

**Shift-potential approaches for determining shape resonances in atoms:  ${}^2P$  Be $^-$  and Mg $^-$** 

Per Kaijser

*Quantum Theory Project, University of Florida, Gainesville, Florida 32611*

Jack Simons

*Department of Chemistry, University of Utah, Salt Lake City, Utah 84112*

(Received 18 September 1979)

It is shown that the positions of atomic shape resonances may be identified by adding to the one-electron Hamiltonian operator an artificial "shift potential" that differentiates between scattering and resonance states by exploiting their different small- $r$  and large- $r$  behavior. We explored the use of shift potentials which are either repulsive for large  $r$  or attractive for small  $r$ . In the first case, resonances correspond to virtual orbitals that are relatively stable in energy. In the latter case the scattering states are stable in energy, and the resonance orbitals are identified by their relatively strong response to the attractive shift potential. The second method is found to be more sensitive and reliable in the application to  ${}^2P$  Be $^-$  and Mg $^-$  presented here. Moreover, it is found that, although the rather simple methods developed here are not capable of giving quantitatively correct resonance energies, they are useful in separating the resonance states from the underlying continuum.

## INTRODUCTION

Several calculational approaches exist for studying electron-atom and electron-molecule shape resonances. The stabilization method of Hazi and Taylor<sup>1,2</sup> makes use of the fact that the orbital energies or configuration interaction (CI) matrix eigenvalues of bound and resonance states are more stable with respect to changes in the basis set than those corresponding to scattering states. By the finite-difference boundary-value method, Truhlar<sup>3-5</sup> successfully determined the resonance state from its independence of the boundary parameter. In their study of atomic resonances, Hunt and Moiseiwitsch<sup>6</sup> used a one-electron operator with a model potential containing one parameter which was determined from a quadratic extrapolation along an isoelectronic sequence. The Harris method<sup>7</sup>, which has recently been applied by Kurtz and Öhrn,<sup>8</sup> uses a scattering wave that is a linear combination of spherical Bessel and Neuman functions and a set of square-integrable functions (virtual Hartree-Fock orbitals). Other successful methods that have received much attention are the method of complex scaling<sup>9-11</sup>, the Weyl theory,<sup>12-14</sup> and the  $R$ -matrix theory<sup>15</sup>.

The present method is based on the fact that an orbital or CI wave function representing a resonance state should have a higher density in the vicinity of the nucleus than those representing scattering states. In this regard it is similar to the first two methods mentioned above.<sup>1,2,3-5</sup> In our approach we add to the electronic Hamiltonian (in the applications presented later we use the Hartree-Fock Hamiltonian) a potential term that differentiates between the regions close to and

far away from the nucleus. If this potential has large positive values in the far region, it will push up the energy levels of the scattering states more than the energy levels of resonance states; whereas the addition of an attractive potential in the interior region will affect the bound and resonance orbitals more strongly than the orbitals of the scattering states. Both these approaches are tested in the present study. The former method, like those of Hazi and Taylor, and of Truhlar, relies on the stability of the energies of the resonance states, and has shown promising results when applied to a model potential.<sup>16</sup> However, when applied to electron scattering from neutral Be and Mg atoms, for which the centrifugal barriers and the attractive potentials in the radial differential equation are very small, we experienced considerable difficulty in identifying a definite resonance state. The alternative procedure of adding an attractive potential to the interior region turns out to be far more sensitive and reliable. In this approach, in contrast to other stabilization methods, we look for the response (energy lowering) from the resonance state and the relative insensitivity of the scattering states.

## PROCEDURE

Our method adopts the analytic Hartree-Fock scheme and hence, describes the shape resonance in the static-exchange approximation. The extension of the approach presented here to include correlation by configuration-interaction or other approaches should be straightforward. The electron density of the target system in an electron-atom shape resonance is described by a basis

set of Slater-type orbitals (STO) of double-zeta or beta quality. To this set we add several STO orbitals of the same symmetry as that of the shape resonance under examination ( ${}^2P$  for  $\text{Be}^-$  and  $\text{Mg}^-$ ). Using this extended basis, a standard Hartree-Fock (HF) calculation is performed for the isolated target atom ( $1s^22s^2$  for Be). In this method the continuum states (either resonance or scattering states) are described by the (square-integrable) virtual HF orbitals with positive energy eigenvalues.

