

Variational calculations of the Fermi contact term for the 2^2S , 2^2P , and 3^2S states of Li and the 2^2S state of Be^+

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The Fermi contact term for the 2^2S , 2^2P , and 3^2S states of Li and the 2^2S state of Be^+ are calculated using high-precision variational wave functions in Hylleraas coordinates. The nonrelativistic Fermi contact terms obtained for these states are 2.905 922(50), $-0.214\ 783(50)$, 0.673 405(50), and 12.497 57(30) a.u., respectively. Estimates of corrections for finite nuclear size, relativistic effects, and QED effects are shown to yield satisfactory agreement with experiment for the 2^2S state of Li and Be^+ , but there remains a substantial disagreement with experiment for the 3^2S state of Li. [S1050-2947(96)04208-4]

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I. INTRODUCTION

The Fermi contact term dominates the hyperfine structure of atomic S states. Although its calculation for lithium has received considerable attention, a high-precision theoretical determination remains a difficult problem. Since the Fermi contact term consists of matrix elements of $\delta(\mathbf{r}_i)$, the calculated results depend critically on the quality of the wave function near the nucleus. A comprehensive summary of early work for the lithium 2^2S contact term can be found in Ref. [1], which contains approximately 50 calculations.

High-precision measurements of hyperfine structure are now available for several states. The atomic beam magnetic resonance measurement of Beckmann, Böklen, and Elke [2] for the lithium 2^2S state yields a derived Fermi contact term accurate to 1 part per 10^6 (ppm). Orth, Ackermann, and Otten [3] measured the lithium 2^2P hyperfine structure using the optical double resonance technique with a somewhat lower accuracy of 0.5%. Very recently, using Stark spectroscopy, Stevens *et al.* [4] measured the hyperfine structure constant for the lithium 3^2S state, with a precision of 0.2%. Using laser-fluorescence mass spectroscopy, Wine-land, Bollinger, and Itano [5] have achieved an accuracy of 2.6 ppm for the Be^+ 2^2S state.

These measurements provide the motivation to improve the atomic theory of hyperfine structure to a corresponding level of accuracy. The first precise calculation of the Fermi contact term was done by Larsson [6] using variational wave functions in Hylleraas coordinates. The value obtained for the 2^2S state is 2.906 a.u. Using the same method, Ahlenius and Larsson [7,8] calculated the 2^2P contact term. However, their value was accurate only to about 1%. Lindgren [9] applied many-body perturbation theory (MBPT) in the coupled-cluster formulation to lithium calculations. The relativistic and finite nuclear size effects to the Fermi contact terms were included for the 2^2S and 2^2P states. These corrections, together with the finite nuclear mass and QED terms, are essential in making any meaningful comparison with high-precision measurements for the 2^2S state. How-

ever, they are not required for the 2^2P state at the present experimental precision. Nevertheless, Lindgren's calculations for the 2^2S and 2^2P contact terms disagree significantly with the measurements. King and co-workers [10–12] calculated the 2^2S contact term using Hylleraas-type wave functions with basis sets containing up to 602 terms. Their results, however, did not significantly improve upon Larsson's value [6]. Blundell *et al.* [13] studied the lithium atom using the relativistic all-order MBPT method. Their contact term for the 2^2S state is close to Lindgren's value [9], and thus is also in disagreement with experiment. Mårtensson-Pendrill and Ynnerman [14] used the coupled-cluster approach to evaluate lithium properties. Their contact term for the 2^2S state is also not accurate. Sundholm and Olsen [15], Carlsson, Jönsson, and Fischer [16], and Tong, Jönsson, and Fischer [17] performed large-scale multiconfiguration Hartree-Fock calculations on the lithium atom. The contact terms obtained by these groups are in reasonable agreement with one another and with the measurements. Based on configuration-interaction (CI) calculations, Esquivel, Bunge, and Núñez [18] developed a method of successively optimizing wave functions by expanding the significant electron-correlation regions. The uncertainty they claimed for the 2^2S contact term is as small as 27 ppm. However, the reliability of their calculation needs to be reexamined. Using multiple basis sets in Hylleraas coordinates [19], McKenzie [20] obtained the most precise value for the 2^2S contact term.

