

## Electron scattering from hydrogen: Collisions in which the total spin quantum numbers change

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In several recent experiments in which spin-polarized electrons were scattered from hydrogen atoms the investigators isolated the spin-exchange effects which arise in the theory from the antisymmetrization of the wave functions of the electrons. Noting the recent advances in techniques of producing and detecting polarized electrons, this paper considers the possibility of finding the terms in the effective transition operator that are spin dependent. The spin-dependent parts of the first Born term in the transverse photon and the instantaneous photon are calculated. The  $1s-1s$ ,  $1s-2s$ , and  $1s-2p$  scattering amplitudes are discussed specifically. A brief comparison is made of the magnitude of these effects and the accuracy of the present experiments.

### I. INTRODUCTION

The recent experiments by Alguard, Hughes, Lubell, and Wainwright<sup>1,2</sup> employing spin-polarized electrons in electron-hydrogen-atom scattering has provided tests of our knowledge of spin-exchange effects in a simple atomic system. These experiments measured the interference between direct and exchange scattering amplitudes in electron impact ionization and elastic scattering off atomic hydrogen over a considerable energy range utilizing spin-polarized electrons and spin-polarized hydrogen atoms. The effects that were measured depend on spin through the exchange terms provided by the Pauli exclusion principle; the effective transition operator for these experiments is indeed spin independent. As such, these spin-exchange effects keep invariant the spin quantum number  $S$  of the scattering electron target and the projection  $M_S$  along the axis of quantization. In the near future, polarized electron scattering experiments of this type will be improved by the use of new methods of producing polarized electron beams, which are expected to increase beam currents from the present 15 nA level to several milliamperes.

In this context this paper considers interactions in which  $S$  and  $M_S$  may change during the scattering. These effects are caused by interaction terms that are spin dependent. We calculate the spin-dependent corrections from one instantaneous photon exchange between the nucleus and the scattered electron (Mott scattering), from one instantaneous photon exchange between the two electrons, and from one-transverse-photon exchange between the two electrons.

Previous theoretical work on total spin-change scattering has been done by Mittleman<sup>3</sup> and by Burke and Mitchell.<sup>4</sup> Mittleman<sup>3</sup> considered a spin-dependent term in the  $1^1S_0 - 2^3S_1$  excitation

of helium by unpolarized electrons and took as an effective spin-dependent potential the spin-other-orbit term that occurs in calculations of the fine-structure energy levels of helium. Arguing that other effects are small at high enough ( $>8$  keV) incident electron energy, he neglects the spin-spin term as well as the relativistic wave function correction for helium. It is this relativistic wave function correction which makes the electron-helium scattering problem at somewhat lower incident electron energy far more complicated than the electron-hydrogen case studied here.

Burke and Mitchell<sup>4</sup> have examined the role the fundamental symmetries play in determining the general form of the interaction in  $s-s$  scatterings in atoms where there is one electron in the outer shell. In addition, they have calculated the transition amplitudes for an electron scattering off a spin-orbit interaction of the form  $\vec{L} \cdot \vec{S} (f(r))$  where  $\vec{L}$  is the total orbital angular momentum operator,  $\vec{S}$  is the total spin operator, and  $f(r)$  which is dependent on the radial distance of the electrons from the nucleus must be determined empirically. This effort is of principal interest in problems where the target is a heavy atom and thus the interaction is too complex to calculate conveniently from first principles and some empirical input is needed.

### II. CALCULATION

The calculation is done using a set of techniques known as time-ordered perturbation theory. There are several books<sup>5,6</sup> that introduce quantum electrodynamics from this point of view. An advantage of the approach is that it is in form very similar to Rayleigh-Schrödinger perturbation theory for nonrelativistic quantum mechanics. The plan in doing these calculations is first to write down the relativistic perturbation amplitudes. A process

known as "nonrelativistic reduction"<sup>7</sup> converts these terms to sufficient accuracy into nonrelativistic amplitudes that are convenient to evaluate.

The starting point of this calculation is an unperturbed Hamiltonian

$$H_0 = H_C^{(1)} + H_{F_r}^{(2)} \quad (1)$$

where  $H_C^{(1)}$  is the Dirac Hamiltonian for an electron in a Coulomb field, the target hydrogen atom, and  $H_{F_r}^{(2)}$  is the Dirac Hamiltonian for the scattering electron. We will ignore the exchange terms. For near forward scattering, which is likely to be the interaction of interest, the direct terms highly dominate at incident electron energy a number of times larger than the ionization energy of hydrogen where this first Born calculation should be useful.