All one-electron orbitals are eigenfunctions of the angular operator  $L^2$ ; for the subspace spanned by the orbitals with eigenvalue  $l(l+1)$ , we can write the kinetic-energy operator in spherical coordinates and atomic units as

$$T_l = -\frac{1}{2r} \frac{d^2}{dr^2} r + \frac{l(l+1)}{2r^2}. \quad (1)$$

The centrifugal barrier, arising from the second term for  $l > 0$ , sharpens the distinction between the resonance and scattering states.

We add to this Hamiltonian operator artificial shift potentials which differentially affect the scattering and resonance states and which leave the bound states relatively unshifted. After adding these new operators we repeat the SCF Hartree-Fock calculations using the basis set employed for the unperturbed problem. Upon examination of the energy eigenvalues of the virtual orbitals, we find that some are shifted much more than others due to the addition of the extra term to the Hamiltonian. With a shift potential which is repulsive for large  $r$ , the orbital energies of the scattering states are pushed upwards more so than are those of the resonance states. For a potential which is attractive in the interior (small- $r$ ) region, the resonance states have their energies lowered and may even become bound states, whereas the scattering states are relatively unaffected (see the tables below).

The repulsive shift potentials which have been tested are of either the exponential or power type, i. e.,

$$V_{\text{exp}}(r) = ae^{br}, \quad (2)$$

$$V_{\text{pow}}(r) = ar^n. \quad (3)$$

Due to the inclusion of diffuse basis orbitals in the HF calculations of the resonance states, constraints must be put on the parameter  $b$  in  $V_{\text{exp}}(r)$  in order to ensure convergence of the integrals of this operator over the atomic-orbital basis. For the applications to electron-neutral-atom scattering described below, these limitations make the exponential shift potential so "flat" that significant differentiation between resonance and scattering states becomes very difficult. The

power potential is of the same kind as that used by Liebman *et al.*<sup>16</sup> In applying this method to our problems, we found the optimal parameter for the model potential used in Ref. 16 to be  $n=8$  with the coefficient  $a$  in the range  $10^{-18}$ – $10^{-9}$  (a. u.).

The scattering electron polarizes the target electron density, giving rise to an additional attractive potential which is not included in the Hartree-Fock potential. The long-range nature of this electron-atom potential is  $-\alpha/2r^4$ , where  $\alpha$  is the static polarizability of the neutral atom. In carrying out the calculation reported below, we include this polarization effect by adding to the Coulomb and exchange operators of the HF Hamiltonian the following cutoff polarization potential:

$$V_{\text{pol}}(r) = \begin{cases} -\frac{\alpha}{2r^4}, & r \geq r_0 \\ -\frac{\alpha r}{2r_0^5}, & r < r_0 \end{cases} \quad (4)$$

in which the cutoff radius  $r_0$  can be treated as an adjustable parameter. This same potential has been used successfully by Truhlar *et al.*<sup>17</sup> and by Kurtz and Öhrn.<sup>8</sup> The cutoff parameter  $r_0$  has been chosen as the distance at which the repulsive-angular-momentum term and the attractive polarization potential cancel each other, i. e.,

$$r_0 = [\alpha/l(l+1)]^{1/2}. \quad (5)$$

In our applications of either of the two repulsive shift potentials  $V_{\text{pow}}(r)$  and  $V_{\text{pow}}(r) + V_{\text{pol}}(r)$  we found that by gradually increasing the parameter  $a$  [Eq. (3)], the energies of the scattering states increase such that one may, for a large enough value of  $a$ , identify the lowest-lying virtual orbital (of this modified HF Hamiltonian) as a resonance state.

We have also explored the possibility of adding only the attractive shift potential  $V_{\text{pol}}(r)$  to the Hamiltonian. For a sufficiently small value of  $r_0$ , this potential is attractive enough to bind one or more of the (previously unbound) virtual orbitals. These virtual orbitals are identified as corresponding to resonance states. The scattering states, on the other hand, are found to be rather stable in their energy under the application of this shift potential. Hence, by carrying out only two calculations, one with a small  $r_0$  and one with no artificial potential added ( $r_0 = \infty$ ), the resonance orbital is easily identified. It can be seen in Tables I and II and in the work of Kurtz and Öhrn that polarization has a drastic influence on the energy of the shape resonance. By performing a third HF calculation in which the po-

TABLE I. Virtual orbital energies (eV) for Be with  $V_{\text{pol}}(r)$  added to the Hamiltonian. The parameter  $r_0$  is in atomic units.

