ω, k, l, and m are positive integers or zero. This wave function helps to incorporate the correlation effect between all the charged particles. To obtain the threshold energy ($E_{\mathrm{He}^+(2s)}$), we have the single-electron wave function,

$$\Psi_1 = \sum_1 C_1[\exp - (\alpha r)] r^1. \tag{2}$$

We have performed the calculations with basis sizes up to $\omega = 15$ ($N = 444$) for the case of a helium atom confined by a spherical cavity. The general expression for the Hamiltonian of the two-electron atom inside a cavity is given by

$$H = -\frac{1}{2}\nabla_1^2 \frac{1}{1}\nabla_2^2 - \frac{z}{r_1} - \frac{z}{r_2} + \frac{1}{r_{12}} + V\left(r_1\right) + V(r_2), \tag{3}$$

where r_1 and r_2 are the position coordinates of two electrons and r_{12} denotes the relative distance between two electrons.

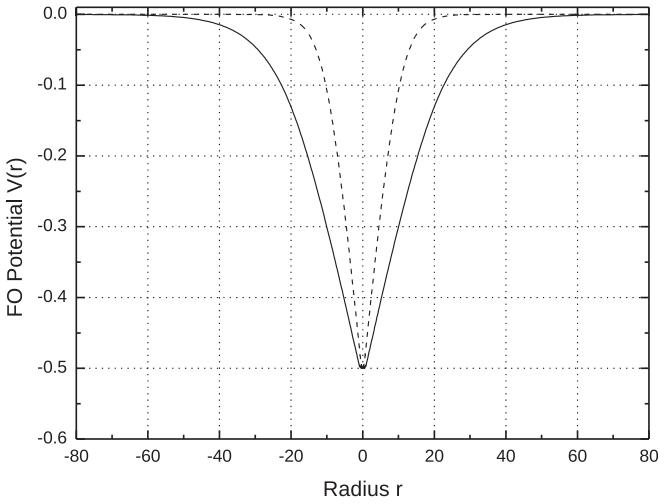

FIG. 1. Shape of the FO potential with $B = 0.1a_0^{-1}$ (solid line) and $B = 0.3a_0^{-1}$ (dashed line) for $A = 0.5$ a.u.

The Hamiltonian of the confined one-electron He^+ ion is given by

$$H = -\frac{1}{2}\nabla^2 - \frac{z}{r} + V\left(r\right). \tag{4}$$

The model of a quantum well that we consider here is of spherical symmetry. We have used the finite oscillator (FO) potential $V(r) = -A(1 + \frac{B}{\sqrt{A}}r)e^{-(B/\sqrt{A})r}$ to represent the quantum-confinement potential where A and B are tuned to set the depth and the width of the spherical cavity [30]. Figure 1 shows the shape of the FO potential for a particular depth ($A = 0.5$ a.u.) with two values of the inverse of the width ($B = 0.1$ and $0.3a_0^{-1}$).

To construct the stabilization plot, we choose a set of nonlinear parameters α [from Eq. (1)] in the vicinity of $2/n$ for the nth threshold of the He^+ ion associated with a particular principal quantum number n. The inner part of a resonance wave function has large amplitude, and it exhibits very stable behavior with the change in nonlinear parameters in wave functions, whereas, the wave functions for scattering states change more drastically. As a result, a stabilized plateau is formed near resonance energy. After constructing the stabilization plateau for the energy eigenvalues, the resonance energy and the width can be extracted from the density of resonance states by using the formula from the stabilization graph [31],

$$\rho^Q(E) = \frac{1}{\alpha_{\max} - \alpha_{\min}} \sum_j \left|\frac{dE_j(\alpha)}{da}\right|^{-1}_{E_j(\alpha)=E}. \tag{5}$$

The contribution to the sum only occurs for the $E_j(\alpha)$ values for which α lies between the intervals $\alpha_{\min}$ and $\alpha_{\max}$ and the sum over the stabilized plateaus inside the interval. For an isolated resonance, $\rho^Q(E)$ can be shown as [32]

$$\rho^Q\left(E\right) \cong \pi^{-1} \frac{\Gamma/2}{\left(E - E_r\right)^2 + \Gamma/4}. \tag{6}$$

Resonance energy E_r and width Γ can be obtained by fitting $\rho^Q(E)$ to Eq. (6).