We obtain the spin-dependent part of the instantaneous photon terms by examining  $M^{(i)}$  where

$$M^{(i)} = \langle F | (-e^2/r_2 + e^2/r_{12}) | I \rangle. \quad (2a)$$

$$M^{(i)} = \left(\frac{e}{2\pi}\right)^2 \int \frac{d^3k}{k} \sum_U \sum_{\vec{\pi}} \langle F | \vec{\alpha}_1 \cdot \vec{\pi} e^{i\vec{k} \cdot \vec{r}_1} | U \rangle \langle U | \vec{\alpha}_2 \cdot \vec{\pi} e^{-i\vec{k} \cdot \vec{r}_2} | i \rangle G_U(k) + (1 \leftrightarrow 2). \quad (3)$$

The sum over  $U$  is taken over all the virtual intermediate states of hydrogen. The symbol  $(1 \leftrightarrow 2)$  represents a term identical to the previous one with electron 1 interchanged with 2 in the transition operator, and  $G_U(k)$  is given by

$$G_U(k) = (E_I - E_U - k)^{-1}. \quad (4)$$

The wave functions  $I$ ,  $U$ ,  $F$  are eigenfunctions of  $H_0$  with  $E_I$ ,  $E_U$ , and  $E_F$  the respective eigenvalues. The Dirac matrices  $\vec{\alpha}_i$  are defined by the standard representation.<sup>10</sup> The quantity  $k$  is the wave number of the Breit photon which is exchanged between

Equation (2a) is the relativistic counterpart of the ordinary first Born amplitude. The vectors  $\vec{r}_1$  and  $\vec{r}_2$  give the position of the bound and the scattering electrons and  $r_{12} = |\vec{r}_1 - \vec{r}_2|$  is the separation. The wave functions  $I$  and  $F$  are the initial and final wave functions of  $H_0$ . The charge of the electron is  $-e$ .

For the calculation of the transverse photon term we take as our perturbing Hamiltonian

$$H' = H'_T, \quad (2b)$$

which in second order gives the interaction for the exchange of a transverse photon (which is often called a Breit photon) between the two electrons. It is convenient to formulate this approach in terms of second quantization, and we give references for such a development.<sup>8</sup>

The contribution to the scattering amplitude from the initial transverse photon interaction in scattering where the initial and final states of the atom are bound is given by  $M^{(i)}$  where we write<sup>9</sup>

the bound and free electron. The sum over  $\vec{\pi}$ , the polarization vector, is over two directions perpendicular to each other and  $\vec{k}$ .

Since we are not concerned with extremely fast incident electrons or bound electrons in an atom of very large atomic number, we may make a nonrelativistic reduction<sup>7</sup> of the matrix operator in (2a) and (3) discarding terms of relative order  $(k^2/m^2)$ ,  $(k_e^2/m^2)$ , and  $(\alpha^2)$ , where  $\alpha$  is the fine-structure constant. It should be noted that we are interested in the spin-dependent transition operator. Obvious spin-independent relativistic corrections are discarded. We write

$$M^{(i)} \approx \langle \psi_f'(\vec{r}_1, \vec{r}_2) | \left( -\frac{e^2}{r_2} + \frac{e^2}{r_{12}} \right) | \psi_i'(\vec{r}_1, \vec{r}_2) \rangle + \frac{i}{2} \left( \frac{e}{2\pi m} \right)^2 \int \frac{d^3k}{k^2} \langle \psi_f'(\vec{r}_1, \vec{r}_2) | \vec{\sigma}_1 \cdot (\vec{k} \times \vec{p}_1) e^{i\vec{k} \cdot (\vec{r}_1 - \vec{r}_2)} - \sigma_2 \cdot (\vec{k} \times \vec{p}_2) e^{-i\vec{k} \cdot \vec{r}_2} (-1 + e^{i\vec{k} \cdot \vec{r}_1}) | \psi_i'(\vec{r}_1, \vec{r}_2) \rangle, \quad (5a)$$