$r_0$	Virtual orbital number											
	1	2	3	4	5	6	7	8	9	10	11	12
4.0	<u>-0.1469</u>	0.0055	0.0230	0.0675	0.1720	0.4134	0.9709	2.2892	5.4121	12.809	34.752	117.12
4.2	<u>-0.0172</u>	0.0055	0.0236	0.0701	0.1791	0.4276	0.9997	2.3349	5.4843	12.958	34.933	117.25
4.23	<u>-0.0030</u>	0.0056	0.0240	0.0709	0.1806	0.4300	1.0040	2.3412	5.4939	12.979	34.956	117.26
4.24	<u>0.0012</u>	0.0058	0.0243	0.0713	0.1812	0.4308	1.0055	2.3433	5.4970	12.986	34.963	117.27
4.25	<u>0.0044</u>	<u>0.0066</u>	0.0246	0.0717	0.1818	0.4316	1.0069	2.3454	5.5001	12.993	34.971	117.27
4.3	0.0054	0.0191	<u>0.0307</u>	0.0744	0.1850	0.4359	1.0142	2.3557	5.5150	13.026	35.006	117.30
4.4	0.0054	0.0220	<u>0.0516</u>	<u>0.0867</u>	0.1933	0.4451	1.0286	2.3752	5.5426	13.090	35.070	117.34
4.6	0.0055	0.0224	0.0613	<u>0.1190</u>	0.2175	0.4656	1.0569	2.4106	5.5896	13.207	35.177	117.41
4.8	0.0055	0.0225	0.0630	<u>0.1351</u>	<u>0.2444</u>	0.4878	1.0837	2.4415	5.6278	13.308	35.262	117.47
5.0	0.0055	0.0226	0.0636	<u>0.1424</u>	<u>0.2663</u>	0.5098	1.1086	2.4683	5.6596	13.395	35.331	117.51
6.0	0.0055	0.0227	0.0645	0.1525	<u>0.3146</u>	<u>0.5929</u>	1.2005	2.5558	5.7723	13.656	35.537	117.63
7.0	0.0055	0.0227	0.0648	0.1550	0.3293	<u>0.6364</u>	1.2509	2.5948	5.8536	13.756	35.619	117.68
10.0	0.0055	0.0227	0.0651	0.1574	0.3442	<u>0.6838</u>	1.3026	2.6379	5.9515	13.844	35.682	117.72
$\infty$	0.0055	0.0228	0.0658	0.1609	0.3562	<u>0.7051</u>	1.3210	2.6669	5.9795	13.866	35.697	117.73

larization potential  $V_{\text{pol}}(r)$  is included but with the more realistic value of the cutoff parameter  $r_0$  given by the criterion<sup>5</sup> above, we can estimate the position (energy) of the shape resonance. This procedure we have found to be a reasonably reliable and very straightforward way of identifying the resonance orbital and energy.

### RESULTS AND DISCUSSION

We applied the method described in the previous section to a study of the  $^2P$  shape resonances of  $\text{Be}^-$  and  $\text{Mg}^-$ . The extended Hartree-Fock solutions of Clementi<sup>18</sup> constitute the basis for the bound electrons in the neutral target atoms. To describe the resonance we augment this basis set on even-tempered STO basis containing twelve  $2P$  orbitals for  $\text{Be}^-$  and ten  $3P$  orbitals for  $\text{Mg}^-$ .<sup>19</sup>

Due to the inclusion of very diffuse functions in the basis sets, modification of the electronic Hamiltonian by adding the exponential potential  $V_{\text{exp}}(r)$

is not computationally tractable for these cases. The addition of  $V_{\text{pow}}(r)$  or  $V_{\text{pow}}(r) + V_{\text{pol}}(r)$  to the Hamiltonian has been found to have the desired effect on the scattering states. As the parameter  $a$  in  $V_{\text{pow}}(r)$  is increased the low-lying virtual orbitals representing scattering states move to higher energy values. However, the orbitals corresponding to the resonance also show some increase in their eigenvalues. Thus, as in Ref. 16, it was found convenient to consider the first-order correction in the eigenvalues, i. e.,

$$E'_i = E_i - \langle \phi_i | V | \phi_i \rangle, \quad (6)$$

where  $V$  is the artificial potential added to the Hamiltonian, and  $\phi_i$  and  $E_i$  are the eigenfunctions and eigenvalues, respectively, of the Hartree-Fock problem with  $V$  included.  $E'_i$  thus has the effect of removing the artificial potential  $V$ . While this process of following orbital eigenvalues as  $a$  is varied allowed for an easy identification of the resonance state in the model potential

TABLE II. Virtual orbital energies (eV) for Mg with  $V_{\text{pol}}(r)$  added to the Hamiltonian. The parameter  $r_0$  is defined in Eq. (4) (a.u.).