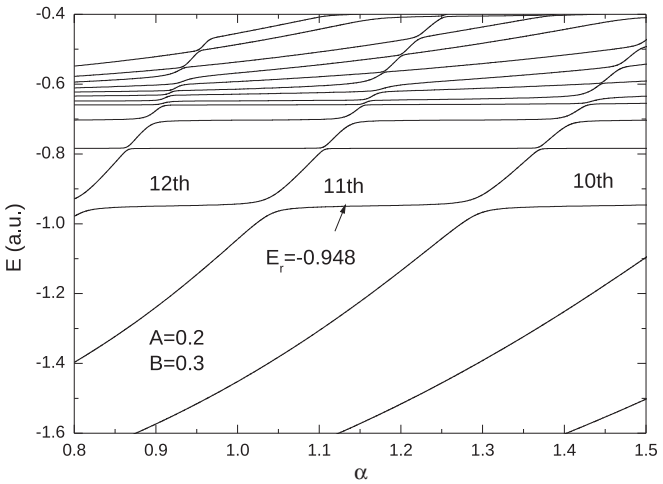

FIG. 2. Energy eigenvalues vs α parameters for the $2s^2\ {}^1S^e$ state of a He atom in a quantum cavity (potential depth $A = 0.2$ a.u.; the inverse of cavity radius $B = 0.3a_0^{-1}$).

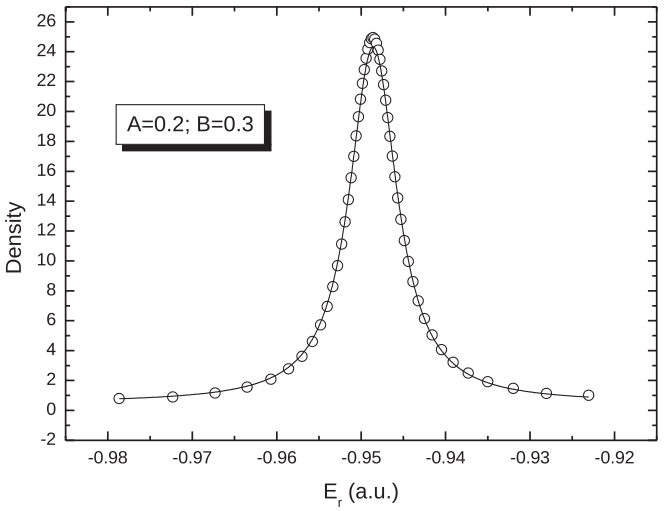

FIG. 3. Calculated density (open circle) and fitted Lorentzian (solid line) for the $2s^2\ {}^1S^e$ state of a He atom in a spherical quantum cavity of depth $A = 0.2$ a.u. and the inverse of radius $B = 0.3a_0^{-1}$.

III. RESULTS AND DISCUSSIONS

In Fig. 2, we plot the S-wave energy eigenvalues vs α for potential depth $A = 0.2$ a.u. and inverse of the width $B = 0.3a_0^{-1}$. The scaling parameter α in the wave function [Eq. (1)] acts as the reciprocal range of a soft wall [31]. The 10th– 23rd eigenvalues in the energy range of -0.4 to -1.6 a.u. are shown here. Stationary behavior is found around $E = -0.948$ a.u., and this stabilized eigenvalue represents the lowest doubly excited $2s^2\ {}^1S^e$ resonance state. From the stabilization plot, we consider the 11th eigenvalue in the range of α from 1.075 to 1.25 and calculate the inverse of its slope to determine the density of states,

$$\rho_n = \frac{\alpha_{n+1} - \alpha_{n-1}}{E_{n+1} - E_{n-1}} = \left|\frac{dE}{d\alpha}\right|^{-1}_{E(\alpha)=E'}. \tag{7}$$

The difference between Eqs. (5) and (7) is that, in Eq. (5), there is an extra multiplication constant $(\alpha_{\max} - \alpha_{\min})^{-1}$. This term will not be involved in the determination of resonance parameters when we fit ρ_n to the Lorentz function,

$$\rho_n(E) = \frac{a\,(\Gamma/2)}{(E - E_r)^2 + \Gamma^2/4} + b. \tag{8}$$

Also, here in Eq. (5), we do not take the sum of the plateaus and then average over them. Instead, we use Eq. (8) to fit the density of the resonance state with one curve at a time. The one that gives the best fit is determined to be the best desired result for that particular resonance [26,31]. Figure 3 represents the Lorentz fitting to our calculated density of states. The open circles stand for the calculated values of ρ_n using Eq. (7), and the solid line is the fitted curve using the Lorentz function of Eq. (8). We obtain the resonance energy $E_r = -0.94857$ a.u. and width $\Gamma = 0.00659$ a.u. from this fitting. In this case, wave functions with basis set $N = 372$ are used.

