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1982 J. Phys. A: Math. Gen. 15 L155

(http://iopscience.iop.org/0305-4470/15/4/002)

J. Phys. A: Math. Gen. **15** (1982) L155–L159. Printed in Great Britain

LETTER TO THE EDITOR

Ground-state logarithmic perturbation theory applied to the Klein–Gordon equation†

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Received 4 January 1982

Abstract. Three-dimensional ground-state logarithmic perturbation theory in non relativistic quantum mechanics is applied to the Klein–Gordon equation. The problem of the π-mesic atoms in an external multiple field is treated in this framework.

A logarithmic perturbation theory for a discrete spectrum in non-relativistic quantum mechanics has recently been developed by Dolgov and Popov (1978, 1979) and Aharonov and Au (1979). In particular, Au and Aharonov (1979) have shown that the ground-state logarithmic perturbation theory can be extended to the three-dimensional problems. Using this technique, they have calculated the first-order correction to the wavefunction and the second-order energy shift for a hydrogen atom in an external multiple field (Dalgarno and Lewis 1955, Bell 1967), and established the connection with Sternheimer's method (1951) and the method of Dalgarno and Lewis (1955).

It is the purpose of this letter to point out that the three-dimensional logarithmic perturbation theory can be extended to a relativistic case in which the Klein–Gordon equation is used. We will use this technique to establish the connection with Sternheimer's method in the Klein–Gordon equation. We will also calculate the second-order energy shift for a π-mesic atom (Corinaldesi and Strocchi 1963) in a $2l$th-order multiple field of the form $V_1 = Q_l r^{l+\varepsilon} P_l(\cos\theta)$, where Q_l is the strength of the multiple field and ε is a relativistic correction factor to be determined.

The Klein–Gordon equation in units $\hbar = e = m = 1$ can be written as (Schiff 1968)

$$(-\nabla^2 + c^2)\psi(r) = c^2(E - V)^2\psi(r), \tag{1}$$

where the potential is most generally given in terms of the perturbation parameter λ

$$V(r) = \sum_{i=0}^{\infty} V_i \lambda^i = V_0 + \lambda V_1 + \lambda^2 V_2 + \ldots . \tag{2}$$

We only consider ground states in which the wavefunction $\psi(r)$ can be put in the form (Au and Aharonov 1979)

$$\psi(r) = \exp[-G(r)]. \tag{3}$$

† Work supported in part by the Natural Sciences and Engineering Research Council of Canada.

Writing that

$$\boldsymbol{g}(\boldsymbol{r}) = \nabla G(\boldsymbol{r}), \tag{4}$$

the Klein–Gordon equation (1) becomes

$$\nabla \cdot \boldsymbol{g} - \boldsymbol{g}^2 = c^{-2}(E - V)^2 - c^2. \tag{5}$$

We assume here that the energy E and the functions $G(\boldsymbol{r})$ and $\boldsymbol{g}(\boldsymbol{r})$ can be expanded as power series of λ,

$$G = \sum_{i=1}^{\infty} G_i \lambda^i = G_0 + \lambda G_1 + \lambda^2 G_2 + \ldots, \tag{6}$$

$$\boldsymbol{g} = \sum_{i=1}^{\infty} \boldsymbol{g}_i \lambda^i = \boldsymbol{g}_0 + \lambda \boldsymbol{g}_1 + \lambda^2 \boldsymbol{g}_2 + \ldots, \tag{7}$$

$$E = \sum_{i=1}^{\infty} E_i \lambda^i = E_0 + \lambda E_1 + \lambda^2 E_2 + \ldots, \tag{8}$$

where E_0 is the unperturbed eigenenergy, and the unperturbed wavefunction ψ_0 is related to G_0 by

$$\psi_0 = \exp(-G_0). \tag{9}$$

If we compare the coefficients of various powers of λ in equation (5), we obtain the following set of differential equations for $\boldsymbol{g}_i$:

$$\nabla \cdot \boldsymbol{g}_0 - \boldsymbol{g}_0^2 = c^{-2}(E_0 - V_0)^2 - c^2, \tag{10}$$

$$\nabla \cdot \boldsymbol{g}_1 - 2\boldsymbol{g}_0 \cdot \boldsymbol{g}_1 = (2/c^2)(E_0 - V_0)(E_1 - V_1), \tag{11}$$

$$\nabla \cdot \boldsymbol{g}_2 - 2\boldsymbol{g}_0 \cdot \boldsymbol{g}_2 = (2/c^2)(E_0 - V_2) + \boldsymbol{g}_1 \cdot \boldsymbol{g}_1 + c^2(E_1 - V_1)^2, \tag{12}$$

$$\begin{aligned} &\nabla \cdot \boldsymbol{g}_i - 2\boldsymbol{g}_0 \cdot \boldsymbol{g}_i \\ &= \frac{2}{c^2}(E_0 - V_0)(E_i - V_i) + \sum_{j=1}^{i-1} \boldsymbol{g}_j \cdot \boldsymbol{g}_{i-j} \\ &\quad + \frac{1}{c^2} \sum_{j=1}^{i-1} (E_j - V_j)(E_{i-j} - V_{i-j}), \qquad i > 1, \end{aligned} \tag{13}$$