$r_0$	Virtual orbital number									
	1	2	3	4	5	6	7	8	9	10
5.0	<u>-1.079 58</u>	0.000 44	0.001 89	0.006 16	0.018 50	0.054 57	0.165 69	0.530 43	1.892 12	7.681 07
5.2	<u>-0.031 77</u>	0.000 44	0.001 89	0.006 19	0.018 80	0.056 17	0.173 01	0.548 17	1.954 66	7.770 03
5.4	0.000 44	0.001 88	0.006 03	<u>0.014 34</u>	<u>0.023 78</u>	0.061 00	0.183 54	0.566 82	2.011 95	7.845 26
5.6	0.000 44	0.001 88	0.006 12	0.017 67	<u>0.042 54</u>	<u>0.076 05</u>	0.197 77	0.585 97	2.063 56	7.909 88
5.8	0.000 44	0.001 88	0.006 13	0.017 94	0.047 57	<u>0.094 02</u>	<u>0.214 67</u>	0.605 19	2.109 41	7.966 09
6.0	0.000 44	0.001 88	0.006 13	0.018 03	0.049 17	<u>0.106 47</u>	<u>0.232 09</u>	0.624 10	2.149 68	8.015 46
6.5	0.000 44	0.001 89	0.006 14	0.018 12	0.050 51	<u>0.121 91</u>	<u>0.268 99</u>	0.668 15	2.228 63	8.115 47
7.0	0.000 44	0.001 89	0.006 14	0.018 15	0.050 97	0.128 51	<u>0.294 34</u>	<u>0.706 09</u>	2.282 91	8.189 69
$\infty$	0.000 44	0.001 89	0.006 16	0.018 37	0.052 78	0.146 98	<u>0.384 78</u>	<u>0.873 85</u>	2.453 38	8.399 18