Recently, significant theoretical progress [21,22] has been made in variational calculations for the lithium atom, using multiple basis sets in Hylleraas coordinates. The nonrelativistic eigenvalues obtained for the 2^2S , 2^2P , and 3^2D states are accurate to a few parts in 10^{10} – 10^{11} . We have also calculated the lithium oscillator strengths to high precision [23]. It is expected that the application of our wave functions to the evaluation of the Fermi contact term will improve upon previous results.

The experimental Fermi contact term f_{expt} for S states is related to the hyperfine constant $A_{1/2}$ by

$$A_{1/2} = \left[\frac{\mu_0 \mu_B \mu_N}{2\pi \hbar a_0^3} \right] \frac{g_e \mu_I f_{\text{expt}}}{3I}, \quad (1)$$

where μ_0 is the vacuum permeability, μ_B and μ_N are the Bohr and nuclear magneton, g_e is the electronic g factor, μ_I is the nuclear magnetic dipole moment, and I is the nuclear spin. Using the most recent adjustment of fundamental constants [24], Eq. (1) becomes

$$A_{1/2}(\text{expt}) = 95.410\,67(7) \frac{g_e \mu_I f_{\text{expt}}}{3I}, \quad (2)$$

in MHz, where the experimental value [2] of the hyperfine constant for the Li 2^2S state is $A_{1/2}(\text{expt}) = 401.752\,043\,3(5)$ MHz, and $\mu_I = 3.256\,426\,8(17)$ [25]. However, there exist inconsistencies in the literature concerning the choice of g_e [9,15,18]. The Dirac value $g_e = 2$ yields $f_{\text{expt}} = 2.909\,393(3)$ a.u.; on the other hand, if the anomalous magnetic moment correction is included, i.e., $g_e = 2(1 + a_e)$ with

$$a_e = \alpha/2\pi - 0.328\,478\,965(\alpha/\pi)^2 + 1.176\,11(\alpha/\pi)^3 + \dots, \quad (3)$$

one obtains instead $f_{\text{expt}} = 2.906\,023(3)$ a.u. In fact, the measured hyperfine constant $A_{1/2}(\text{expt})$ can be written symbolically as

$$A_{1/2}(\text{expt}) = 2(1 + a_e) C_{\text{rel}} C_M C_R C_{\text{QED}} 95.410\,67(7) \frac{\mu_I}{3I} f_c, \quad (4)$$

where a_e is the anomalous magnetic moment correction, C_{rel} is the relativistic correction factor, C_M and C_R are the finite nuclear mass and size correction factors, and C_{QED} is the QED correction factor other than the anomalous magnetic moment correction. The remaining factor f_c is the uncorrected Fermi contact term defined by

$$f_c = 4\pi \left\langle \Psi \left| \sum_{i=1}^3 \delta(\mathbf{r}_i) \sigma_{zi} \right| \Psi \right\rangle, \quad (5)$$

where $\hbar \sigma_{zi}/2$ is the spin operator of electron i in the z direction, and Ψ is the nonrelativistic wave function of lithium. From Eqs. (2) and (4) we then have

$$f_{\text{expt}} = \frac{2(1 + a_e)}{g_e} C_{\text{rel}} C_M C_R C_{\text{QED}} f_c. \quad (6)$$

It is obvious that if the experimental Fermi contact term is derived from Eq. (2) by use of $g_e = 2$, then f_{expt} should be compared with f_c with the anomalous magnetic moment correction and the others included, whereas if $g_e = 2(1 + a_e)$ is chosen, then the anomalous magnetic moment correction should not be included. In a recent paper, Esquivel, Bunge, and Núñez [18] also discussed the choice of g_e , but evidently they came to the opposite conclusion, thereby omitting the a_e correction in their comparison with experiment. In the present work, we choose the definition of $g_e = 2(1 + a_e)$ in Eq. (2).

TABLE I. Convergence of the nonrelativistic Fermi contact term for the lithium 2^2S and 2^2P states, in atomic units.

No. of terms	2^2S	No. of terms	2^2P
19	2.779 030	20	-0.211 726
50	2.972 074	55	-0.213 876
120	2.931 676	138	-0.213 227
256	2.910 944	306	-0.218 712
502	2.906 045	622	-0.214 937
918	2.906 253	1174	-0.214 947
1589	2.905 981	1715	-0.214 860
∞	2.905 922(50)	∞	-0.214 783(50)

For the case of $^9\text{Be}^+$, the same argument applies except that the nuclear magnetic moment is $\mu_I = -1.177\,432(3)$ [26].