$$M^{(i)} \approx \left( \frac{e}{2\pi m} \right)^2 \int \frac{d^3k}{k} \sum_u \sum_{\vec{\pi}} \langle \psi_f'(\vec{r}_1, \vec{r}_2) | e^{i\vec{k} \cdot \vec{r}_1} [\vec{p}_1 \cdot \vec{\pi} + \frac{1}{2} i \vec{\sigma}_1 \cdot (\vec{k} \times \vec{\pi})] | u \rangle \langle u | [\vec{p}_2 \cdot \vec{\pi} - \frac{1}{2} i \vec{\sigma}_2 \cdot (\vec{k} \times \vec{\pi})] \times e^{-i\vec{k} \cdot \vec{r}_2} | \psi_i'(\vec{r}_1, \vec{r}_2) \rangle \tilde{G}_u(k) + (1 \leftrightarrow 2), \quad (5b)$$

where  $\vec{p}_1$  and  $\vec{p}_2$  are the momentum operators for the corresponding electrons. The first term in (5a) is the leading spin-independent transition operator taken between wave functions  $\psi'$  which

have the spin-same-orbit interaction included as a perturbation. The spin-orbit interaction gives rise to a spin-dependent contribution. For scattering between  $s$  states the spin-orbit correction

vanishes. For this case we can replace  $\psi'$  by  $\psi$  the nonrelativistic (Pauli approximation) wave functions. In the general excitation problem we need to include the spin-orbit wave function correction. A discussion is given in the Appendix. The second part of (5a) is clearly a spin-dependent contribution. Equation (5b) also has a spin-dependent and a spin-independent contribution. The spin-independent part is of order  $\alpha^2$  less than the leading Born approximation and therefore we neglect it.

In Eq. (5) the  $\sigma_i$  matrices are Pauli spin matrices.  $\tilde{G}_u(k)$  is a nonrelativistic approximation of  $G_u(k)$  with  $E_I$  and  $E_U$  replaced by their nonrelativistic counterparts  $W_i$  and  $W_u$ , respectively. Specifically, we write

$$W_i = k_i^2/2m + \epsilon_i = k_f^2/2m + \epsilon_f \quad (6)$$

and

$$W_u = k_u^2/2m + \epsilon_u, \quad (7)$$

where  $k_i$ ,  $k_u$ , and  $k_f$  are momenta of the free electron, and the  $\epsilon$  are the nonrelativistic energies of the target atom.

We write for the wave functions  $\psi_f$  and  $\psi_i$

$$\psi = \phi(\vec{r}_1)\theta(\vec{r}_2)\chi, \quad (8)$$

where the  $\phi$ 's are eigenfunctions of the target atom, the  $\chi$ 's are two-particle spinors and the  $\theta$ 's are free particle plane-wave states of the form  $\exp(i\vec{k}_{i,f} \cdot \vec{r})/(2\pi)^{3/2}$ .

Inserting (8) in (5a) and (5b), we integrate over the spatial coordinate  $\vec{r}_2$  of the scattering electron and in (5b) sum over the polarization vector  $\vec{\pi}$ . After some manipulation and discarding of the spin-independent terms, we obtain the leading part  $\mathfrak{M}_S^{(t)}$  of the spin-dependent part of  $M$ . With  $\vec{q} = \vec{k}_i - \vec{k}_f$  we write for the transverse photon term

$$\begin{aligned} \mathfrak{M}_S^{(t)} \approx & \tilde{A}(q) \langle \chi_f | i\vec{\sigma}_1 \cdot (\vec{k}_i \times \vec{k}_f) F_1 - i\vec{\sigma}_2 \cdot (\vec{q} \times \vec{F}_2) \\ & - \frac{1}{2}(q^2 \vec{\sigma}_1 \cdot \vec{\sigma}_2 - \vec{\sigma}_1 \cdot \vec{q} \vec{\sigma}_2 \cdot \vec{q}) F_1 | \chi_i \rangle \end{aligned} \quad (9)$$

and for the instantaneous photon term

$$\begin{aligned} \mathfrak{M}_S^{(i)} \approx & \tilde{B}(q) \langle \chi_f | i\vec{\sigma}_2 \cdot (\vec{k}_i \times \vec{k}_f) (\delta_{f_i} - F_1) \\ & + i\vec{\sigma}_1 \cdot (\vec{q} \times \vec{F}_2) | \chi_i \rangle + \mathfrak{M}_S^{wf} \end{aligned} \quad (10)$$

where the spin-dependent wave-function correction  $\mathfrak{M}_S^{wf}$  is discussed in the Appendix.