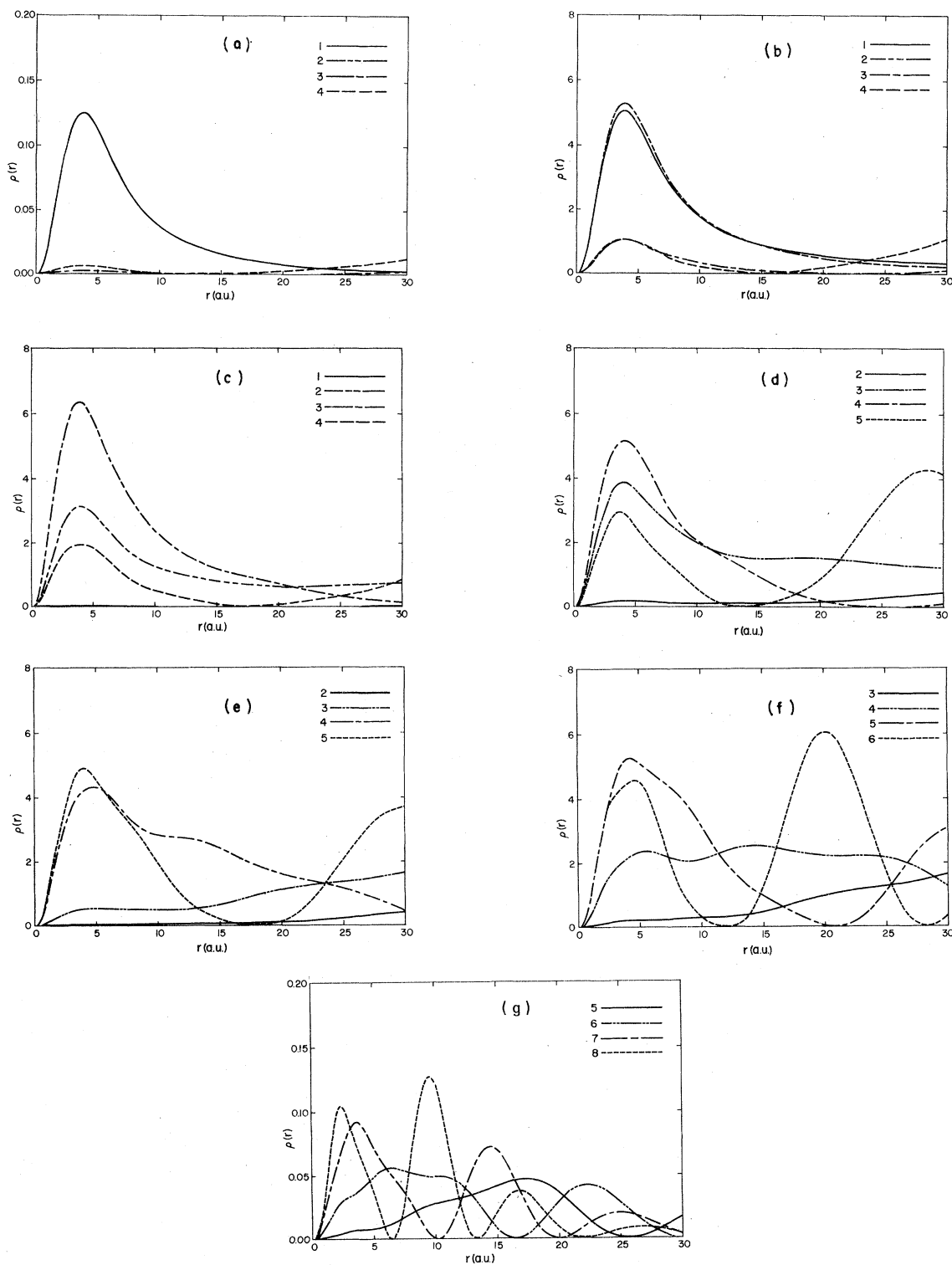


FIG. 1. The radial density (arbitrary units) for  $0 \leq r \leq 30$  a.u. for virtual orbitals of Be. The integrated norms to 30 a.u. are for  $\gamma_0=4.2$ : orb. 1, 0.97; orb. 2, 0.00; orb. 3, 0.02; orb. 4, 0.11;  $\gamma_0=4.25$ : orb. 1, 0.45; orb. 2, 0.45; orb. 3, 0.08; orb. 4, 0.13;  $\gamma_0=4.3$ : orb. 1, 0.01; orb. 2, 0.35; orb. 3, 0.56; orb. 4, 0.17;  $\gamma_0=4.4$ : orb. 2, 0.05; orb. 3, 0.56; orb. 4, 0.44; orb. 5, 0.49;  $\gamma_0=4.6$ : orb. 2, 0.03; orb. 3, 0.25; orb. 4, 0.65; orb. 5, 0.57;  $\gamma_0=4.8$ : orb. 3, 0.20; orb. 4, 0.61; orb. 5, 0.62; orb. 6, 0.71;  $\gamma_0=\infty$ : orb. 5, 0.61; orb. 6, 0.85; orb. 7, 0.92; orb. 8, 0.95.

