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Unstable States in Quantum Many-Body Theory

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Abstract

Unstable states of a general type of many-body system characterized by a combination of outgoing waves and bound states in all channels are investigated. It is seen, that the time-development in general will contain both oscillating and exponentially decaying terms.

1. Introduction

We shall here consider the problem of unstable states in the general case of a number of interacting particles and fields of different kinds.

We assume that the system has a Hamiltonian H which includes all fields, responsible for the interactions, and that the system at time $t = 0$ is in the state $|a\rangle$. The energy of the system is not sharply defined but the mean energy $\langle a|H|a\rangle$ is above threshold for decay into two or more fragments, or it may decay by electromagnetic radiation etc. The state $|a\rangle$ is approximately confined in a volume Ω_a.

Now, the time development of the system, which we shall only evaluate for $t \geqslant 0$ is given by

$$|a(t)\rangle = e^{-iHt}|a\rangle \tag{1.1}$$

(Here and in the following $\hbar = 1$).

This time development may be studied by different methods [1] e.g. by means of an expansion of $|a(t)\rangle$ in terms of the stable eigenstates of H [2]. We shall here consider another approach based on the boundary conditions corresponding to the decay of the system.

The decay is accompanied by outflow of particles through a sphere of large radius R around the volume Ω_a. We shall assume that R is sufficiently large so all space integrals in H are taken inside the sphere R. The total probability inside R $A_R(t) = \int_0^R (4\pi/3)\, \mathrm{d}r\, r^2 \langle a(t)|a(t)\rangle$ is defined by the equation

$$\partial_t A_R(t) = -J_R(t) \quad J_R(t) = \langle a(t)|J_R|a(t)\rangle \tag{1.2}$$

$$A_R(0) = 1$$

(we use normalization in the volume Ω_a). We suppose that H_R has no complex interactions. Therefore $J_R \neq 0$ if the kinetic term H_R^0 is not hermitian for the decay problem. In the case e.g. of a system of nonrelativistic fermions the kinetic term of H is

$$H_R^0 = -\frac{1}{2m}\int_{r \leqslant R} \mathrm{d}\mathbf{r}\, \psi_{\mathbf{r}}^{+} \nabla^2 \psi_{\mathbf{r}} \tag{1.3}$$

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and the flow operator becomes

$$J_R = i(H^0 - H^{0+})_R = \frac{-i}{2m}\int_{(R)} \mathrm{d}\mathbf{S}(\psi_{\mathbf{R}}^{+}\nabla_{\mathbf{R}}\psi_{\mathbf{R}} - (\nabla_{\mathbf{R}}\psi_{\mathbf{R}}^{+})\psi_{\mathbf{R}}) \tag{1.4}$$

where $\mathrm{d}\mathbf{S}$ is the surface element of the sphere R, ψ^+ and ψ are the creation and annihilation operators of the fermions. Analogue expressions may be written for any systems and J_R contains the currents of the particles and the surface integral on the sphere of large R.

In their physical consequences the different methods of describing decaying states or in general, resonances are essentially equivalent [1, 2, 3]. Our aim is therefore mainly to point at some general concepts and features of decaying states of many-body systems.

2. The Schrödinger equation for the unstable state

Let us consider the Schrödinger equation

$$(\epsilon - H)\psi = 0 \tag{2.1}$$

for various boundary conditions. The most appropriate method for analysis of the solutions of (2.1) seems to us to be the projection operators method [4].

Let p and q be projection operators on the continuous and discrete spectrum of some complete set of state vectors so

$$p + q = 1 \quad p^2 = p \quad q^2 = q \quad pq = 0$$

The choice of such a set is determined by the system considered. For instance, for nuclei it is natural to use the set of eigenstates of the shell model Hamiltonian without residual interactions.

