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Predicted energy shifts for “paronic” helium

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It has been shown recently that one can construct a local relativistic quantum field theory which admits small violations of the Pauli exclusion principle by introducing “paronic” states which obey para-Fermi statistics of order 2. Paronic shifts are calculated for the low-lying states of helium to aid in the design of experiments either to detect paronic helium, or place upper limits on its possible existence.

Greenberg and Mohapatra¹ have recently argued that one can construct a local relativistic quantum field theory which admits a small violation of the Pauli exclusion principle. Their construction derives from a model of a single oscillator² which mainly obeys Fermi statistics, but which allows double occupancy with a small amplitude β . Such a state obeys para-Fermi statistics of order 2 such that when two fermions are brought together, there is a probability $\beta^2/2$ that they will form a doubly occupied (symmetric) state. Following Greenberg *et al.*,¹ the term *paronic* will be used to denote such states.

A serious objection to these proposals is raised in an earlier paper by Govorkov³ which shows that paronic states as constructed above generate a Hilbert space with negative norm. However, since other mechanisms may still exist for producing the same phenomenology,⁴ it remains of interest to look for evidence for paronic states in the spectra of atoms and molecules.

Kelleher *et al.*⁵ have recently proposed an experiment involving the excitation spectrum of helium which would be sensitive to the presence of paronic states. The experiment would place an upper limit on possible violations of the Pauli exclusion principle much lower than the relatively weak value $\beta^2/2 \leq 10^{-7}$ which can be inferred from existing spectra.⁵ The purpose of this paper is to present theoretical values for the transition frequencies of paronic helium on which the experiment is based.

In the nonrelativistic *LS* coupling approximation, the wave functions for paronic helium are identical to those for normal helium except that the singlet and triplet spin functions are interchanged so as to form a totally *symmetric* wave function. The nonrelativistic energies are

therefore identical, but there are small paronic shifts relative to normal helium of order α^2 from the spin-dependent terms in the Breit interaction, and of order α^3 and higher from the anomalous magnetic moment and other quantum electrodynamic corrections. The relationship between the energy levels of normal helium and paronic helium is shown in Fig. 1.

The energy levels of normal helium are well known

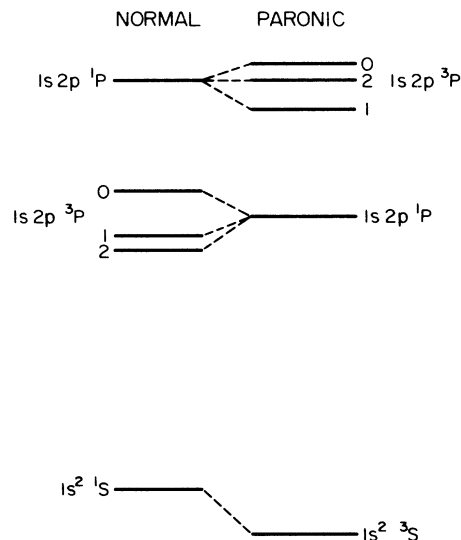


FIG. 1. Schematic diagram showing the paronic helium states relative to the normal helium reference states.

from Martin's⁶ tabulations of experimental data, and high-precision theoretical calculations.⁷⁻¹² The terms included in the present work are

$$E = E_{\text{NR}} + \langle B_p \rangle + \Delta E_{\text{RR}} + \Delta E_{\text{QED}}, \quad (1)$$

where E_{NR} is the nonrelativistic energy (including first- and second-order mass-polarization corrections), B_p is the Pauli form of the Breit interaction, ΔE_{RR} are relativistic reduced-mass corrections of $O(\alpha^2\mu/M)$, and ΔE_{QED} are quantum electrodynamic corrections of $O(\alpha^3)$.

The results are expressed in terms of the shift of the paronic state relative to the normal state of opposite spin; i.e., with singlet and triplet states interchanged. Specifically, the paronic shift is defined to be

$$\Delta E(nLSJ) = E(nLSJ)_{\text{paronic}} - E(nL\tilde{S}\tilde{J})_{\text{normal}}, \quad (2)$$

with

$$\tilde{S} = S \pm 1,$$

$$\tilde{J} = \begin{cases} L & \text{for } L \geq 1 \\ \tilde{S} & \text{for } L = 0. \end{cases}$$