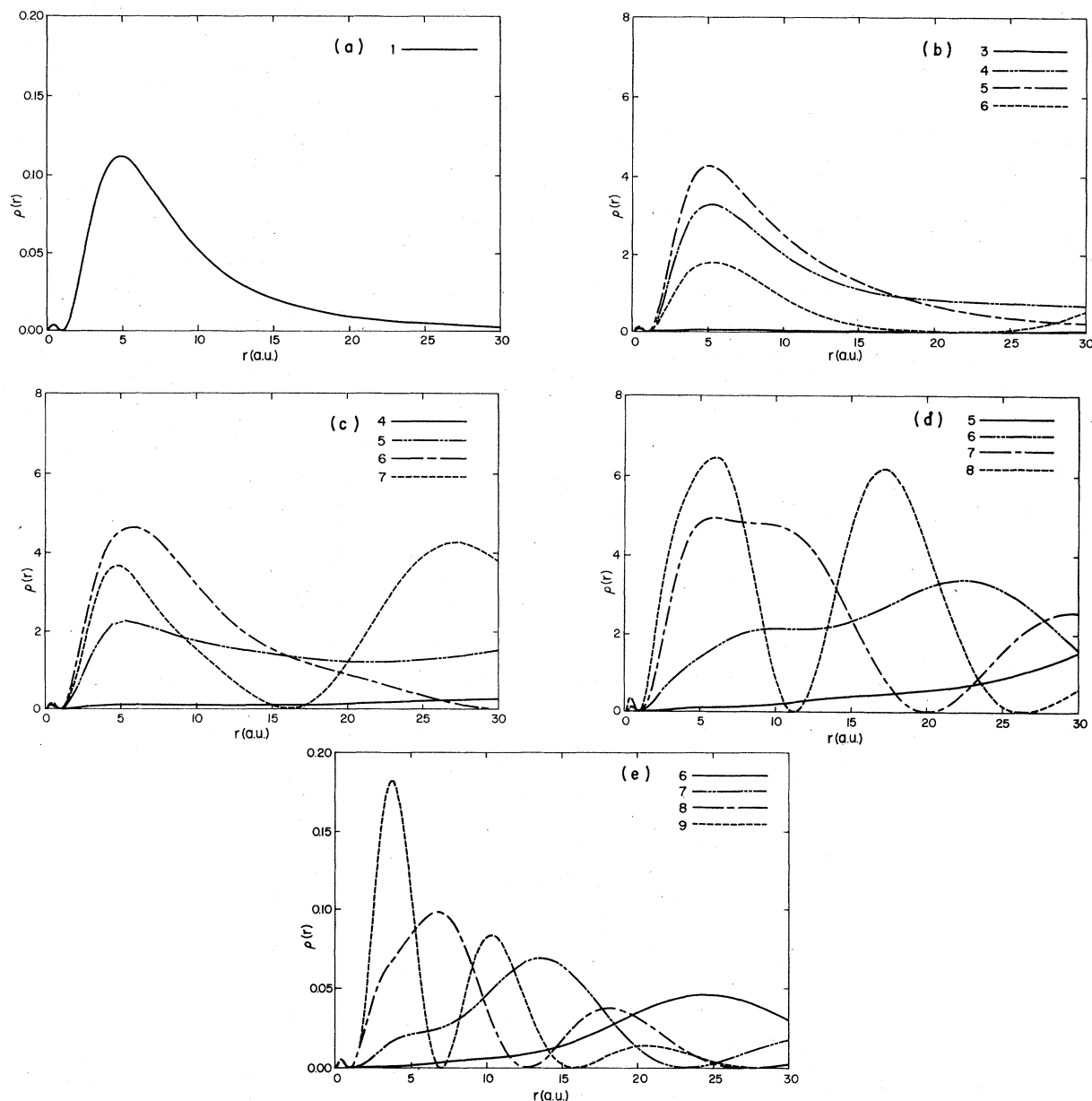


FIG. 2. The radial density (arbitrary units) for  $0 \leq r \leq 30$  a.u. for virtual orbitals of Mg. The integrated norms to 30 a.u. are for  $\gamma_0=5.2$ : orb. 1, 0.98;  $\gamma_0=5.4$ : orb. 3, 0.01; orb. 4, 0.41; orb. 5, 0.45; orb. 6, 0.16;  $\gamma_0=5.6$ : orb. 4, 0.04; orb. 5, 0.43; orb. 6, 0.52; orb. 7, 0.61;  $\gamma_0=6.5$ : orb. 5, 0.14; orb. 6, 0.66; orb. 7, 0.73; orb. 8, 0.83;  $\gamma_0=\infty$ : orb. 6, 0.60; orb. 7, 0.76; orb. 8, 0.90; orb. 9, 0.95.

considered in Ref. 16, the situation is not so clear cut for  $\text{Be}^-$  and  $\text{Mg}^-$ . Although the resonance orbital may be identified after several ( $\sim 10$ ) HF calculations with different values of  $a$ , we consider this method to be less useful for applications to the electron-neutral-atom scattering. This we claim is mainly due to the small centrifugal barrier in the radial differential equation for these neutral atoms, which makes the separation into resonance and scattering states less sharp than

in the model potential case.

The use of the attractive potential  $V_{\text{pot}}(r)$  only in identifying the desired root is demonstrated in Tables I and II and Figs. 1 and 2. In the tables we give the eigenvalues of the virtual  $p$  orbitals of the Be and Mg atoms as a function of the cutoff parameter  $\gamma_0$  defined in Eq. (4). Comparing the top and bottom lines of Table I for beryllium (with  $\gamma_0=4.0$  and  $\gamma_0=\infty$ , respectively), we see that orbitals 9–12 are stable, and that orbitals

2–6 in the first row have energies which are nearly the same as those of orbitals 1–5 in the bottom row. Orbitals 6 and 7 (for  $r_0 = \infty$ ) responded most strongly to the attractive shift potential. We can gradually follow the orbitals in the resonance-energy range as the value of the parameter  $r_0$  is decreased from infinity to 4.0. These are the underlined orbitals in the two tables and can be identified as the resonance-energy and orbital region for that particular value of the polarization potential.