The form factors  $F_1$  and  $\vec{F}_2$  are given by

$$F_1(\vec{q}) = \langle \phi_f(\vec{r}_1) | e^{i\vec{q} \cdot \vec{r}_1} | \phi_i(\vec{r}_1) \rangle \quad (11)$$

the generalized oscillator strength,<sup>11</sup> and

$$\vec{F}_2(\vec{q}) = \langle \phi_f(\vec{r}_1) | e^{i\vec{q} \cdot \vec{r}_1} \vec{p}_1 | \phi_i(\vec{r}_1) \rangle. \quad (12)$$

The overall factors  $\tilde{A}(q)$  and  $\tilde{B}(q)$  are defined by

$$\tilde{A}(q) = [e^2/(8\pi^2 m^2 q)] [(\epsilon_i - \epsilon_f - q)^{-1} + (\epsilon_f - \epsilon_i - q)^{-1}] \quad (13)$$

and

$$\tilde{B}(q) = \frac{1}{2} [e/(2\pi m q)]^2. \quad (14)$$

Equation (10) includes the spin-dependent part of the scattering of the incident electron by the nuclear Coulomb field. The  $\delta_{fi}$  symbol connected with this contribution stands for the overlap of the initial and final spatial wave functions.

Examining the transverse photon (9) contribution, we find that the first two terms inside the matrix element are spin-other-orbit interactions, and the remaining part is the spin-spin interaction. The instantaneous (10) term contains spin-other-orbit contributions.

For convenience we redefine our coordinate system with the directions suggested by the collision process<sup>12</sup>

$$\begin{aligned} \hat{q} &= (\vec{k}_i - \vec{k}_f) / |\vec{k}_i - \vec{k}_f|, \\ \hat{p} &= (\vec{k}_i + \vec{k}_f) / |\vec{k}_i + \vec{k}_f|, \\ \hat{n} &= (\vec{k}_i \times \vec{k}_f) / |\vec{k}_i \times \vec{k}_f|, \end{aligned} \quad (15)$$

with  $\hat{n}$  which points out of the scattering plane the quantization axis. We rewrite (9) and (10) using our new coordinate system.

$$\begin{aligned} \mathfrak{M}_S^{(t)} \approx & \tilde{A}(q) \langle \chi_f | [i\vec{\sigma}_1 \cdot \hat{n} k_i k_f \kappa \\ & + \frac{1}{2} q^2 (\vec{\sigma}_1 \cdot \vec{\sigma}_2 - \vec{\sigma}_1 \cdot \hat{q} \vec{\sigma}_2 \cdot \hat{q})] F_1 \\ & - i\vec{\sigma}_2 \cdot (\vec{q} \times \vec{F}_2) | \chi_i \rangle, \end{aligned} \quad (16a)$$

$$\begin{aligned} \mathfrak{M}_S^{(i)} \approx & \tilde{B}(q) \langle \chi_f | i\vec{\sigma}_2 \cdot \hat{n} k_i k_f \kappa (\delta_{f_i} - F_1) \\ & + i\vec{\sigma}_1 \cdot (\vec{q} \times \vec{F}_2) | \chi_i \rangle + \mathfrak{M}_S^{wf}, \end{aligned} \quad (16b)$$

where

$$\kappa = [1 - (\hat{k}_i \cdot \hat{k}_f)^2]^{1/2}. \quad (17)$$

In (16a) and (16b) are contained the spin-dependent parts of the transition amplitude. Let us consider some special cases. For  $s$ -to- $s$  scattering the vector  $\vec{q} \times \vec{F}_2$  vanishes. The spin-spin terms in (16a) and (16b) cause spin-flip transitions in which the change of  $M_S$  [ $\Delta M_S = M_S(f) - M_S(i)$ ] is  $\pm 2$ . In collisions where the  $\delta$  function  $\delta_{fi}$  is one the spin-orbit term can cause a  $\Delta S = \pm 1$ ,  $\Delta M_S = 0$  scattering. Scattering events where  $\Delta M_S$  equals  $\pm 1$  are not allowed as can be seen from examination of (16a) and (16b) or from fundamental grounds because of space reflection invariance.<sup>4</sup>