II. VARIATIONAL CALCULATIONS

The variational wave functions used to calculate f_c are constructed from multiple basis sets in Hylleraas coordinates, as described in Ref. [21]. The explicit form for the wave functions is

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \mathcal{A} \sum_t \sum_{\mu_t} a_{t, \mu_t} \phi_{t, \mu_t}(\alpha_t, \beta_t, \gamma_t) \times (\text{angular function}) \times (\text{spin function}), \quad (7)$$

where

$$\phi_{t, \mu_t}(\alpha_t, \beta_t, \gamma_t) = r_1^{j_1} r_2^{j_2} r_3^{j_3} r_{12}^{j_{12}} r_{23}^{j_{23}} r_{31}^{j_{31}} e^{-\alpha_t r_1 - \beta_t r_2 - \gamma_t r_3}, \quad (8)$$

where μ_t denotes a sextuple of integer powers $j_1, j_2, j_3, j_{12}, j_{23}$, and j_{31} , index t labels different sets of nonlinear parameters α_t, β_t , and γ_t , and \mathcal{A} is the three-particle antisymmetrizer. Except for various truncations, all terms are included such that

$$j_1 + j_2 + j_3 + j_{12} + j_{23} + j_{31} \leq \Omega, \quad (9)$$

and the convergence studied as Ω is progressively increased. A complete optimization is then performed with respect to all the nonlinear parameters. These techniques yield much improved convergence relative to single basis set calculations.

Table I contains the convergence studies of Fermi contact terms for both 2^2S and 2^2P states as the size of the basis set progressively increases. Table II presents a comparison of our nonrelativistic results with some selected previous calculations. Table II indicates that the present result for the 2^2S contact term agrees with and improves the best previous value of McKenzie [20]. Furthermore, the Hylleraas-type variational calculations of Larsson [6], King and Shoup [10], and King [11], and the multiconfigurational Hartree-Fock calculations of Sundholm and Olsen [15], Carlsson, Jönsson, and Fischer [16], and Tong, Jönsson, and Fischer [17] agree to about four figures with our result. However, Lindgren's result [9] of many-body perturbation theory and the CI result of Esquivel, Bunge, and Núñez [18] deviate significantly.

TABLE II. Comparison of the nonrelativistic Fermi contact term for the lithium 2^2S and 2^2P states, in atomic units.

Author	Method	Ref.	2^2S	2^2P
Larsson (1968)	100-term Hylleraas	[6]	2.906	
Ahlenius <i>et al.</i> (1973)	78-term Hylleraas	[7]		-0.216 2
Ahlenius <i>et al.</i> (1978)	97-term Hylleraas	[8]		-0.208 6
Lindgren (1985)	MBPT	[9]	2.917 26(5)	-0.2208(1)
King <i>et al.</i> (1986)	352-term Hylleraas	[10]	2.904(2)	
King (1989)	602-term Hylleraas	[11]	2.906 359	
King <i>et al.</i> (1990)	296-term Hylleraas	[12]	2.907 051	
Blundell <i>et al.</i> (1989)	all-order MBPT ^a	[13]	2.9119(4)	
Sundholm <i>et al.</i> (1990)	MCHF	[15]	2.903 9(20)	-0.215 8(15)
Esquivel <i>et al.</i> (1991)	CI	[18]	2.908 56(8)	
McKenzie (1991)	1134-term Hylleraas	[20]	2.906 0(3)	
Carlsson <i>et al.</i> (1992)	MCHF	[16]	2.904 7	-0.215 5
Tong <i>et al.</i> (1993)	MCHF	[17]	2.905 1	-0.217 05
This work			2.905 922(50)	-0.214 783(50)

^aIncludes relativistic wave-function corrections, but not the Breit interaction.

Although Esquivel, Bunge, and Núñez claimed that their contact term converges to a definite value, the convergence may not be complete to the figures they quote. This can be seen, for example, from their convergence study of the matrix element of $\sum_{i=1}^3 1/r_i$. The value they reported is 5.717 929 a.u., whereas the Hylleraas variational value is 5.718 110 883 61(13) [21].

