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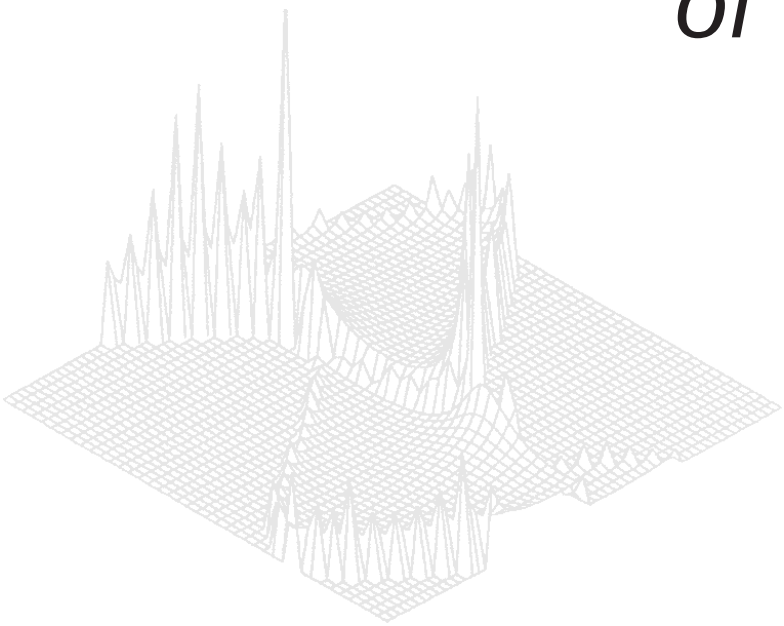
Australian Journal of Physics

Volume 53, 2000



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Aust. J. Phys., 2000, **53**, 631–640

Position Indeterminacy

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Abstract

Calculations assuming position indeterminacy in the Dirac equation are reported. Energy shift contributions for low-lying states of hydrogen-like atoms are calculated by treating the position indeterminacy as a perturbation additional to standard quantum mechanics. The results are consistent with the current discrepancy between theory and experiment for Lamb shifts in hydrogen, deuterium and the helium ion.

1. Introduction

As is well known, Heisenberg considered the possibility of a fundamental length (Carazza and Kragh 1995). The mathematically significant feature of such a concept is the replacement of the previous differential equations of quantum mechanics with difference equations. The present work examines the related concept of position indeterminacy. Specifically, the results of calculations on the Lamb shifts of hydrogen-like atoms, resulting from introducing position indeterminacy in the Dirac equation, are reported.

An expression for position indeterminacy is obtained (see the Appendix) by imposing a maximal acceleration in the dynamics of the uncertainty relations. Maximal acceleration is a concept previously introduced by Caianiello (1981, 1984). The following relation for the position indeterminacy length is obtained:

$$\delta = \hbar c \Delta E / 2E_0^{\,2} \quad . \tag{1}$$

A consequence of this indeterminacy is to impose a limit to which the precision of the quantum particle position can be determined. Mathematically, the consequence of position indeterminacy is similar to that of a fundamental length, in that the finite difference operator replaces the differential operator in quantum mechanics. The momentum operator is then a difference operator. Using basic definitions of the difference and differential operators, restricted to one dimension, the following series relation is obtained:

$$p_i\Psi = -i\hbar\Delta\Psi = -i\hbar(\partial/\partial x_i + \delta\,\partial^2/\partial x_i^{\,2}/2 + \delta^2\partial^3/\partial x_i^{\,3}/6 + \ldots)\Psi \,, \tag{2}$$

where Δ and $\partial/\partial x_i$ have the usual definitions. Terms of increasing order in δ give position indeterminacy contributions additional to standard quantum mechanics. Consistency with standard theory is nevertheless maintained. The standard momentum operator is the zero order term of this series. Further, since the position indeterminacy length is small, terms of higher order in δ will only contribute as perturbations on standard quantum mechanics.