Note for  $q$  much greater than  $|\epsilon_f - \epsilon_i|$ , which will be correct for other than a most restricted region where the scattering angle is less than  $2|\epsilon_f - \epsilon_i|/k_i$ , we may replace  $\vec{A}(q)$  by  $-2\vec{B}(q)$ . In this approximation we write for the sum of the instantaneous and transverse contribution

$$\begin{aligned} \mathfrak{M}_S \approx & \vec{B}(q) \langle \chi_f | i \vec{\sigma}_2 \cdot \hat{n} k_i k_f \kappa \delta_{fi} \\ & - i(2\vec{S} + \vec{\sigma}_1) \cdot \hat{n} k_i k_f \kappa F_1 + i(2\vec{S} + \vec{\sigma}_2) \cdot (\vec{q} \times \vec{F}_2) \\ & - [q^2(\vec{\sigma}_1 \cdot \vec{\sigma}_2) - \vec{\sigma}_1 \cdot \hat{q} \vec{\sigma}_2 \cdot \hat{q}] F_1 | \chi_i \rangle + \mathfrak{M}_S^{wf}, \end{aligned} \quad (18)$$

where  $\vec{S}$  is the sum of spins of the two electrons. If either  $\chi_i$  or  $\chi_f$  is a spin-zero state, the  $\vec{S}$ -dependent terms are zero. In addition, the operator  $\vec{S} \cdot \hat{n}$  vanishes for  $\chi_i$  or  $\chi_f$  a  $S=1$ ,  $M_S=0$  state.

For  $1s$ - $1s$  and  $1s$ - $2s$  scattering we give the corresponding values of the form factor  $F_1$ :

$$F_1(\vec{q}; 1s-1s) = 2^4 / [a_0^4(q^2 + 4/a_0^2)^2], \quad (19)$$

$$F_1(\vec{q}; 1s-2s) = 4\sqrt{2} q^2 / \{a_0^4 [q^2 + 9/(4a_0^2)]^3\} \quad (20)$$

where  $a_0$  is the Bohr radius.

The next special case we examine is  $s$ - $p$  scattering. It is convenient to write our  $p$ -wave functions in the coordinate basis given by (15). The form factors  $F_1$  and  $\vec{F}_2$  in the form  $\hat{q} \times \vec{F}_2$  for  $1s$  -  $2p$  scattering where  $\hat{\lambda}$  is either  $\hat{p}$ ,  $\hat{q}$ , or  $\hat{n}$  are given below<sup>13</sup>

$$F_1(\vec{q}; 1s-2p\hat{\lambda}) = \frac{12i\sqrt{2}}{a_0^5} \frac{\vec{q} \cdot \hat{\lambda}}{(q^2 + 9/4a_0^2)^3}, \quad (21)$$

$$\hat{q} \times \vec{F}_2(\vec{q}; 1s-2p\hat{\lambda}) = \frac{i\sqrt{2}}{a_0^5} \frac{\hat{q} \times \hat{\lambda}}{(q^2 + 9/4a_0^2)^2}. \quad (22)$$

In general, for  $s$ - $p$  excitations the expression  $\vec{q} \times \vec{F}_2$  does not vanish. As a consequence  $\Delta M_S = \pm 1$  transitions are allowed.

### III. CONCLUSION

Since scattering events in which  $S$  and  $M_S$  change can not be produced by the spin-independent interaction, it would seem logical in order to detect the spin-dependent part of the transition operator to employ perfectly polarized electron and atomic beams and examine only those events that change either of the total spin quantum numbers. Experimental difficulties prevent us from obtaining anywhere near perfectly polarized beams. In the experiment<sup>1</sup> mentioned earlier the beam polarizations were 63% for the electrons and 50% for the atoms. As a result, in an attempt to detect changes in  $S$  and  $M_S$ , one will have to perform many different experiments and determine the spin-dependent parts of the transition operator in interference terms with the spin-independent part. A discussion of using partially polarized beams to determine the spin-dependent transition operator in  $s$ - $s$  excitations has been given by Burke and Mitchell.<sup>3</sup>

In general we find that the spin-dependent corrections are of order  $\alpha^2$  smaller than the spin-independent part. We compare this to the present level of accuracy<sup>14</sup> of the experiment by Alguard *et al.*,<sup>1</sup> which is 4 parts in  $10^4$ . With a GaAs photoemission polarized electron source capable of high intensity and optical polarization reversal, differential scattering experiments sensitive to the level of less than 1 part in  $10^4$  in the parallel-antiparallel cross-section asymmetry appear possible. Whether this advance will allow the detection of terms in the transition operator which can change the total spin quantum numbers remains to be seen.