where the unperturbed Klein–Gordon equation (11) is assumed to have exact solutions. We see from equations (12)–(13) that they all have the same structure and may be able to be solved in the same manner. It is observed (Aharonov and Au 1979) that the square of the unperturbed wavefunction

$$\rho = \psi_0^2 = \exp(-2G_0) \tag{14}$$

constitutes an integrating factor for equations (12)–(13). Multiplying equation (12) by the integrating factor and integrating over all space, we obtain

$$\frac{2}{c^2} \int (E_0 - V_0)(E_1 - V_1)\rho \, \mathrm{d}^3 r = \int \nabla \cdot (\boldsymbol{g}_1 \, \mathrm{e}^{-2G_0}) \, \mathrm{d}^3 r = 0. \tag{15}$$

From equation (15), we find for the first-order energy coefficient E_1

$$E_1 = \frac{1}{N} \int V_1 (E_0 - V_0)\rho \, \mathrm{d}^3 r, \tag{16}$$

where the normalisation factor is $N=\int (E_0-V_0)\rho\, \mathrm{d}^3r$. In a similar manner, the ith-order energy coefficient E_i can be found as

$$E_i=\frac{1}{N}\Big(\int V_i(E_0-V_0)\rho\, \mathrm{d}^3r-\frac{c^2}{2}\sum_{j=1}^{i-1}\int \boldsymbol{g}_j\cdot\boldsymbol{g}_{i-j}\rho\, \mathrm{d}^3r-\frac{1}{2}\sum_{j=1}^{i-1}\int (E_j-V_j)(E_{i-j}-V_{i-j})\rho\, \mathrm{d}^3r\Big). \tag{17}$$

We note here that, in the non-relativistic limit $c\to\infty$, equations (16) and (17) reduce to the results obtained by Au and Aharonov (1979).

By following the same procedure as done for the Schrödinger equation by Au and Aharonov (1979), we establish the connection with Sternheimer's method (1951) in the Klein–Gordon equation. From equation (3), we obtain for the first-order correction to the wavefunction

$$\psi_1=-G_1\,\mathrm{e}^{-G_0}=-G_1\psi_0. \tag{18}$$

Taking the Laplacian of ψ_1, we find

$$\nabla^2\psi_1=-\nabla^2(G_1\,\mathrm{e}^{-G_0})=\psi_1[\nabla^2G_0-(\nabla G_0)^2]-\psi_0(\nabla^2G_1-2\nabla G_0\cdot\nabla G_1). \tag{19}$$

With the aid of equations (11) and (12), equation (19) can be rewritten as

$$-[\nabla^2+(1/c^2)(E_0-V_0)^2-c^2]\psi_1=(2/c^2)(E_0-V_0)(E_1-V_1)\psi_0. \tag{20}$$

Equation (20) is the Sternheimer equation, when the Klein–Gordon equation is used instead of the Schrödinger equation. Using the same argument, we can obtain, from equation (13), the following generalised Sternheimer equation:

$$-\Big(\nabla^2+\frac{1}{c^2}(E_0-V_0)^2-c^2\Big)G_i\psi_0 =\Big(\frac{2}{c^2}(E_0-V_0)(E_i-V_i)+\sum_{j=1}^{i-1}\boldsymbol{g}_j\cdot\boldsymbol{g}_{i-j}+\frac{1}{c^2}\sum_{j=1}^{i-1}(E_j-V_j)(E_{i-j}-V_{i-j})\Big)\psi_0, \tag{21}$$

where V_i is the ith-order potential coefficient in λ. Because of the vector nature of $\boldsymbol{g}_i=\nabla G_i$ in the three-dimensional problems, equations (20) and (21) may not be easily solved.

As one application of the above relativistic perturbation theory, we calculate the first-order correction to the wavefunction and the second-order energy shift of a π-mesic atom (Corinaldesi and Strocci 1963) in an external multiple field. This problem in the non-relativistic case has been treated by Dalgarno and Lewis (1955) and Bell (1967). It is also discussed by Au and Aharonov (1979) in the framework of the logarithmic perturbation theory. The perturbation interaction V_1 for a π-mesic atom in a $2l$th-order multiple field should be written as

$$V_1=Q_lr^{l+\varepsilon}P_l(\cos\theta), \tag{22}$$

where Q_l is the strength of the interaction, and ε is a relativistic correction factor to be determined from equation (12). Under this perturbation, equation (22) becomes

$$\nabla^2G_1-2\nabla G_0\cdot\nabla G_1=-(2/c^2)(E_0/c+\gamma/r)Q_lr^{l+\varepsilon}P_l(\cos\theta), \tag{23}$$

where $\gamma=Z/c$, Z is the charge of the nucleus, and the unperturbed value E_0 for the ground state is given by (Schiff 1968)

$$E_0=\frac{c^2}{[1+\gamma^2/(s+1)^2]^{1/2}}, \qquad s=-\tfrac{1}{2}+(\tfrac{1}{4}-\gamma^2)^{1/2}. \tag{24}$$