With standard treatments of the momentum operator (Dirac 1958; Landau and Lifshitz 1977), the right operator is obtained before taking the differential limit. Other definitions

 10.1071/PH99076 0004-9506/00/050631$05.00

of the difference operator could be considered; however, with these initial calculations consistency with the standard definition is used. The Dirac equation should then be a second order difference equation. Such equations maintain the basic quantum mechanical requirements of real eigenvalues and orthonormal eigenfunctions.

2. Calculations

The momentum difference operator yields a perturbation series to increasing order of δ in the Dirac Hamiltonian as

$$H' = -i\hbar c \Sigma \alpha_I \, (\delta \, \partial^2/\partial x_i^{\,2}/2 + \delta^2 \partial^3/\partial x_i^{\,3}/6 + \ldots) \, , \;\; i = x,y,z \, , \tag{3}$$

where α_i are the usual Dirac matrices, and the summation is over coordinate directions. Standard perturbation theory (Roman 1965) is then used to obtain the energy shift contributions for low-lying states of hydrogen-like atoms. While the first order operator in (3) is not hermitian conjugate, the unitarity of the *S*-matrix is preserved as this operator gives zero in first order.

First and second order terms used in these perturbation calculations follow from the definition of the *T*-matrix (Roman 1965) as

$$T_{ii} = \; \langle i \, | H' \, | \, i \, \rangle + \; \Sigma \; T_I T^*_I / (E_i - E_I) \, . \tag{4}$$

In obtaining this expression, the hermiticity of the perturbation Hamiltonian is not explicitly used. Rather, the orthonormality of the full wavefunctions is used via the use of the closure relation. Since the full wavefunctions are solutions of second order difference equations, orthonormality and hence closure, are maintained. Iterating gives to second order

$$T_{ii} = \langle i|H'|i\rangle + \Sigma \, |\langle i|H'|I\rangle|^2/(E_i - E_I). \tag{5}$$

Summation, in the second term, is over intermediate states. The normalisation constant in the *T* matrix for discrete states is approximately unity. This is due to the smallness of the position indeterminacy as a perturbation.

From second order quasi-degenerate perturbation (Corson 1951), at the lowest order term in (3), the energy shift corrections for the $n = 2$ states (i.e. $2S_{1/2}$, $2P_{1/2}$, $2P_{3/2}$) are calculated. The perturbation series given by (3) is additional to standard quantum mechanics, which includes QED. It is then appropriate to assume that for these calculations the degeneracy of the $2S_{1/2}$, $2P_{1/2}$ states (which is present in the Dirac equation) is previously removed. Since contributions arising from (3) are much smaller than QED contributions, this assumption in the order of perturbation is acceptable.

A question arises on the choice of wavefunctions. The $2S_{1/2}$, $2P_{1/2}$ wavefunctions used in this perturbation should then be the Dirac functions modified by QED as a first perturbation. However, it is readily seen that the degree of mixing is small. This is due to the $2S_{1/2}$ QED energy shift, of order 1040 MHz, being much greater than the $2P_{1/2}$, which is of order 12 MHz. Hence, the wavefunctions used here are just the Dirac functions. This approximation is appropriate in obtaining leading term contributions arising from (3).

Further approximations are also used. The relativistic components of the Dirac wavefunctions (Rose 1961) are taken to first order in $Z\alpha$, introducing a low Z approximation. Also, for second order perturbation, given by equation (5), leading contributions

Table 1. Radial functions

$N = (Z/2a_0)^{3/2}e^{-\rho/2}$ and $\rho = Zr/a_0$, where a_0 is the Bohr radius

State	Nonrelativistic component	Relativistic component
$2S_{1/2}$	$N(2-\rho)$	$-N(Z\alpha/4)(4-\rho)$
$2P_{1/2}$	$-(N/\sqrt{3})\rho$	$-(N/\sqrt{3})(Z\alpha/4)(2-\rho/3)$
$2P_{3/2}$	$(N/\sqrt{3})\rho$	$-(N/\sqrt{3})\,(Z\alpha 4)\rho$

arise from intermediate states within the same principal quantum number. This is due to the energy separation in the denominator being several orders of magnitude smaller for such states. Hence, calculations are restricted to intermediate states within the same principal quantum number. With leading term approximations discussed above, the radial functions are given in Table 1. Angular and spin components are as referenced in Rose (1961).