The nonrelativistic energy in Eq. (1) then cancels, and only the spin-dependent parts of the remainder survive. The $O(\alpha^2)$ terms are¹³

$$B_p = H_3 + H_5, \quad (3)$$

with

$$H_3 = H_{\text{SO}} + H_{\text{SOO}}, \quad (4)$$

$$H_5 = -\frac{8\pi}{3} \left(\frac{e}{mc} \right)^2 \mathbf{s}_1 \cdot \mathbf{s}_2 \delta(\mathbf{r}_{12}) + H_{\text{SS}}. \quad (5)$$

In the above H_{SO} and H_{SOO} are the usual spin-orbit and spin-other-orbit interactions, and H_{SS} is the rank-2 spin-spin interaction. The remaining small corrections in Eq. (1) can be written in the form^{10,11,14}

$$\Delta E_{\text{RR}} = (\Delta E_{\text{RR}})_M + (\Delta E_{\text{RR}})_X, \quad (6)$$

with

$$(\Delta E_{\text{RR}})_M = \Delta_1 - (2m/M)[\langle H_{\text{SOO}} \rangle + \langle H_5 \rangle], \quad (7)$$

$$\Delta_1 = \sum_{\substack{k,l \\ k \neq l}} \left[\frac{Ze^2}{mMc^2 r_k^3} \right] \mathbf{r}_k \times \mathbf{p}_l \cdot \mathbf{s}_k,$$

and

$$\Delta E_{\text{QED}} = (\alpha/\pi)(\langle H_{\text{SO}} \rangle + \frac{2}{3}\langle H_{\text{SOO}} \rangle + \langle H_5 \rangle). \quad (8)$$

The terms in $(\Delta E_{\text{RR}})_M$ correspond to using the reduced-mass Rydberg $R_M = (1 - \mu/M)R_\infty$ in converting the B_p matrix elements from a.u. to cm^{-1} . The remaining part $(\Delta E_{\text{RR}})_X$ is the second-order cross term of $O(\alpha^2\mu/M)$ resulting from using mass-polarization-corrected wave functions in evaluating matrix elements of B_p . The matrix elements are listed in Table I in terms of the infinite nuclear-mass part $\langle T_0 \rangle$ and a finite-mass correction $(\mu/M)\langle T_1 \rangle$. Finally, the terms in ΔE_{QED} are the spin-dependent anomalous magnetic-moment corrections.

The matrix elements were evaluated with correlated variational wave functions in Hylleraas coordinates, using the double basis set method described previously¹⁰⁻¹² together with a complete optimization of the nonlinear parameters. The uncertainties in the matrix elements in Table I represent the degree of convergence obtained with basis sets containing up to 840 terms.

For S states, all of the terms in Eqs. (3), (6), and (8) vanish except for the $\delta(\mathbf{r}_{12})$ contact term in (5). Using

$$\langle \mathbf{s}_1 \cdot \mathbf{s}_2 \rangle = \frac{1}{2}[S(S+1) - \frac{3}{2}], \quad (9)$$

the 3S -state paronic shift is

$$\Delta E = -\frac{8\pi}{3}(1 - 2m/M) \left[1 + \frac{\alpha}{\pi} \right] \alpha^2 \langle \delta(\mathbf{r}_{12}) \rangle \quad (10)$$

in units of $2R_M$ with

$$R_M = 109\,722.2735 \text{ cm}^{-1}.$$

This gives the shift of the triplet paronic S state relative to the normal singlet state. The shift is zero for the singlet paronic S state.

TABLE I. Values of matrix elements (in a.u.) required for the calculation of paronic energy shifts in helium. For ^4He , $\mu/M = 1.3\,707\,456 \times 10^{-4}$. Numbers in parentheses denote errors.

Paronic state	$\langle \delta(\mathbf{r}_{12}) \rangle$	$\langle \ H_{\text{SO}}\ \rangle^2$	$\langle \ H_{\text{SOO}}\ \rangle^2$	$\langle \ H_{\text{SS}}\ \rangle^2$	$\langle \ \Delta_1\ \rangle / (\alpha^2 m/M)$
1^3S	0.334 093 86(4) -0.038 707 μ/M	0	0	0	0
2^3S	0.027 169 90(3) -0.005 553 3 μ/M	0	0	0	0
2^3P	0.002 309 601(1) -0.010 853 μ/M	0.115 001 314 57(1) -0.318 14 μ/M	-0.084 605 704 4(1) -0.008 84 μ/M	-0.083 009 487(2) +0.138 85 μ/M	0.200 710 7(1)
2^3P-^1P	0	0.107 319 480 7(3) -0.054 970 μ/M	0.038 762 042 24(2) -0.032 041 μ/M	0	-0.076 465 28(2)
3^3P	0.000 791 739(1) -0.003 317 μ/M	0.031 481 175(3) -0.090 28 μ/M	-0.021 518 850(5) -0.010 89 μ/M	-0.231 993 74(2) +0.032 50 μ/M	0.069 095 2(3)
3^3P-^1P	0	0.031 488 222(1) -0.022 263 μ/M	0.010 777 285(2) -0.010 64 μ/M	0	-0.021 455 01(3)

TABLE II. Calculated shifts of the paronic helium states, relative to the normal helium reference states (in cm^{-1}) as defined by Eq. (2).