For a π-mesic atom with nuclear charge Z in the ground state, the function G_0 is given by (Schiff 1968)

$$G_0 = \frac{Z}{[(s+1)^2+\gamma^2]^{1/2}} r - s \ln r + \text{constant} = br - s \ln r + \text{constant} \tag{25}$$

where $b = Z/[(s+1)^2+\gamma^2]^{1/2}$. The gradient of G_0 is then

$$\nabla G_0 = (b - s/r)\boldsymbol{i}_r. \tag{26}$$

We see from equation (23) that $G_1(r)$ must take the form

$$G_1(r) = R(r)P_l(\cos\theta) = (u(r)/r)P_l(\cos\theta). \tag{27}$$

Substituting equations (26) and (27) into (23), we obtain the following inhomogeneous equation for $u(r)$:

$$\frac{d^2u}{dr^2} - 2(br-s)\frac{d}{dr}\left(\frac{u}{r}\right) - \frac{l(l+1)}{r^2}u = -\frac{2E_0Q_l}{c^2}r^{l+1+\varepsilon} - \frac{2\gamma Q_l}{c}r^{l+\varepsilon}. \tag{28}$$

As $\gamma \to 0$ in the non-relativistic limit, equation (28) reduces to the known non-relativistic equation (Au and Aharonov 1979).

The particular solution for equation (28) can be written as

$$u(r) = Q_l(d_1 r^{l+1+\varepsilon} + d_2 r^{l+2+\varepsilon}). \tag{29}$$

Inserting equation (29) into equation (28), we find

$$\varepsilon = -(l+s+\tfrac{1}{2}) + [(l+s+\tfrac{1}{2})^2 - 2sl]^{1/2},$$

$$d_1 = \frac{E_0(l+s+\varepsilon+1) + Zb(l+\varepsilon+1)}{c^2b^2(l+\varepsilon+1)(l+\varepsilon)}, \qquad d_2 = \frac{E_0}{c^2b(l+\varepsilon+1)}, \tag{30}$$

where E_0 and s are defined by equation (24), and b by equation (25). If we set $\gamma = 0$, equation (30) reduces to the non-relativistic result: $\varepsilon = 0$, $d_1 = 1/l$ and $d_2 = 1/(l+1)$ (Au and Aharonov 1979). From equations (29) and (30), the first-order correction to the wavefunction is then given by

$$\psi_1 = -G_1 e^{-G_0} = -(1/N_1)(d_1 r^{l+1+s+\varepsilon} + d_2 r^{l+2+s+\varepsilon}) e^{-br}, \tag{31}$$

where $N_1 = [4\pi(2+2s)!/(2b)^{3+2s}]^{1/2}$ is the normalisation factor for the unperturbed wavefunction ψ_0. With the known value of G_1, we can then calculate the second-order energy shift with the aid of equation (17). After a lengthy calculation, we obtain finally for E_2

$$E_2 = -\frac{Q_l^2(2l+2s+2\varepsilon+2)!}{2(2l+1)(2b)^{2l+2\varepsilon}}\left(\frac{2b^2d_1^2[(l+\varepsilon)^2+l(l+1)]}{(l+s+\varepsilon+1)(2l+2s+2\varepsilon+1)}\right.$$
$$+\frac{2bd_1d_2[(l+\varepsilon)(l+\varepsilon+1)+l(l+1)]}{l+s+\varepsilon+1}$$
$$\left.+d_2^2[(l+\varepsilon+1)^2+l(l+1)]+\frac{1}{c^2}\right)\left(\frac{E_0}{c^2}(2+2s)!+\frac{2\gamma b}{c}(1+2s)!\right)^{-1}. \tag{32}$$

Equation (32), in the non-relativistic limit, yields the well known result for a hydrogen atom in the multiple field (Dalgarno and Lewis 1955, Bell 1967, Au 1978, Au and

Aharonov 1979):

$$E_2 = -Q_l^2[(2+2)!(l+2)/l(l+1)2^{2l+2}]. \tag{33}$$

We note here that, in using the Klein–Gordon equation to solve the problem of a π-mesic atom in a $2l$th-order multiple field, the perturbation V_1 must be written in the form given by equation (22). If we set the relativistic correction factor ε to be zero, we cannot find any solution for G_1 in analytic form. It is evident from the above calculation that the same procedure can be used to calculate the higher-order energy shifts.

In conclusion, we have extended the three-dimensional non-relativistic logarithmic perturbation theory to the relativistic case in which the Klein–Gordon equation is used. We have derived the generalised Sternheimer equations resulting from the Klein–Gordon equation. We have then calculated the second-order energy shift of a π-mesic atom in a $2l$th-order multiple field and found that the perturbation contains a relativistic correction factor in the form $V_1 = Q_l r^{l+\varepsilon} P_l(\cos\theta)$.

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