In the figures, we plot the radial density [ $r^2 \int d\Omega \psi^*(\vec{r})\psi(\vec{r})$ ] of four orbitals whose energies are close to that of the resonance for a selected set of values for the parameter  $r_0$ . The small “bumps” occurring for small  $r$  in the Mg case originate from the orthogonality constraint with the occupied  $2p$  orbitals and are absent in Be, which has no  $p$  orbital occupancy. The general character of those scattering states with energies less than the resonance is a flat and extremely slow-rising radial density in the interior region, as can be seen from the solid line in Figs. 1(c)–1(g) and 2(b)–2(e). Those scattering states with energies above the resonance show a regular oscillatory behavior as the dashed lines in Figs. 1(d)–1(g) and 2(c)–2(e) indicate. The orbitals in the resonance range display rather different structure from the two types of scattering states mentioned above which possess a regular behavior and hence are easily distinguished.

The first two figures display the radial density out to 30 a. u. In order to more clearly judge the extensions of the orbitals, we have included in the figure text the integrated norms within this distance, i.e.,

$$\int_0^{30 \text{ a.u.}} r^2 dr \int d\Omega \psi^*(\vec{r})\psi(\vec{r}),$$

which, of course, are a fraction of unity for these normalized orbitals. It is interesting to see that orbitals 1 and 2 in Fig. 1(b) are very similar in the range  $0 \leq r \leq 30$  a. u. That they are indeed orthogonal can be seen from Fig. 3, which displays them in the range  $0 \leq r \leq 200$  a. u. Orbital 1 in Fig. 1(a) has the form of a bound orbital, as expected from the negative value of its orbital energy. A negative orbital energy is, however, not a necessity for this localized form, since this orbital is almost indistinguishable from orbital 1 for Be for  $r_0 = 4.24$  a. u., which has a positive orbital energy.

To estimate the energy range of the  $^2P$  shape resonances of  $\text{Be}^-$  and  $\text{Mg}^-$ , we use the criterion of Eq. (5) for estimating the correct  $r_0$ . With a value of  $\alpha = 46$  a. u. for the static polarizability of Be, we compute  $r_0 = 4.8$  a. u., and with  $\alpha = 84$  a. u. for Mg, we compute  $r_0 = 6.5$  a. u. With these

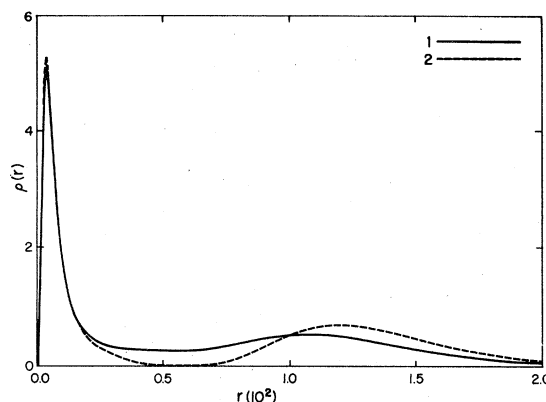


FIG. 3. The radial density (arbitrary units) for  $0 \leq r \leq 200$  a. u. for virtual orbitals 1 and 2 for Be with the value 4.25 for the cutoff parameter  $r_0$  in  $V_{\text{pol}}(r)$ . The integrated norms are 0.99 and 0.98, respectively.

values we obtain energy ranges of 0.14–0.24 eV for  $\text{Be}^-$  and 0.12–0.27 eV for  $\text{Mg}^-$ . In the latter case orbital 7 shows a much more localized structure than orbital 6 [Fig. 2(d)], which indicates that the center of the resonance is closer to 0.27 eV. Experimentally, the energy of the  $^2P$  shape resonance for Mg has been determined to 0.15 eV (Ref. 20). To our knowledge, no experimental values have been obtained for beryllium. Although it is obvious that these predictions are rather approximate, it should be pointed out that these simple calculations give results which are in good agreement with those of calculations of a much more sophisticated nature.<sup>6,8,10</sup>

The predictions of resonance energies and orbitals we obtained are not artifacts of the basis sets. Even though all virtual orbitals are found to change their eigenvalues when the basis is modified, the scheme of adding the attractive potential  $V_{\text{pol}}(r)$  to the Hamiltonian always gave the same resonance-energy range.

The use of the repulsive shift potential  $V_{\text{pow}}(r)$  or  $V_{\text{pow}}(r) + V_{\text{pol}}(r)$  corresponds to raising the scattering states with energies less than the resonance to levels above the resonance energy in Table I for  $r_0 = \infty$  and 4.8 a. u., respectively, and in Table II for  $r_0 = \infty$  and 6.5 a. u., respectively. Thus, when we successfully identify the resonance orbital, we will be in agreement with the method of using the attractive potential  $V_{\text{pol}}(r)$  only. In this way we realize that the two former schemes are essentially included (special cases) of the latter.