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### APPENDIX: SPIN-DEPENDENT TRANSITION OPERATORS ARISING FROM SPIN-ORBIT WAVE-FUNCTION CORRECTIONS

As was mentioned in Sec. II, the spin-same-orbit corrections to the initial and final wave functions can give a spin-dependent amplitude. We consider the first term in Eq. (5a) as a sum of the ordinary nonrelativistic Born approximation plus the spin-orbit wave-function correction. After

integrating over  $\vec{r}_2$ , we obtain the amplitude

$$M_{wf}^{(i)} = (e^2/2\pi^2q^2) [\langle \phi_f(\vec{r}_1) | X | \phi_i(\vec{r}_1) \rangle \langle \chi_f | \chi_i \rangle + \langle \phi_f(\vec{r}_1) \chi_f | X g_i H'_{s-so} + H'_{s-so} g_f X | \phi_i(\vec{r}_1) \chi_i \rangle \quad (A1)$$

where

$$X = -1 + e^{i\vec{q}\cdot\vec{r}_1},$$

$$g_i = (\epsilon_i - \tilde{H} + i\eta)^{-1},$$

$$g_f = (\epsilon_f - \tilde{H} + i\eta)^{-1},$$

$\tilde{H}$  is the nonrelativistic hydrogen Hamiltonian, and  $\eta$  is an arbitrarily small positive constant that reminds us to take the principal part. There are additional relativistic spin-independent corrections that are ignored here since these corrections are negligible compared to the nonrelativistic amplitude. To distinguish between these two spin-independent contributions would require extraordinarily precise absolute scattering experiments which are unlikely. The spin-same-orbit

perturbation  $H'_{s-so}$  is given by

$$H'_{s-so} = (e^2/4m^2r_1^2) \vec{\sigma}_1 \cdot \vec{l}_1, \quad (A2)$$

where  $\vec{l}_1$  is the angular momentum of the bound electron. If the initial and final states are both ( $l_1=0$ ) s states, there is no contribution from this term. In the more general case the  $H'_{s-so}$  part of Eq. (A1) simplifies to

$$\mathfrak{M}_s^{wf} = (e^2/2\pi^2q^2) \langle \phi_f(\vec{r}_1) | e^{i\vec{q}\cdot\vec{r}_1} g_i A + A g_f e^{i\vec{q}\cdot\vec{r}_1} | \phi_i(\vec{r}_1) \rangle, \quad (A3)$$

where  $A$  is given by

$$A = \langle \chi_f | H'_{s-so} | \chi_i \rangle. \quad (A4)$$

The expression in (A1) can be evaluated using an explicit representation of the Coulomb-Green's function and related techniques.<sup>15</sup> The corresponding wave-function corrections from a transverse photon exchange appear to be somewhat smaller since the terms corresponding to  $g_i$  and  $g_f$  in this case are smaller.

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<sup>8</sup>J. J. Sakurai, *Advanced Quantum Mechanics* (Addison-Wesley, Reading, Mass., 1973), p. 20; H. A. Bethe and E. E. Salpeter, in Ref. 7, p. 170.

<sup>9</sup>We use the set of units where  $\hbar=c=1$ .

<sup>10</sup>J. J. Sakurai, in Ref. 8, p. 81, Eq. (3.40).

<sup>11</sup>M. Inokuti, Rev. Mod. Phys. 43, 297 (1971).

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<sup>13</sup>In Eq. (19)-(22) are used the forms of the wave functions that have real positive normalization factors. In particular,  $\phi_{2p\lambda} = \pi^{-1/2} (2a_0)^{-5/2} \vec{r} \cdot \hat{\lambda} \exp(-r/2a_0)$  is employed for the  $2p_\lambda$  state.

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