Paronic state	Normal reference state	Paronic shift
$1s^2\ ^3S_1$	$1s^2\ ^1S_0$	-10.4322
$1s2s\ ^3S_1$	$1s2s\ ^1S_0$	-0.8484
$1s2s\ ^1S_0$	$1s2s\ ^3S_1$	0
$1s2p\ ^3P_2$	$1s2p\ ^1P_1$	0.0196
$1s2p\ ^3P_1$	$1s2p\ ^1P_1$	-0.2935
$1s2p\ ^3P_0$	$1s2p\ ^1P_1$	0.1328
$1s2p\ ^1P_1$	$1s2p\ ^3P_1$	0.0672
$1s3p\ ^3P_2$	$1s3p\ ^1P_1$	0.00905
$1s3p\ ^3P_1$	$1s3p\ ^1P_1$	-0.09473
$1s3p\ ^3P_0$	$1s3p\ ^1P_1$	0.01627
$1s3p\ ^1P_1$	$1s3p\ ^3P_1$	0.01783

The situation is more complicated for the 3P paronic states because the matrix elements of H_{SO} , H_{SOO} , and H_{SS} must be recomputed using the spacially symmetric $1snp$ nonrelativistic wave functions in place of the antisymmetric ones. The results are listed in Table I in terms of the reduced matrix elements

$$\langle \gamma' L' S' J M | H_{SO} | \gamma L S J M \rangle \\ = (-1)^{L+S'+J} \begin{Bmatrix} J & S' & L' \\ 1 & L & S \end{Bmatrix} \langle \gamma' L' S' | H_{SO} | \gamma L S \rangle,$$

and

$$\langle \gamma' L' S' J M | H_{SS} | \gamma L S J M \rangle \\ = (-1)^{L+S'+J} \begin{Bmatrix} J & S' & L' \\ 2 & L & S \end{Bmatrix} \langle \gamma' L' S' | H_{SS} | \gamma L S \rangle. \quad (12)$$

For the diagonal elements, the multiplying factors are $-\frac{1}{3}$, $-\frac{1}{6}$, and $\frac{1}{6}$ in Eq. (11), and $\frac{1}{3}$, $-\frac{1}{6}$, and $\frac{1}{30}$ in Eq. (12) for 3P_J states with $J=0, 1,$ and 2 , respectively. For the off-diagonal elements of Eq. (11) with $S'=1, S=0$, and $J=1$ the factor is $\frac{1}{3}$. The final eigenvalues for the 3P_1 and 1P_1 states include the singlet-triplet mixing correction.

Table II lists the paronic shifts for the low-lying S and P states of helium. The uncertainty is estimated to be $\pm 0.2(\alpha Z)^4 = \pm 0.002 \text{ cm}^{-1}$ from uncalculated terms of this order. The largest effect is clearly a downward shift of 10.4322 cm^{-1} for the $1s^2\ ^3S_1$ ground state. For the excited states, it is interesting that the ordering of the 3P_J states has changed. Whereas the normal states are completely inverted with $E_0 > E_1 > E_2$, the paronic states are ordered according to $E_0 > E_2 > E_1$. The actual transition frequencies can easily be obtained by adding the difference of the paronic shifts to the known transition frequencies⁶ for the normal reference states of opposite spin. For example, the predicted $1^3S_1 - 2^3P_1$ transition frequency for paronic helium of $(171\,145.14 \pm 0.15) \text{ cm}^{-1}$ is obtained by adding the paronic shift of $(-0.2935 + 10.4322) \text{ cm}^{-1} = 10.1387 \text{ cm}^{-1}$ (see Table II) to the experimental $1^1S_0 - 2^1P_1$ transition frequency for normal helium⁶ of $(171\,135.00 \pm 0.15) \text{ cm}^{-1}$. The calculated shift is much more accurate than the $\pm 0.15\text{-cm}^{-1}$ experimental uncertainty in the ground-state energy.

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