For the ground state, contributions arising from second order perturbation at the first order term in (3) are several orders of magnitude smaller than for the $n = 2$ states. This is due to the energy separation, in the denominator of the second order perturbation term, being of the order of electron-volts for the ground state, compared with the much smaller fine structure and Lamb shift energy separations of the $n = 2$ states. The leading term contribution for the ground state is found to come from the second term in (3) at first order perturbation. This results in a different Z dependence for leading term contributions for $n = 1$ (Z^8) and $n = 2$ (Z^{10}) levels.

The remaining unknown is the energy uncertainty. We assume this to be the root mean square excitation energy calculated from standard quantum mechanics (Bethe and Salpeter 1957) which gives $\Delta E_{\rm rms} = pZ^2$ Ry, where Ry is the Rydberg energy and p is a number dependent on the principal and angular momentum quantum numbers. For the $1S_{1/2}$, $2S_{1/2}$ and the 2P states, p^2 is calculated to be 1.33, 0.238 and 0.033 respectively. The resulting expressions for the energy shifts are

$$\begin{aligned}
\Delta E(1S_{1/2}) &= (-)\, p^2 Z^8 \alpha^6 \mathrm{Ry}/320\,, \\
\Delta E(2S_{1/2}) &= p^2 Z^{10} \alpha^6 \mathrm{Ry}^2 [1.0/\Delta E_1 - 5.0/3\Delta E_2]/80^2\,, \\
\Delta E(2P_{1/2}) &= (-) p^2 Z^{10} \alpha^6 \mathrm{Ry}^2 (1.0/\Delta E_1)/80^2\,, \\
\Delta E(2P_{3/2}) &= p^2 Z^{10} \alpha^6 \mathrm{Ry}^2/(80^2 \Delta E_2)\,,
\end{aligned} \tag{6}$$

where ΔE_1 is the classic Lamb shift and ΔE_2 is the $2P_{3/2}$–$2S_{1/2}$ energy separation.

Two features are experimentally significant. The high Z dependence ensures increasing magnitudes of these contributions with increasing atomic number. Further, the $2S_{1/2}$–$2P_{1/2}$ contribution is much larger than the ground state. Effectively, the Z dependence for $n = 2$ level reduces to approximately Z^6 due to an approximate Z^4 dependence in the energy separations in the denominator of (6).

These energy contributions then introduce an approximate $(Z\alpha)^6$ term in the classic Lamb shift contributions of low Z hydrogen-like atoms. This is of the same magnitude as the accuracy of current QED theory and experiment for Lamb shifts, thereby enabling direct comparison with experiment. Energy expressions given in (6) were also obtained with standard perturbation in the Pauli approximation. The $2S_{1/2}$, $2P_{1/2}$ degeneracy is

Table 2. $2S_{1/2}$–$2P_{1/2}$ Lamb shifts

Ion	Experiment	Theory (QED)	Position indeterminacy contribution
H	1057845(9) kHz [a]	1057829(4)(4) kHz [b]	13 kHz
	1057851.6 (2.1) [b]	1057825(6) [d]	
	1057844.6 (2.9) [c]	1057830(6) [d]	
D	1059233.7(2.9) [c]	1059210(7) [e]	
He	14042.52 (16) MHz [f]	14040.98(18) MHz [d]	1.0 MHZ
Li	62765 (21) MHz [g]	62737 (6) MHz [h]	13 MHz
O	2192 (15) GHz [h]	2196.14 (21) GHz [h]	6.9 GHz
	2215.6 (7.5) GHz [h]		
	2202.7 (11.0) GHz [h]		