In Table I, we illustrate the investigation for the $2s^2\ {}^1S^e$ resonant state with a particular potential depth $A = 0.2$ a.u. and $B = 0.3, 1.5a_0^{-1}$ and $A = 0.5$ a.u. and $B = 0.4, 3a_0^{-1}$ as the sample studies. We have performed the calculations for three different values of $\omega = 13$ ($N = 308$), 14 ($N = 372$), and 15 ($N = 444$) in the basis expansion to achieve converged results. Table I shows that all the resonant parameters have almost reached the converged digits with expansion length $N = 372$ ($\omega = 14$) terms. The converged results of the resonant position and width for the $2s^2\ {}^1S^e$ state are -0.9485 a.u. and 0.00659 a.u., respectively, for $A = 0.2$ a.u. and $B = 0.3a_0^{-1}$ and for $B = 1.5a_0^{-1}$, with the same A value, are -0.7884 and 0.00430 a.u., respectively. Similarly, for $A = 0.5$ a.u., we have the converged resonance parameters -1.3115 a.u. (resonance position) and 0.00955 a.u. (resonance width) with $B = 0.4a_0^{-1}$, whereas, $B = 3a_0^{-1}$ presents converged resonance energy -0.7968 a.u. and width 0.0039 a.u. The remaining results reported in this paper are also converged with the basis size $N = 372$ (not shown).

Next, we calculate the resonance energy and width of the free helium atom ($2s^2\ {}^1S^e$ state) by using the above-mentioned

TABLE I. The He ($2s^2\ {}^1S^e$) resonance of confined He.

A in a.u.	B in a_0^{-1}	ω	N	Resonance energy (E_r) in a.u.	Resonance width (Γ) in a.u.
0.2	0.3	13	308	−0.948 61	0.006 59
		14	372	−0.948 57	0.006 59
		15	444	−0.948 57	0.006 59
	1.5	13	308	−0.788 48	0.004 30
		14	372	−0.788 46	0.004 30
		15	444	−0.788 45	0.004 30
0.5	0.4	13	308	−1.311 64	0.009 57
		14	372	−1.311 57	0.009 55
		15	444	−1.311 54	0.009 55
	3	13	308	−0.796 85	0.003 99
		14	372	−0.796 84	0.003 97
		15	444	−0.796 84	0.003 96

TABLE II. Comparison of the present $2s^2\ ^1S^e$ resonance energies E_r and resonance widths Γ of a He atom with earlier predictions [26–29].

Method	Resonance energy E_r (a.u.)	Resonance width Γ (a.u.)
Present paper	−0.77781	0.00454
CR [24]	−0.77787	0.00454
[27]	−0.777867	0.004541
[28]	−0.777867636	0.004541306
ECCESE [29]	−0.77786815	0.00454230
SM [26]	−0.77783	0.004549

computational procedure. In Table II, we compare our results with the existing values obtained by using the complex rotation method [24,27,28], the method with explicitly correlated complex eigenvalue Schrödinger equations (ECCESEs), [29] as well as the stabilization method (SM) [26]. The present predicted resonance energy $E_r = -0.77781$ a.u., resonance width $\Gamma = 0.00454$ a.u., and those of earlier calculations [26–29] are identical up to the fourth and fifth decimal places, respectively.

In the present paper, we are interested with the autoionizing resonant states of the confined He atom for different potential depths with various cavity sizes. We list our predictions in Table III for resonance energies, widths, and corresponding threshold energies for the potential depth of quantum cavity $A = 0.2$ and 0.5 a.u. and radius $(1/B)$ starting from 0.05 to $200a_0$. Very large values of B correspond to very small widths

TABLE III. The $2s^2\ ^1S^e$ resonance energies E_r and resonance widths Γ of a He atom and threshold energies of $He^+(2s)$ in a quantum cavity for various potential depths and widths.

Potential Depth A (a.u.)	Cavity size $B^{-1}(a_0^{-1})$	Resonance Energy E_r (a.u.)	Resonance Width Γ (a.u.)	Threshold Energy $He^+(2s)$ (a.u.)
0.2	0.05	−0.7778	0.004 54	−0.5000
	0.1	−0.7781	0.004 54	−0.5003
	0.2	−0.7795	0.00451	−0.5013
	0.5	−0.7849	0.004 31	−0.5050
	1.0	−0.7996	0.004 55	−0.5131
	2.5	−0.8972	0.006 27	−0.5648
	10	−1.1115	0.005 67	−0.6704
	20	−1.1552	0.005 00	−0.6902
	100	−1.1766	0.004 58	−0.6995
	200	−1.1776	0.004 55	−0.6999
0.5	0.05	−0.7783	0.004 53	−0.5004
	0.1	−0.7800	0.004 49	-0.5021
	0.2	−0.7872	0.004 25	−0.5071
	0.5	−0.8137	0.004 15	−0.5226
	1.0	−0.9289	0.006 79	−0.5825
	2.5	−1.3116	0.009 55	−0.7768
	10	−1.6978	0.006 05	−0.9646
	20	−1.7526	0.005 08	−0.9892
	100	−1.7766	0.004 57	−0.9994
	200	−1.7777	0.004 54	−0.9999

