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1979 J. Phys. A: Math. Gen. 12 1321

(http://iopscience.iop.org/0305-4470/12/8/024)

J. Phys. A: Math. Gen., Vol. 12, No. 8, 1979. Printed in Great Britain

Energy shifts and the S matrix in degenerate perturbation theory

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Received 15 November 1978

Abstract. Adiabatic perturbation theory is employed to establish a relationship between the S matrix and the averaged energy shift of a degenerate level.

Field-theoretical methods have proved extremely useful in perturbation theory for stationary energy–eigenvalue problems. In particular, a simple connection between the energy shift and the scattering matrix in the Feynman formalism has been applied before to lowest-order processes; such a connection may already be understood heuristically on the basis of the Born approximation (e.g. Akhiezer and Berestetskii 1953). A general relationship has been obtained by Rodberg (1958), who used a linked-cluster expansion and showed how the energy shift of a non-degenerate state then follows from the connected part of the S matrix (see also Michels and Suttorp 1978).

The linked-cluster expansion in fact relies upon the choice of the non-degenerate unperturbed state as a new vacuum state; consequently Rodberg's treatment cannot be applied in degenerate perturbation theory. Yet a generalisation of his final result does exist for the averaged energy shift of a degenerate level, as we shall prove now along different lines.

We study a time-independent Hamiltonian H that is the sum of an unperturbed part H_0 and a perturbation $H_1 = \lambda V$. Let E_0 be a degenerate eigenvalue in the discrete part of the spectrum of H_0, and let $|\psi_\alpha\rangle$ be normalised eigenstates of H with eigenvalues $E_\alpha = E_0 + \Delta E_\alpha$ that reduce to E_0 for λ tending to zero. Since $\lambda \mathrm{d}H/\mathrm{d}\lambda = H_1$ and $\lambda \mathrm{d}/\mathrm{d}\lambda \langle\psi_\alpha|\psi_\alpha\rangle = 0$ we may write for the energy shifts ΔE_α:

$$\lambda(\mathrm{d}/\mathrm{d}\lambda)\Delta E_\alpha = \lambda(\mathrm{d}/\mathrm{d}\lambda)\langle\psi_\alpha|H - E_0|\psi_\alpha\rangle = \langle\psi_\alpha|H_1|\psi_\alpha\rangle \tag{1}$$

(cf. Pines 1961) and hence for the average $\overline{\Delta E}$ of these energy shifts:

$$\lambda(\mathrm{d}/\mathrm{d}\lambda)\overline{\Delta E}\,\mathrm{Tr}\,P = \mathrm{Tr}(H_1 P), \tag{2}$$

with $P = \Sigma_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$ the projector onto the subspace of perturbed eigenstates.

Starting from the identity (2) we shall derive the connection between $\overline{\Delta E}$ and the S matrix. To that end we go over to the time-dependent interaction representation; moreover the perturbation is switched on adiabatically, so that it takes the form:

$$H_{1\epsilon}(t) = \lambda_\epsilon(t)\exp(\mathrm{i}H_0 t)V\exp(-\mathrm{i}H_0 t), \qquad \lambda_\epsilon(t) = \lambda\exp(-\epsilon|t|). \tag{3}$$

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0305-4470/79/081321+03$01.00

The time dependence of the perturbed system is governed by the unitary evolution operator $U_\epsilon(t, t')$, which satisfies the differential equation

$$\mathrm{i}(\partial/\partial t)U_\epsilon(t, t') = H_{1\epsilon}(t)U_\epsilon(t, t'), \qquad U_\epsilon(t, t) = 1. \tag{4}$$

In terms of this operator one can prove the following relation between the projector P and the corresponding projector P_0 of the unperturbed level (Dmitriev 1975):

$$P = \lim_{\epsilon \to 0} U_\epsilon(0, \pm\infty)P_0U_\epsilon(\pm\infty, 0). \tag{5}$$

If the perturbation is sufficiently small the operations PP_0 and P_0P constitute a non-singular linear mapping between the perturbed and the unperturbed states. Consequently we may write the projector P as:

$$P = P_-P_0(P_0P_+P_-P_0)^{-1}P_0P_+, \tag{6}$$

with $P_\pm = P$ given by (5). Upon substituting (6) with (5) into (2) and using $\mathrm{Tr}\, P = \mathrm{Tr}\, P_0$ we obtain for the averaged energy shift in the adiabatic formalism:

$$\lambda(\mathrm{d}/\mathrm{d}\lambda)\overline{\Delta E}\,\mathrm{Tr}\, P_0 = \lim_{\epsilon \to 0} \mathrm{Tr}[(P_0U_\epsilon(\infty, -\infty)P_0)^{-1}P_0U_\epsilon(\infty, 0)H_1U_\epsilon(0, -\infty)P_0]. \tag{7}$$

Between the square brackets at the right-hand side the adiabatic S matrix $S_\epsilon \equiv P_0U_\epsilon(\infty, -\infty)P_0$ shows up. To deal with the remaining part of (7) let us consider the identity:

$$\mathrm{i}(\partial/\partial t)\{U_\epsilon(t'', t)\mathrm{i}\lambda_\epsilon(t')(\delta/\delta\lambda_\epsilon(t'))U_\epsilon(t, t'')\} = U_\epsilon(t'', t')H_{1\epsilon}(t')U_\epsilon(t', t'')\delta(t'-t), \tag{8}$$

which follows by first applying (4), and then (3) and the definition:

$$(\delta/\delta\lambda_\epsilon(t'))\lambda_\epsilon(t) = \delta(t'-t) \tag{9}$$

of the functional derivative. From (8) we get after integration over t from t'' to t:

$$\mathrm{i}\lambda_\epsilon(t')(\delta/\delta\lambda_\epsilon(t'))U_\epsilon(t, t'') = U_\epsilon(t, t')H_{1\epsilon}(t')U_\epsilon(t', t''), \qquad (t > t' > t''). \tag{10}$$