III. SMALL CORRECTIONS

The calculated nonrelativistic value of f_c must be corrected for various effects before it can be compared with experiment, especially for the 2^2S states. These effects include the finite nuclear mass and size corrections, relativistic corrections, and quantum electrodynamic (QED) corrections.

A. Finite nuclear mass correction

The finite nuclear mass correction should include both the mass scaling and mass polarization contributions, the latter

being neglected in most previous calculations. In fact, the mass polarization term often tends to cancel the mass scaling correction. The mass scaling correction for ^7Li can be obtained simply by multiplying the calculated value by a factor

$$(1 + m_e/M)^{-3} = 0.999\,7654,$$

where m_e is the electron mass and M is the nuclear mass. The mass polarization correction can be taken into account by including $-(\mu/M)\sum_{i<j}\nabla_i\cdot\nabla_j$ explicitly in the Hamiltonian, where $\mu = m_e M/(m_e + M)$ is the reduced mass. The wave function thus obtained is used to calculate the contact term once again, from which the mass polarization contribution can be extracted by subtraction. The results are listed in Table III. Although the mass polarization correction turns out to be small for 2^2S states, it is the dominant source of uncertainty in the variational results. For the 2^2P state, it is 3 times larger in magnitude than the mass scaling term and of opposite sign. The effect is unusually large for 2^2P states

TABLE III. Comparison of theoretical and experimental Fermi contact terms for the Li 2^2S , 2^2P , and 3^2S states and for the Be^+ 2^2S state, expressed in atomic units.

Contribution	Li 2^2S	Li 2^2P	Li 3^2S	Be^+ 2^2S
Nonrelativistic	2.905 922(50)	-0.214 783(50)	0.673 405(50)	12.497 57(30)
Mass scaling	-0.000 682	0.000 050	-0.000 158	-0.002 28
Mass polarization	0.000 027(71)	-0.000 159(71)	0.000 007(71)	0.000 07(42)
Relativistic	0.002 49(18)	-0.000 105 ^a	0.000 577(43)	0.019 9(11)
Nuclear size	-0.001 082(94)		-0.000 251(20)	-0.006 18(19)
QED	-0.000 918(47)		-0.000 213(11)	-0.005 29(34)
Total	2.905 75(22)	-0.214 997(71)	0.673 368(86)	12.503 8(12)
Experiment	2.906 023(3) ^b	-0.213 5(10) ^c	0.684 8(16) ^d	12.503 528(33) ^e
Difference	-0.000 27(22)	-0.001 5(10)	-0.011 4(16)	0.000 3(12)

^aCombined relativistic and nuclear size correction from Ref. [9].

^bReference [2].

^cReference [3].

^dReference [4].

^eReference [5].

because the mass polarization correction to the wave function does not vanish in a Hartree-Fock approximation.

B. Relativistic corrections

Accurate calculations of the correction factors C_{rel} , C_R , and C_{QED} are not available. The aim of this and the following subsections is to show that reasonable estimates of these terms can account for the differences between theory and experiment. In considering the various contributions, it is important to remember that in a Hartree-Fock approximation, f_c comes entirely from the outer ns electron since the contributions from the $1s^2\ ^1S$ core electrons cancel. In this regard, the corrections are quite different from those for excited states of Li^+ where the unpaired $1s$ electron gives the dominant contribution [27].

As first discussed by Breit [28], the one-electron relativistic correction to f_c comes from the replacement

$$|\psi(0)|^2 \rightarrow \frac{1}{\alpha a_0 \pi} \int_0^\infty g_{ns}(r) \frac{1}{r^2} f_{ns}(r) r^2 dr, \quad (10)$$

where $a_0 = \hbar^2/m_e e^2$ is the Bohr radius, and $g_{ns}(r)$ and $f_{ns}(r)$ are the large and small radial components of the Dirac wave function for an ns electron. Breit obtained results for $n=1$ and 2. We have extended his results to arbitrary n to obtain

$$|\psi(0)|^2 \rightarrow \frac{Z^3}{\pi a_0^3 n^3} \left[1 + \left(\frac{9n + 11n^2 - 11}{6n^2} \right) (\alpha Z)^2 + O(\alpha^4 Z^4) \right]. \quad (11)$$

