

Energy shifts and the S matrix in degenerate perturbation theory

M A J Michels[†] and L G Suttorp

Instituut voor Theoretische Fysica, Universiteit van Amsterdam, Valckenierstraat 65, Amsterdam, The Netherlands

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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 $\lambda dH/d\lambda = H_1$ and $\lambda d/d\lambda \langle \psi_\alpha | \psi_\alpha \rangle = 0$ we may write for the energy shifts ΔE_α :

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

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

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

with $P = \sum_\alpha |\psi_\alpha\rangle \langle \psi_\alpha|$ 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:

$$H_{1\epsilon}(t) = \lambda_\epsilon(t) \exp(iH_0 t) V \exp(-iH_0 t), \quad \lambda_\epsilon(t) = \lambda \exp(-\epsilon|t|). \quad (3)$$

[†] Present address: Koninklyke/Shell-Laboratorium, Amsterdam.

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

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

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):

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

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:

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

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

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

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:

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

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

$$(\delta/\delta\lambda_\epsilon(t'))\lambda_\epsilon(t) = \delta(t' - t) \quad (9)$$

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

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

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:

$$\lambda(d/d\lambda)\overline{\Delta E} \text{Tr } P_0 = \lim_{\epsilon \rightarrow 0} i\lambda_\epsilon(0)(\delta/\delta\lambda_\epsilon(0)) \text{Tr } \ln S_\epsilon. \quad (11)$$

So the averaged energy shift $\overline{\Delta E}$ can be obtained from the adiabatic S matrix by performing a functional differentiation of $\text{Tr } \ln S_\epsilon$ 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 $\text{Tr } \ln S_\epsilon$, namely,

$$\text{Tr } \ln S_\epsilon = \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} dt_1 \dots dt_n \text{Tr}(P_0T(t_1, \dots, t_n)P_0)\lambda_\epsilon(t_1) \dots \lambda_\epsilon(t_n); \quad (12)$$

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

$$T(t_1 + \tau, \dots, t_n + \tau) = \exp(iH_0\tau)T(t_1, \dots, t_n)\exp(-iH_0\tau). \quad (13)$$

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

$$\overline{\Delta E} \text{Tr } P_0 = \sum_{n=1}^{\infty} i \lambda^n \int_{-\infty}^{\infty} dt_1 \dots dt_n \frac{1}{n} \sum_{m=1}^n \delta(t_m) \text{Tr}(P_0 T(t_1, \dots, t_n) P_0), \quad (14)$$

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 $\text{Tr} \ln S_0$, the only difference being, apart from a factor $i/\text{Tr } P_0$, 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):

$$\begin{aligned} \overline{\Delta E} \text{Tr } P_0 &= \sum_{n=1}^{\infty} i \exp(i(E_f - E_i)\tau) \lambda^n \int_{-\infty}^{\infty} dt_1 \dots dt_n \frac{1}{n} \\ &\times \sum_{m=1}^n \delta(t_m + \tau) \text{Tr}(P_0 T(t_1, \dots, t_n) P_0). \end{aligned} \quad (15)$$

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

$$-2\pi i \delta(E_f - E_i) \overline{\Delta E} \text{Tr } P_0 = \text{Tr} \ln S_{fi}. \quad (16)$$

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 $P_0 T(t_1, \dots, t_n) P_0$ of these Feynman diagrams in such a way that each term may be calculated separately in the limit $\epsilon \rightarrow 0$.

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