[a] Lundeen and Pipkin (1981) [b] Eides *et al.* (1995) [c] Schwob *et al.* (1999)
[d] Mallampalli and Sapirstein (1998) [e] de Beauvoir *et al.* (1997)
[f] van Wijngaarden *et al.* (1991) [g] Leventhal (1975) [h] Drake *et al.* (1988)

Table 3. Hydrogen ground state Lamb shift

Experiment	Theory (QED)	Position indeterminacy contribution to experiment
8172837(22) kHz [a]	8172731(40) kHz [b]	(−)31 kHz
8172874(60) kHz [c]	8172691(40) kHz [b]	(−)40 kHz
8172798(46) kHz [d]		(−)32 kHz
8172827(51) kHz [e]		(−)40 kHz
		(Subtract from experiment)

[a] Schwob *et al.* (1999) [b] Mallampalli and Sapirstein (1998) [c] Weilz *et al.* (1995)
[d] Bourzeix *et al.* (1996) [e] Berkeland *et al.* (1995)

again assumed to be removed by QED. The Pauli approximation is more useful for future investigations in atomic helium and positronium.

Using current values for the fine structure and the Rydberg constants, the energy shift contributions are calculated for the above equations. All results are summarised in Tables 2 and 3. Comparison is shown with QED theory and experiment.

3. Experimental Comparison

For the classic Lamb shift, position indeterminacy contributions of 13 kHz and 1 MHz are predicted for hydrogen and the helium ion respectively. A discrepancy of this magnitude currently exists between QED theory and experiment. With QED theory two-loop Lamb shift calculations are incomplete. However, the current discrepancy would not be removed by QED unless remaining terms show striking nonperturbative behaviour (Mallampalli and Sapirstein 1998). More recent calculations (Goidenko *et al.* 1999) for $Z > 3$ show the results are consistent with the perturbation theory expansion. Suggesting a non-perturbative behaviour is unlikely to remove the current discrepancy.

The $2S_{1/2}$–$2P_{3/2}$ hydrogen separation lacks the precision of the classic Lamb shift, the experimental value being 9911.200(12) MHz (Hagley and Pipkin 1994). A theoretical value can be inferred by subtracting the recent classic Lamb shift evaluation of Mallampalli

and Sapirstein (1998) from the well-known $2P_{1/2}$–$2P_{3/2}$ shift of 10969.0394(2) MHz, giving a derived value of 9911.209 MHz. The position indeterminacy contribution reduces the theoretical value by 7 kHz. This contribution is smaller than the experimental uncertainty; however, a better centring between theory and experiment is obtained.

For the hydrogen ground state Lamb shift the situation is most interesting. Position indeterminacy predicts a negligible discrepancy at the current experimental precision. However, the ground state Lamb shift is obtained experimentally by transitions involving several levels, thereby introducing the Lamb shifts of such levels. For example, with the most recent and precise value (Schwob *et al.* 1999), the ground state Lamb shift is determined from a set of simultaneous equations involving the experimentally obtained 1S–2S and 2S–8D, 2S–12D transition frequencies. If the position indeterminacy discrepancies for the $2S_{1/2}$, $2P_{1/2}$ levels are included the experimental ground state Lamb shift is reduced by 32 kHz, greatly improving agreement with theory. Similar calculations with other recently obtained ground state Lamb shifts are given in Table 3. Improved agreement with theory is highlighted in all these various values.

An interesting inferred ground state QED value can be obtained from the following calculations. Since the $2P_{1/2}$ and $L' = L_{1S}–8L_{2S}$ QED Lamb shifts are known to high precision [i.e. −12835.99(8) kHz and −187.226(5) MHz receptively], an inferred QED ground state shift, (i.e. L_{1S}) can then be obtained. Using the most recent experimental classic Lamb shift an inferred ground shift of 8172.843 MHz is obtained. This value is about 100 kHz larger than current QED theory. However, if the discrepancy predicted here is included, the QED ground state Lamb shift would be predicted to be 8172.739 MHz. This results shows greater consistency, to within uncertainties, with current values.