When this result, with $t = \infty$, $t' = 0$, $t'' = -\infty$, is inserted in (7) the right-hand side is expressed completely in terms of S_ϵ. In view of the trace operation we may formally write:

$$\lambda(\mathrm{d}/\mathrm{d}\lambda)\overline{\Delta E}\,\mathrm{Tr}\, P_0 = \lim_{\epsilon \to 0} \mathrm{i}\lambda_\epsilon(0)(\delta/\delta\lambda_\epsilon(0))\,\mathrm{Tr}\ln S_\epsilon. \tag{11}$$

So the averaged energy shift $\overline{\Delta E}$ can be obtained from the adiabatic S matrix by performing a functional differentiation of $\mathrm{Tr}\ln S_\epsilon$ with respect to the time-dependent coupling constant.

From the well-known Dyson series expansion of the operator U_ϵ in powers of λ an expansion of the same general structure follows for $\mathrm{Tr}\ln S_\epsilon$, namely,

$$\mathrm{Tr}\ln S_\epsilon = \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}t_1 \ldots \mathrm{d}t_n\, \mathrm{Tr}(P_0T(t_1, \ldots, t_n)P_0)\lambda_\epsilon(t_1)\ldots\lambda_\epsilon(t_n); \tag{12}$$

here the operator $T(t_1, \ldots, t_n)$ need not be specified in detail, apart from its behaviour under time translation:

$$T(t_1+\tau, \ldots, t_n+\tau) = \exp(\mathrm{i}H_0\tau)T(t_1, \ldots, t_n)\exp(-\mathrm{i}H_0\tau). \tag{13}$$

Combining (12) with (11) and (9) we find:

$$\overline{\Delta E}\,\mathrm{Tr}\,P_0 = \sum_{n=1}^{\infty} \mathrm{i}\lambda^n \int_{-\infty}^{\infty} \mathrm{d}t_1 \ldots \mathrm{d}t_n \frac{1}{n} \sum_{m=1}^{n} \delta(t_m)\,\mathrm{Tr}(P_0 T(t_1, \ldots, t_n) P_0), \tag{14}$$

where in the integral at the right-hand side the adiabatic limit has been taken. Comparison of (12) and (14) shows that $\overline{\Delta E}$ may be calculated in the same way as $\mathrm{Tr}\ln S_0$, the only difference being, apart from a factor $\mathrm{i}/\mathrm{Tr}\,P_0$, the suppression of one time integration.

Let us now formally put the energies of the final and initial projectors in (12) and (14) equal to E_f and E_i, respectively; the scattering matrix S_0 will accordingly be denoted as S_{fi}. When the time variables t_j in (14) are replaced by $t_j + \tau$ we then have in view of (13):

$$\overline{\Delta E}\,\mathrm{Tr}\,P_0 = \sum_{n=1}^{\infty} \mathrm{i}\exp(\mathrm{i}(E_\mathrm{f} - E_\mathrm{i})\tau]\lambda^n \int_{-\infty}^{\infty} \mathrm{d}t_1 \ldots \mathrm{d}t_n \frac{1}{n}$$

$$\times \sum_{m=1}^{n} \delta(t_m + \tau)\,\mathrm{Tr}(P_0 T(t_1, \ldots, t_n) P_0). \tag{15}$$

Upon bringing the factor $\mathrm{i}\exp[\mathrm{i}(E_\mathrm{f} - E_\mathrm{i})\tau]$ to the left-hand side, integrating from $\tau = -\infty$ to $\tau = \infty$ and using (12) we arrive at the relation

$$-2\pi\mathrm{i}\delta(E_\mathrm{f} - E_\mathrm{i})\overline{\Delta E}\,\mathrm{Tr}\,P_0 = \mathrm{Tr}\ln S_{\mathrm{fi}}. \tag{16}$$

This is a generalisation of Rodberg's result, which was also obtained by adiabatic perturbation theory, but in a completely different way. In particular our starting equation (7) for the energy shift in the adiabatic formalism does not contain an explicit factor ϵ, owing to which the step of actually putting $\epsilon = 0$ is facilitated.

The above expressions enable one to obtain the averaged energy shift $\overline{\Delta E}$ of a stationary system by applying the covariant Feynman formalism. It should be noticed, however, that in general this cannot be achieved by a straightforward evaluation of the S matrix, since the existence of the adiabatic limit is not proved for the individual Feynman diagrams contributing to (14). In a forthcoming paper we shall develop a systematic method for resumming the integrands $P_0 T(t_1, \ldots, t_n) P_0$ of these Feynman diagrams in such a way that each term may be calculated separately in the limit $\epsilon \to 0$.

Acknowledgments

This investigation is part of the research program of the Stichting voor Fundamenteel Onderzoek der Materie (FOM) which is financially supported by the Nederlandse Organisatie voor Zuiver-Wetenschappelijk Onderzoek (ZWO).

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