One of the most important differences between the addition of the attractive potential  $V_{\text{pol}}(r)$  and the repulsive potential  $V_{\text{pow}}(r)$  is the qualitative effects these potentials have on the boundary conditions of the solutions to the Schrödinger differential equation. In the former case no change

occurs, whereas for the repulsive potentials, the problem has been turned into the solution of a particle in a box, or more accurately a bowl. We find it more appealing to leave the original structure of the differential equation and its boundary condition intact, and hence favor not using the power repulsive potential.

Improvements to the above method involving  $V_{\text{pol}}(r)$  should be pursued by using a more realistic polarization potential. We have used, for reasons of computational simplicity, the long-range form of the potential modified by a simple cutoff. Because the resonance orbital has substantial ampli-

tude in the vicinity of the target's valence orbitals, it is expected that improvements in the form of the potential  $V_{\text{pol}}(r)$  will be of significant importance.

#### ACKNOWLEDGMENTS

The authors wish to acknowledge the financial support of the National Science Foundation (Grants Nos. DMR 76-84577 and CHE 75-19476). The authors thank Professor K. Jordan for useful discussions and comments. J. S. acknowledges support of the Camille and Henry Dreyfus, J. S. Guggenheim, and David P. Gardner Foundations.

<sup>1</sup>A. U. Hazi and H. S. Taylor, *Phys. Rev. A* **1**, 1109 (1970).

<sup>2</sup>H. S. Taylor and A. U. Hazi, *Phys. Rev. A* **14**, 2075 (1976).

<sup>3</sup>D. G. Truhlar, *J. Comput. Phys.* **10**, 123 (1972).

<sup>4</sup>D. G. Truhlar, *Chem. Phys. Lett.* **15**, 483 (1972).

<sup>5</sup>D. G. Truhlar, *Chem. Phys. Lett.* **26**, 377 (1974).

<sup>6</sup>J. Hunt and B. L. Moiseiwitsch, *J. Phys. B* **3**, 892 (1970).

<sup>7</sup>F. E. Harris, *Phys. Rev. Lett.* **19**, 173 (1967).

<sup>8</sup>H. A. Kurtz and Y. Öhrn, *Phys. Rev. A* **19**, 43 (1979).

<sup>9</sup>*Proceedings of the 1978 Sanibel Work Shop*, *Int. J. Quantum. Chem.* **14**, 4 (1978).

<sup>10</sup>T. N. Rescigno, C. W. McCurdy, and A. E. Orel, *Phys. Rev. A* **17**, 1931 (1978).

<sup>11</sup>N. Moiseyev, P. R. Certain, and F. Weinhold, *Mol. Phys.* **36**, 1613 (1978).

<sup>12</sup>M. Hehenberger, H. V. McIntosh, and E. Brändas, *Phys. Rev. A* **10**, 1494 (1974).

<sup>13</sup>M. Hehenberger, B. Laskowski, and E. Brändas, *J. Chem. Phys.* **65**, 4559 (1976).

<sup>14</sup>M. Hehenberger, P. Froelich, and E. Brändas, *J. Chem. Phys.* **65**, 4571 (1976).

<sup>15</sup>P. G. Burke and W. D. Robb, *Adv. At. Mol. Phys.* **11**, 143 (1975).

<sup>16</sup>J. F. Liebman, D. L. Yeager, and J. Simons, *Chem. Phys. Lett.* **48**, 227 (1977).

<sup>17</sup>D. G. Truhlar, J. K. Rice, S. Trajmar, and D. C. Cartwright, *Chem. Phys. Lett.* **9**, 229 (1971).

<sup>18</sup>E. Clementi, *Tables of Atomic Functions* (IBM, San Jose, Calif., 1965).

<sup>19</sup>The twelve orbital exponents for Be were chosen to be 2.0, 1.5, 1.0, 0.75, 0.5, 0.375, 0.25, 0.18, 0.125, 0.09, 0.06, 0.03, and the ten orbital exponents for Mg, 1.000, 0.5995, 0.3594, 0.2154, 0.1292, 0.774, 0.464, 0.0278, 0.0167, 0.0100.

<sup>20</sup>P. D. Burrow, J. A. Mischejda, and J. Comer, *J. Phys. B* **9**, 3255 (1976).