S-Matrix Formalism for Level-Shift Calculations*

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An exact formula for the level shift is given in terms of the adiabatic S-matrix constructed from the perturbation which produces the shift. The formula is used to discuss the role of the subsidiary condition in quantum electrodynamic level-shift calculations.

INTRODUCTION

LET $|\alpha\rangle$ be an eigenstate of a zero-order Hamiltonian H_0, $|\beta\rangle$ that eigenstate of a perturbed Hamiltonian $H=H_0+gH_1$ into which $|\alpha\rangle$ goes as g, the coupling constant, increases from zero. Thus

$$H_0|\alpha\rangle=E_0|\alpha\rangle, \quad H|\beta\rangle=E|\beta\rangle, \quad \lim_{g\to 0}|\beta\rangle=|\alpha\rangle. \tag{1}$$

With now standard techniques it may be shown[1] that the level shift $\Delta E=E-E_0$ is given by

$$\Delta E=\lim_{\epsilon\to 0}\left(\mp i\epsilon g\frac{\partial}{\partial g}\ln\langle\alpha|U(0,\pm\infty;\epsilon)|\alpha\rangle\right), \tag{2$\pm$}$$

where

$$U(t_1,t_2;\epsilon)=P\left[\exp\left(-i\int_{t_1}^{t_2}e^{iH_0t}gH_1e^{-iH_0t-\epsilon|t|}dt\right)\right] \tag{3}$$

is the so-called "adiabatic" U matrix. (P represents Dyson's chronological operator.) We wish to point out that Eq. (2) may be replaced by the more symmetrical formula

$$\Delta E=\lim_{\epsilon\to 0}\left(\tfrac{1}{2}i\epsilon g\frac{\partial}{\partial g}\ln\langle\alpha|U(\infty,-\infty;\epsilon)|\alpha\rangle\right), \tag{4}$$

which provides a direct connection between the level shift and the adiabatic S matrix

$$S_\epsilon=U(\infty,-\infty;\epsilon). \tag{5}$$

The great advantage of Eq. (4) over Eq. (2$\pm$) is that, for the case of interacting fields, the former allows the use of Feynman's covariant techniques whereas the latter does not, there being no energy conservation at a vertex.

Equation (4) provides an elementary derivation of methods used in the calculation of the second- and fourth-order radiative corrections[2] to the energy levels of hydrogen, no prescriptions about oscillating terms at infinity being necessary. It shows how, in principle, such calculations may be extended to all orders in the coupling constant, in a covariant way.

A simple proof of Eq. (4) is given in Sec. I. In Sec. II, Eq. (4) is applied to a discussion of the role of the Fermi subsidiary condition,

$$(\partial A_u/\partial x_u)|\psi\rangle=0, \tag{F}$$

in the calculation of level shifts in quantum electrodynamics.

I. PROOF OF EQUATION (4)

Direct calculation shows that[3]

$$(H-E_0)U(0,\pm\infty;\epsilon)|\alpha\rangle=\mp i\epsilon g\frac{\partial}{\partial g}U(0,\pm\infty;\epsilon)|\alpha\rangle. \tag{6$\pm$}$$

Multiplication of Eq. (6$-$) by $\langle\beta|$, defined by Eq. (1), gives

$$\Delta E=i\epsilon g\langle\beta|U(0,-\infty;\epsilon)|\alpha\rangle^{-1}\times\left\langle\beta\left|\frac{\partial}{\partial g}U(0,-\infty;\epsilon)\right|\alpha\right\rangle. \tag{7}$$

Now $|\beta\rangle$ may be constructed from $|\alpha\rangle$ by a limit process[3]

$$|\beta\rangle=\lim_{\delta\to 0}\left(\frac{U(0,\pm\infty;\delta)|\alpha\rangle}{\langle\alpha|U(0,\pm\infty;\delta)|\alpha\rangle}\right). \tag{8$\pm$}$$

Insertion of $|\beta\rangle$ in the form given by Eq. (8+) into Eq. (7) gives

$$\Delta E=\lim_{\delta\to 0}F(\delta,\epsilon), \tag{9}$$

where

$$F(\delta,\epsilon)=i\epsilon g\langle\alpha|U(\infty,0;\delta)U(0,-\infty;\epsilon)|\alpha\rangle^{-1}\times\left\langle\alpha|U(\infty,0;\delta)\frac{\partial}{\partial g}U(0,-\infty;\epsilon)|\alpha\right\rangle. \tag{10}$$

Here use has been made of

$$U^\dagger(0,+\infty;\epsilon)=U(\infty,0;\epsilon). \tag{11}$$

Equation (9) implies

$$\Delta E=\lim_{\epsilon\to 0}[\lim_{\delta\to 0}F(\delta,\epsilon)]. \tag{12}$$

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[1] See, e.g., Bryce S. De Witt, University of California Radiation Laboratory Report UCRL-2884 (unpublished), Eq. 6.24.