For the hydrogen ground state and classic Lamb shift, discussion of possible sources of discrepancy between experiment and QED theory has focused on nuclear-dependent corrections, specifically the size of the proton radius. A detailed review of more usual proton radius determinations is available (Karshenboim 1999). The widely used value of 0.862(12) fm leads to the QED discrepancy quoted above.

A proton radius determination can also be made by assuming the completeness of QED theory, and then extracting a value from the experimental data. A value of 0.890(14) fm is thus obtained (Udem *et al.* 1997) from experimental ground state Lamb shift values. The procedure is to subtract from the experimental ground state Lamb shift all QED theory excluding the nuclear-dependent term. The proton radius is then obtained from

$$aR^2_{QED} = L_{EXP} - L_{QED}\,, \tag{7}$$

where aR^2_{QED} is the nuclear-dependent term (Karshenboim 1999), and L_{EXP}, L_{QED} are the experimental and theory ground state Lamb shifts. As discussed above, position indeterminacy reduces the experimental Lamb shift, thereby modifying the QED derived proton radius. This gives a modified value of

$$R^2_{MOD} = R^2_{QED} - \gamma/a\,, \tag{8}$$

where γ/a is the position indeterminacy contribution. For the Udem *et al.* and Schwob *et al.* experimental procedure this term equals 0.0202 fm^2. As will be seen, the modified value is sensitive to the precision of both the experimental and QED theory Lamb shift. For the Udem *et al.* data a modified proton radius of 0.878(14) fm is obtained. For the more recent and precise experimental value (Schwob *et al.* 1999), and again using the

QED value of Mallampalli and Sapirstein (1998), a QED proton radius of 0.900 fm is obtained. The modified value is 0.889 fm, which is slightly outside the range of uncertainties with the non-QED proton radius of 0.862(12) fm.

However, the more recent theoretical QED (Goidenko *et al.* 1999) suggests that in the low Z region the Mallampalli and Sapirstein (1998) contribution of −71 kHz is overestimated by more than 50%. Neglecting this contribution gives a QED radius of 0.875 fm and a modified value of 0.862 fm. At 50% contribution, the modified proton radius becomes 0.876 fm. Both modified values remove the discrepancy between the QED and non-QED proton radius to within the uncertainty in theory and experiment.

As this paper was in preparation, Melnikov *et al.* (2000) reported a new theoretical ground state Lamb shift of 8172778(16)(32) kHz, using the usual 0.862(12) fm proton radius. Agreement with experiment is obtained using a reanalysed larger proton radius of 0.877(24) fm. Alternatively, they obtain a QED extracted proton radius of 0.883(14) fm, which is not consistent with the usual non-QED value. For the Melnikov *et al.* extracted value, position indeterminacy contributions give a modified proton radius of 0.871 fm. This value is consistent with both the usual non-QED, as well as the reanalysed value quoted by Melnikov *et al.* Incorporating the position indeterminacy contributions introduced here maintains consistency between theory and experiment, to within current uncertainties, for all the various proton radius values used.

Using the method outlined above, the classic Lamb shift can be calculated from the Melnikov *et al.* ground state value. Agreement with experiment again requires a larger value of the proton radius. Alternatively, new contributions of the same magnitude as that presented here need to be considered.

For the He^+ ion, the discussion on the discrepancy focuses on a possible experimental uncertainty (van Wijngaarden *et al.* 1998). Work on a repeat measurement is apparently in progress. Attention is drawn to the concluding sentence of the van Wijngaarden *et al.* paper, namely, that 'some additional contribution that scales as Z^6 is required to account for the discrepancy in He^+'.