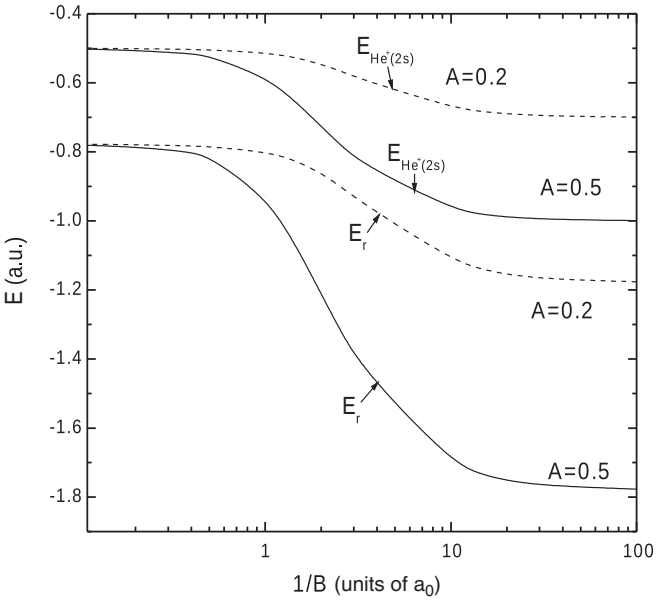

FIG. 4. The $2s^2\ ^1S^e$ resonance energies E_r of a He atom and the threshold energy of $He^+(2s)$ in a quantum cavity with potential depth $A = 0.2$ a.u. (dashed line) and 0.5 a.u. (solid line) vs $1/B$ values.

$(1/B)$ of the confined potential, and it is found that, in this situation, the helium atom nearly acts as an atom without a confinement. When the potential size increases, the resonance energy as well as the threshold energy monotonically decrease due to enhancement in the strength of the confining potential. Beyond $1/B = 100a_0$, the resonance energy is shifted to −1.177 a.u. for the potential depth $A = 0.2$ a.u. and to −1.777 a.u. for $A = 0.5$ a.u., whereas, the threshold energies become −0.6999 and −0.9999 a.u. for $A = 0.2$ and 0.5 a.u., respectively. This establishes the fact that, for the very large values of $1/B$, the resonance energy of the two-electron atom is shifted down by a value of about $2A$, and the threshold energy for the one-electron subsystem is reduced by an amount almost A.

We also tabulate the resonance width for different depths as well as the ranges of the confining potential in the same table. When the cavity radius is increased, the resonance width Γ is first decreased to reach a minimum and, subsequently, increases to a maximum value as the cavity radius is increased further. Then, the width starts to decrease when the range of the potential is increased further, and eventually, it approaches the free-atom value when $1/B$ reaches about 100 a_0, as shown in Table III.

Figure 4 separately depicts the resonance energy of the $2s^2\ ^1S^e$ state associated with its threshold $He^+(2s)$ as a function of different cavity sizes for two potential depths. When the cavity radius, i.e., $1/B$ is very small, and hence, the effect on the helium atom is not too large and the curves for the resonance energies start with the same energy −0.778 a.u. as expected, it is very close to the resonance energy for the free-atom case. Similarly, for the case of the $He^+(2s)$ threshold, when the $1/B$ value is very small, the curves for two different potential depths show the same energy −0.5 a.u. ($n = 2$ threshold energy of free He^+ ion). When the width of the spherical cavity is relatively broad, with an increase in $1/B$, the resonance energy as well as the $n = 2$ threshold energy of the confined helium are