[2] See R. Mills and N. M. Kroll, Phys. Rev. 98, 1489 (1955), and references cited therein.

[3] M. Gell-Mann and F. Low, Phys. Rev. 84, 350 (1951), Appendix, or reference 1.

With perhaps the exception of unphysical cases, the path of approach to the point (0,0) of the (δ,ϵ) plane used in Eq. (12) can be deformed to the path $\delta=\epsilon$ without changing the result. Thus we find

$$\Delta E=\lim_{\epsilon\to 0}F(\epsilon,\epsilon), \tag{13}$$

or

$$\Delta E=\lim_{\epsilon\to 0}i\epsilon g\langle\alpha|U(\infty,-\infty;\epsilon)|\alpha\rangle^{-1} \times\left\langle\alpha\left|U(\infty,0;\epsilon)\frac{\partial}{\partial g}U(0,-\infty;\epsilon)\right|\alpha\right\rangle, \tag{14-}$$

using the group property of $U(t_1,t_2;\epsilon)$.

Multiplication of the Hermitian conjugate of Eq. (6+) by $|\beta\rangle$, in the form of Eq. (8−), yields, as above,

$$\Delta E=\lim_{\epsilon\to 0}i\epsilon g\langle\alpha|U(\infty,-\infty;\epsilon)|\alpha\rangle^{-1} \times\left\langle\alpha\left|\left[\frac{\partial}{\partial g}U(\infty,0;\epsilon)\right]U(0,-\infty;\epsilon)\right|\alpha\right\rangle. \tag{14+}$$

The addition of Eqs. (14−) and (14+) results in

$$\Delta E=\lim_{\epsilon\to 0}\left(\tfrac{1}{2}i\epsilon g\langle\alpha|S_\epsilon|\alpha\rangle^{-1}\times\left\langle\alpha\left|\frac{\partial}{\partial g}S_\epsilon\right|\alpha\right\rangle\right), \tag{15}$$

which is just the statement of Eq. (4).

II. ROLE OF THE SUBSIDIARY CONDITION IN LEVEL-SHIFT CALCULATIONS

The problem of the subsidiary condition (F) in the calculation of level-shifts does not appear to have been discussed in the literature—it has generally been assumed that (F) can be ignored. As is well known, this is the case for scattering problems. In the calculation of the second-order radiative corrections to the hydrogenic energy levels, it can be seen by direct computation that (F) can be ignored.[4] Equation (4) now shows in a simple way that this holds to all orders in the coupling constant. For, $\langle\alpha|S_\epsilon|\alpha\rangle$ is computed as the "forward scattering amplitude" of the Dirac state $|\alpha\rangle$ by the operator S_ϵ, constructed in the bound interaction representation. This operator differs from the usual S operator only in that the electron propagator is $(\not{p}-\not{V}-m)^{-1}$ instead of $(\not{p}-m)^{-1}$. Since correspondingly, $(\not{p}-\not{V}-m)|\alpha\rangle=0$, Feynman's proof[5] of the ignorability of (F) for scattering problems can be taken over almost word for word, if his "$\not{p}$" is everywhere replaced by "$\not{p}-\not{V}$."

Similar considerations hold for more complex problems. Equation (4) could be used as the starting point of a calculation of the energy levels of a two-electron atom with large Z, the electrons not interacting in lowest approximation, and the covariant gauge could be employed profitably. However, one could also use Coulomb gauge for the photon lines representing electron-electron interaction and covariant gauge for the self-energy lines, just as in the corresponding scattering problem, Eq. (4) making the analogy between these complete. For $Z=2$ this point becomes important, for it shows that in the corresponding Bethe-Salpeter equation[6] the gauges may be mixed in this manner. Such a possibility is essential if the difficulties of renormalization in the Coulomb gauge are to be avoided, but a rapidly convergent perturbation method[6] for the solution of such an equation is to be developed. Mixed gauges have been used by Fulton and Martin in their treatment of positronium,[7] without, however, any discussion. The above argument, although not directly applicable to their case without modification, serves to justify such a mixing in the case of positronium also.

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[4] W. Heitler, *The Quantum Theory of Radiation* (Clarendon Press, Oxford, 1954), third edition, Sec. 34.

[5] R. P. Feynman, Phys. Rev. **76**, 769 (1949), Sec. 8.

[6] J. Sucher and H. M. Foley (to be published).

[7] T. Fulton and P. Martin, Phys. Rev. **95**, 811 (1954).