A discrepancy between theory and experiment also currently exists with the hyperfine splitting of positronium and the decay of ortho-positronium (Czarnecki *et al.* 1999*a*, 1999*b*). The experimental situation for the latter is at present unclear. Possible position indeterminacy contributions for orthopositronium decay are given in an accompanying paper (Ruzzene 2000; present issue, see p. 641).

For the Li and O ions, position indeterminacy contributions of 13 MHz and 6.9 GHz are predicted. Current precision in theory and experiment neither confirm nor negate such contributions. However, the largeness of these values suggests that these ions are suitable for further study.

For the higher Z region, experimental values lack sufficient precision to test possible position indeterminacy contributions. For hydrogen-like nickel ($Z = 28$) the ground state Lamb shift is 5.07(10) and 5.096(4) eV for experiment and theory respectively. Position indeterminacy gives a contribution of −0.003 eV to the theory value. Since the experimental value is obtained from the 2P–1S transition, position indeterminacy contributions will also affect the value measured via the 2P state. However, such contributions are small compared with the present experimental uncertainty.

4. Conclusion

Although the basic concept of position indeterminacy is clearly speculative, the actual calculations are not. All terms have been calculated using only standard quantum mech-

anics. Furthermore, there is no free parametrisation to set the overall magnitude, which is determined by the size of the position indeterminacy.

This work does not introduce radical new thought. Heisenberg did consider the related idea of a fundamental length, including the use of difference equations, to address the formal singularities of QED.

These calculations show that position indeterminacy can be expressed mathematically while still maintaining consistency with standard quantum mechanics, yet be testable against current developments in theory and experiment.

This work has deliberately refrained from exploring the philosophical implications of the concept of position indeterminacy on deeper questions on the physical meaning of quantum mechanics. Nevertheless, the expression for position indeterminacy has been obtained from an operational analysis of the uncertainty principle. Hence, these calculations are open to whatever interpretations of the uncertainty principle are available.

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Appendix

The concept of a maximal acceleration has been introduced as

$$A_{max} = 2m_0c^3/\hbar \ . \tag{9}$$

A maximal acceleration implies, from the basic definition of impulse, a maximal change in momentum as

$$\Delta p_{max} = (2m_0{}^2c^3/\hbar)\Delta t^1 \ , \tag{10}$$

where Δt^1 is the time duration of the impact. Classical thinking underlies both (9) and (10). Their relevance to quantum mechanics could be considered conceptually ambiguous. However, the uncertainty principle has its physical justification in operational analysis of various physical systems. Basic classical principles are used throughout the analysis (see de Broglie 1990 and Bohm 1951). The uncertainty relations

$$\delta x \ \delta p \geq \beta\hbar, \ \ \delta t \Delta E \geq \beta\hbar \tag{11}$$

are well known. These are not the generalised relations (where the uncertainties are defined as standard deviations). Ambiguity exists for the lower bound, which is set at β. The quantities in (11) are interpreted operationally as a consequence of 'measuring', in principle, the position and momentum of the quantum particle. 'Measuring' the position and momentum, will determine the position by up to δx, and the momentum by up to δp, thereby introducing uncertainties of δx and δp. The energy–time uncertainty is interpreted, somewhat differently, as the time elapsed δt required to 'observe' an energy change ΔE. At a shorter time interval, the uncertainty in energy would be greater than the energy changed. In this case it would not be possible to know that the energy has actually changed. Analysis of the electron–photon interaction introduces several constraints on these inequalities. The minimum possible uncertainty in position is required. Accordingly, the change in momentum resulting from 'measurement' is set at the maximal momentum change given by (10). The most accurate 'measurement' of position is then $\delta = \beta\hbar/\Delta p_{max}$. Likewise, the minimum time elapsed 'measurable' for the electron to change in energy by ΔE is $\delta t = \beta\hbar/\Delta E$. However, this is also the smallest time elapsed 'measurable' to ensure that the interaction with the photon has actually occurred. The time elapsed for the impulse in (10) can only be 'known' to δt, so $\Delta t^1 = \delta t$. Substituting we will get relation (1). The lower bound factor β cancels.