For $n=1$ and 2, this reproduces the known Breit correction coefficients $3/2$ and $17/8$, and for $n=3$ the coefficient is $115/54$. The coefficient of the next term of $O(\alpha^4 Z^4)$ works out to be [29]

$$\frac{189 - 330n - 134n^2 + 225n^3 + 203n^4}{72n^4}. \quad (12)$$

The values for $n=1, 2,$ and 3 are $17/8, 449/128,$ and $2279/648,$ respectively. The $2s-1s$ difference of $177/128$ is close to, but not quite the same as, the value $179/128$ quoted by Prior and Wang [30].

Knowledge of the general n dependence contained in Eq. (11) may help in identifying an equivalent operator whose matrix elements with respect to nonrelativistic wave functions would yield the same result. Such an operator could then be used to calculate the relativistic correction starting from the nonrelativistic wave function for a many-electron atom. However, this is an interesting problem, which to our knowledge has not been solved. In the absence of better estimates, we take the relativistic correction factor to be

$$C_{\text{rel}} = 1 + \left(\frac{9n + 11n^2 - 11}{6n^2} \right) (\alpha Z^*)^2, \quad (13)$$

where $Z^* = Z - \sigma$ is an effective screened nuclear charge for a single ns electron. One would expect σ to be small because the effect comes primarily from the region near the nucleus. The choice $\sigma = 0.25 \pm 0.10$ gives a relativistic correction of 855 ± 63 ppm for $\text{Li}(2^2S)$, in reasonable accord

with the range of values 775–1080 ppm obtained by Lindgren and Rosén [31] from Hartree-Fock calculations, depending on the model chosen. In the absence of better calculations, we use the same value of σ to extrapolate to $\text{Li}(3^2S)$ and to $\text{Be}^+(2^2S)$. The results are listed in Table III. The smaller correction of ~ 560 ppm adopted by Lindgren [9] and by Mårtensson-Pendrill and Yennerman [14] includes also the finite nuclear size correction discussed in the next section.

C. Finite nuclear size corrections

For a one-electron ion, the finite nuclear size correction is simply the Zemach correction [32],

$$C_R = 1 - 2Z \langle R_{\text{em}} \rangle / a_0, \quad (14)$$

where $\langle R_{\text{em}} \rangle$ is an average electromagnetic charge radius for the nucleus obtained by folding together the electric charge and magnetization densities. The result depends somewhat on the model chosen for the two distributions. If R_e and R_m denote the rms radii for the electric and magnetic distributions, respectively, then for an exponential $e^{-\Lambda r}$ distribution with $R_e = R_m$,

$$\langle R_{\text{em}} \rangle = 35R_e / (16\sqrt{3}). \quad (15)$$

The multiplying factor of $35/(16\sqrt{3}) \approx 1.263$ substantially enhances the effect relative to the point magnetic dipole case for which $R_m = 0$ and $\langle R_{\text{em}} \rangle = R_e$. For a Gaussian charge distribution, the multiplying factor would be $4/\sqrt{3\pi}$ in place of $35/(16\sqrt{3})$. This comparison illustrates the degree of sensitivity on the assumed form of the nuclear charge distribution. Models that incorporate a more detailed account of nuclear spin structure are discussed by Shabaev [33].

There is considerable spread in the values of R_e and R_m tabulated by de Jager, de Vries, and de Vries [34], particularly for R_m . The average values are $R_e = 2.40$ fm and $R_m = 2.80$ fm for ^7Li , and $R_e = 2.51$ fm and $R_m = 2.67$ fm for ^9Be . We take the averages of these, i.e., $\bar{R} = 2.60 \pm 0.20$ for ^7Li and $\bar{R} = 2.59 \pm 0.08$ for ^9Be to calculate $\langle R_{\text{em}} \rangle$ from Eq. (15). The results are listed in Table III. The finite nuclear size calculation done by Lindgren [9] corresponds to the choice $\langle R_{\text{em}} \rangle = R_e$ for the case of pointlike nuclear moments. If the resulting correction of -272 ppm for $\text{Li}(2^2S)$ is added to the relativistic correction of 855 ppm from Sec. III B, the total of 583 ppm agrees with the total calculated by Lindgren [9] (i.e., 0.0011 a.u. with his definition of f_c). However, his calculation does not include the magnetic moment distribution represented by the Zemach effect.