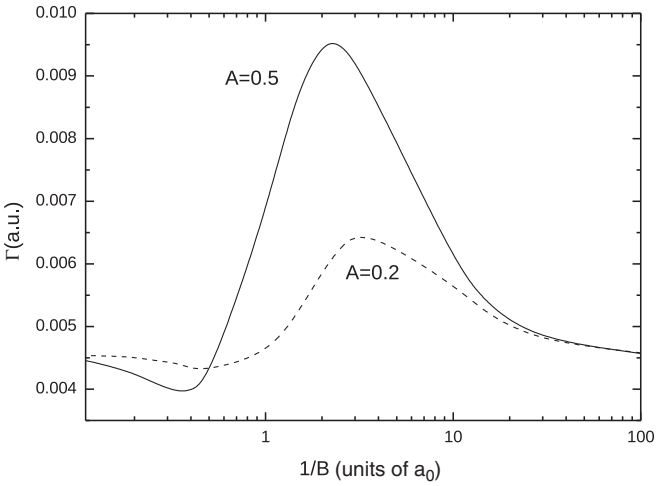

FIG. 5. The $2s^2\ {}^1S^e$ resonance width Γ of a He atom in a quantum cavity with potential depth $A = 0.2$ a.u. (dashed line) and 0.5 a.u. (solid line) vs $1/B$ values.

decreased and gradually approach a steady value of -1.177 and -0.6995 a.u., respectively, at around $1/B = 100a_0$ for the potential depth $A = 0.2$ a.u. This result of the resonant position of the $2s^2\ {}^1S^e$ state is decreased by an amount almost equal to twice the potential depth ($2A$) to -0.778 a.u. that has already been mentioned. Similarly, the resonance curve for $A = 0.5$ a.u. shows the same nature and reaches -1.777 a.u. for very large values of $1/B$ (around 100 a.u.). Figure 4 also shows that, for large values of $1/B$, the energy of a single electron in the $2s$ state ($E_{\mathrm{He}^+(2s)}$) is decreased by a value of about A (potential depth).

Figure 5 shows the confining potential effect on resonance width of a helium atom inside a quantum cavity. When the size of the cavity is small (large B), the autoionization width first is decreased slightly from its free-atom value. For the case of $A = 0.2$, when $1/B$ reaches about 0.7 (or 0.4 for the case of $A = 0.5$), the width starts to increase and reaches a maximum value of about at $B^{-1} = 3.3$ (or 3 for the case of $A = 0.5$). After reaching their maxima, the widths start to decrease when the size of the cavity is increased further (increasing $1/B$) and, eventually, reach the free-atom values when B approaches a very small value. While the behaviors for the widths near both ends of the B values (very small and very large cavities) are understood as they resume the free-atom value, the oscillatory character (first decreases, then increases and decreases) is quite interesting. Such a phenomenon can be explained as follows. For the free-atom case, the wave function of a doubly excited autoionization state has large amplitude in the inner region and has oscillatory character in the outer region. Now, when the helium atom is confined in a quantum cavity, the node or antinode of the resonance wave function lies on the edge of the quantum cavity, destructive interference or constructive interference takes place inside the cavity, leading to shortening or prolonging of the autoionization lifetime. As a result, the width exhibits oscillatory behavior when the size of the cavity is changed. The large amplitude of the resonance wave function leads to the large bump in the width vs the cavity-size curve. As compared to the two cases with different A values, for $A = 0.5$ and when the cavity size is large, the energy of the resonance state reaches a lower value than that of the $A = 0.2$ case. As a result, the amplitude of the inner part of the resonance wave function for the former case is larger than the latter amplitude, which in turn, leads to an even larger bump in the figure for width vs $1/B$ (cavity size). This phenomenon is very much like the electric-field effect on the hydrogenic impurity inside a spherical quantum dot with finite confinement [12,13]. It was revealed that the width for the autoionizing hydrogen state under an external dc electric field shows oscillatory behavior when the size of the quantum dot is changed.

IV. CONCLUSIONS

We analyze the general behaviors of the lowest S-wave resonant state of the He atom confined in a spherical quantum cavity by using the stabilization method. We use a FO potential in which two parameters can be tuned arbitrarily to achieve a specific depth and range of the potential. In this paper, we have shown how the confining potential strength affects the resonance parameters of a two-electron atomic system. From the results, it is apparent that a very small cavity radius does not influence the resonance energies as well as the resonance width. But when the size of the cavity increases, the width starts to have an oscillatory behavior and eventually returns back to the free-atom value for a very large cavity. Working with a highly correlated Hylleraas-type wave function, we are able to obtain accurate resonance parameters, which are well converged with the basis size $N = 444$. We investigate the effect of confinement on autoionizing resonance states of two-electron atomic systems. We hope our findings will stimulate others to further investigate resonances of many-electron atoms with confining potentials.

ACKNOWLEDGEMENT

This work was supported by the National Science Council of Taiwan.

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