Alternatively, the same expression can be obtained without direct use of maximal acceleration. In general, the transfer of energy per unit time is, by definition, given by $\Delta E/\Delta t$. Using the energy–time uncertainty relation at the minimum time, leading to a maximum in the energy transfer per unit time, gives $(\Delta E)^2\, 2/\hbar$. For a particle with rest energy E_0, the maximum energy change possible (i.e. a total transfer) is $\Delta E = E_0$. This gives an expression for the maximum possible energy transfer per unit time as $E_0^2 2/\hbar$. Returning to the particle–quanta interaction, with an energy change ΔE, and assuming that the energy transfer occurs at the maximum possible rate per unit time, then $\Delta E/\Delta t = E_0^2 2/\hbar$. Using $\delta = c\Delta t$, as discussed, yields relation (1). Since the maximal acceleration is readily obtained from the maximum energy transfer per unit time, the different approaches are related.

The electron is 'viewed' as interacting with virtual photons via the Coulomb field and self-interaction. Since the electron can only have energies equal to the energy of the different states, its energy can only change by amounts equal to the energy difference between states. The energy chang ΔE in (1) is then identified as the energy separation between states.

The mean value of ΔE is then the mean excitation energy. This is calculated with the same underlying assumptions used by Bethe in the initial Lamb shift calculation (Bethe 1947). The significance of (1) for the electron–photon interaction is that a space separation δ is required for the process to occur. It cannot be considered a point interaction.

Position indeterminacy results from imposing upper limits to either the change in momentum, or the energy transfer per unit time. As such no additional dynamics are introduced to the uncertainty principle. This has an important consequence. Position indeterminacy does not require altering the Dirac equation to include dynamics additional to standard quantum mechanics. These calculations thereby differ from calculations introducing maximal acceleration directly into the Dirac equation (Lambiase *et al.* 1997).

For the uncertainty principle, operational analysis focuses on conceptual questions of 'measurability' of, for example, position. With this analysis, there is a slight difference. The physical basis of (1) is the particle–quanta interaction. The consequence of (1) is that, in the presence of interaction, the particle position is 'measurable' only to a precision of δ in space separation. For the electron this distinction is only conceptual since interaction is always present, even as self-interaction. Popper (1985) took the realist view that the uncertainty relations are scatter relations expressing limits on the scatter of particles. Further realist thinking has explored the possibility that quantum mechanics is based on self-interaction (Hestendes 1985).

According to the uncertainty principle, position and momentum cannot be precisely determined simultaneously. However, each can be precisely determined individually. Position indeterminacy imposes a limit to the determined position of a quantum particle even individually. If the quantum mechanically defined position of a particle is imprecisely defined, then a precise knowledge of position cannot be included in the wavefunction. The wavefunction is likewise undefined within a minimum length.

Position indeterminacy, as expressed by relation (1), is a quantum mechanical feature arising from the uncertainty relations. Hence it affects the quantum mechanical wavefunction but does not impose a discreteness on the structure of space. The concept is thereby different from that of a fundamental length.

For the atomic electron, Welton (1948) showed that the Lamb shift could be attributed to fluctuations in the electron position due to zero point variation in the radiation field.

Such a fluctuation in the electron position differs from the concept of position indeterminacy.

For the hydrogen electron in the ground state, rms fluctuations in position per Bohr radius are obtained from the Welton (1948) expression as $6\alpha^{3/2}$, where the Bethe upper and lower energy cut-offs are used. Position indeterminacy per Bohr radius at the hydrogen ground state goes as $\alpha^3/4$, which is some four orders of magnitude smaller.

The Welton expression describes fluctuations in position due to the electron experiencing a force. Position indeterminacy imposes a limit to which the quantum mechanical position can be determined. Indeed fluctuations in the electron position as described by Welton can only be determined to a precision given by the position indeterminacy.

Manuscript received 24 August 1999, accepted 3 May 2000