D. Quantum electrodynamic corrections

The largest QED correction is the free-electron anomalous magnetic moment factor $(1 + a_e)$ in Eq. (6). Beyond this are the binding energy corrections contained in C_{QED} . In a one-electron approximation, they are given for the $2s$ state by

$$C_{\text{QED}} = 1 + \alpha(Z\alpha)(\ln 2 - \frac{5}{2}) - \frac{\alpha(Z\alpha)^2}{\pi} \left[\frac{8}{3} \ln^2(Z\alpha) + 1.1675 \ln(Z\alpha) - 9.83 \pm 0.29 \right]. \quad (16)$$

The above is obtained by adding the $1s$ shift [35] to the $2s - 1s$ difference quoted by Prior and Wang [30]. The leading terms of order $\alpha(Z\alpha)$ and $\alpha(Z\alpha)^2 \ln^2(Z\alpha)$ are state independent-correction factors multiplying the Fermi contact term. They therefore apply to any state, and in particular to each term in the linear combination of hydrogenic Slater determinants describing lithium. For this reason, it is appropriate to take Z to be the full nuclear charge, at least for these leading terms. The same reasoning leads to the state-independent part of the Lamb shift derived by Kabir and Salpeter [36] for helium, and verified to high precision [37]. The remaining terms are state dependent, but their contribution is small. Equation (16) should therefore provide a reasonably good account of the QED correction, with the entire state-dependent part taken as the uncertainty. The results are listed in Table III.

IV. DISCUSSION

Despite the approximate nature of the correction factors C_{rel} , C_R , and C_{QED} discussed in Sec. III, the results in Table III indicate that they all have about the same magnitude, and all must be included in a comparison with experiment. It is noteworthy that there is substantial cancellation among the various corrections. The agreement with the measurement of Beckmann, Böklen, and Elke [2] for $\text{Li}(2^2S)$ is somewhat outside the range of uncertainty when the various contributions are added in quadrature, but not when the uncertainties are added linearly. The greatest source of error comes from the relativistic correction. The agreement with the measurement of Wineland, Bollinger, and Itano [5] for $\text{Be}^+(2^2S)$ is as good as can be expected. Here, the one-electron approximations used for the small corrections should be more reliable. There is also good agreement with the measurement of

Orth, Ackermann, and Otten [3] for the $\text{Li}(2^2P)$ state, but here the corresponding corrections are much smaller, and the experimental accuracy is not sufficient to be sensitive to them. However, there is a large discrepancy of $-0.0114(16)$ between theory and experiment for the $\text{Li } 3^2S$ state. This is clearly larger than what could be explained by any reasonable adjustment of the relativistic, nuclear size, and QED correction factors.

Further improvements are possible for the calculation of the nonrelativistic f_c . A global operator equivalent of $\delta(\mathbf{r}_i)$, which samples the wave function over all space, would undoubtedly yield better convergence. The Hiller-Sucher-Feinberg operator [38], which has been used in helium calculations [39], could be extended to the lithium case. This has not yet been done because the calculation of more highly singular operators in Hylleraas coordinates is required. There is a need for further developments in techniques for evaluating these more highly singular integrals.

In summary, we have calculated the Fermi contact term for the $\text{Li } 2^2S$, 2^2P , and 3^2S states and the $\text{Be}^+ 2^2S$ state, using high-precision variational wave functions in Hylleraas coordinates. We have shown that reasonable estimates of the relativistic, finite nuclear size, and QED corrections give acceptable agreement with experiment for the 2^2S states of Li and Be^+ , but there is a significant discrepancy for the $\text{Li } 3^2S$ state. The high precision that is now available for the basic nonrelativistic part of f_c makes it worthwhile to consider more sophisticated calculations of the various small corrections. This would be straightforward for the finite nuclear size effect, but advances in theory are required in order to find appropriate operators for the relativistic and QED corrections. Once these problems are solved, the comparison with experiment could be interpreted as a probe of nuclear structure. This remains a challenge for the future.

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