The confined character of $|a\rangle$ is given by

$$q|a\rangle = a\rangle \tag{2.2}$$

and R must be chosen larger than the characteristic dimension of the considered system of q states (atomic, nuclear etc.). Projecting with p and q, we may write (2.1) as the system of equations

$$(\epsilon - H_{qq})\psi_q = H_{qp}\psi_p \quad \psi_q \equiv q\psi$$

$$(\epsilon - H_{pp})\psi_p = H_{pq}\psi_q \quad H_{qp} \equiv qHp \text{ etc.} \tag{2.1a}$$

Now, instead of these equations let us consider the equations (not equivalent to (2.1)) with ϵ as a parameter

$$(E_n(\epsilon) - H_{qq})|n_q(\epsilon)\rangle = H_{qp}|n_p(\epsilon)\rangle$$

$$(\epsilon - H_{pp})|n_p(\epsilon)\rangle = H_{pq}|n_q(\epsilon)\rangle \tag{2.3}$$

Because of the definition of p and q spaces

$$H^+_{qq} = H_{qq};\quad H^+_{pq} = H_{qp}\quad J_R = \mathrm{i}(H_{pp} - H^+_{pp}) \tag{2.4}$$

(note, that only the p-space is responsible for the outgoing waves). So we have from (2.3, 4) that the imaginary part of $E_n(\epsilon)$ is connected directly to the flow of particles

$$2\,\mathrm{Im}\,E_n(\epsilon) = -\frac{1}{\langle n_q(\epsilon)|n_q(\epsilon)\rangle}\langle n_p(\epsilon)|J_R\,|n_p(\epsilon)\rangle \tag{2.5}$$

In analogy to the boundary condition for discrete eigenstates (no particles in the continuous spectrum when $H_{pq}\to 0$) we may write $|n_p(\epsilon)\rangle$ for real ϵ in the form

$$|n_p(\epsilon)\rangle = \frac{1}{\epsilon - H_{pp} + \mathrm{i}\alpha}H_{pq}\,|n_q(\epsilon)\rangle \qquad (\alpha\to 0^+) \tag{2.6}$$

If ϵ is larger than the threshold energy ϵ_t of the continuous spectrum of H_{pp}, the function, $|n_p(\epsilon)\rangle$ describes outgoing particles due to the source $H_{pq}\,|n_q(\epsilon)\rangle$. Using (2.6) we have to remember that $H_{pp}\neq H^+_{pp}$ and therefore e.g. we may write

$$\frac{1}{\epsilon - H_{pp} + \mathrm{i}\alpha} - \frac{1}{\epsilon - H^+_{pp} - \mathrm{i}\alpha} = -\mathrm{i}\frac{1}{\epsilon - H^+_{pp} - \mathrm{i}\alpha}\times J_R\frac{1}{\epsilon - H_{pp} + \mathrm{i}\alpha} \tag{2.7}$$

By substituting (2.6) into the first of eqs. (2.3) we have

$$(E_n(\epsilon) - \mathcal{H}_q(\epsilon))|n_q(\epsilon)\rangle = 0 \tag{2.8}$$

$$\mathcal{H}_q(\epsilon) = H_{qq} + \Delta_q(\epsilon),\quad \Delta_q(\epsilon) = H_{qp}\frac{1}{\epsilon - H_{pp} + \mathrm{i}\alpha}H_{pq}$$

This is an eigenvalue equation in the q space for the Hamiltonian $\mathcal{H}_q(\epsilon)$, where ϵ is considered as a parameter.

(i) In the region of real $\epsilon < \epsilon_t$ the Hamiltonian $H_q(\epsilon)$ is hermitian and the eigenvalues $E_n(\epsilon)$ are real and discrete for any interactions. Eq. (2.3) turns into eq. (2.1) if the roots of the equation

$$E_n(\epsilon_n) = \epsilon_n \qquad (\epsilon_n < \epsilon_t) \tag{2.9}$$

exist. In this case we have simply

$$H|n\rangle = \epsilon_n|n\rangle,\quad |n\rangle = (|n_p(\epsilon)\rangle + |n_q(\epsilon)\rangle)_{\epsilon=\epsilon_n}$$

$$\langle n'|n\rangle = \delta_{nn'}\langle n_q|n_q\rangle\left(1 - \frac{\partial E_n(\epsilon)}{\partial\epsilon}\right)_{\epsilon=\epsilon_n} = \delta_{nn'} \tag{2.10}$$

Thus $|n\rangle$ and ϵ_n are the eigenstates and eigenvalues of the discrete spectrum of the total Hamiltonian H ($\langle n_p|J|n_p\rangle = 0$).

(ii) In the region of real $\epsilon > \epsilon_t$ the eigenvalues $E_n(\epsilon)$ are complex and the solution of (2.9) does not exist.

(iii) For the complex ϵ ($\epsilon\to z = \epsilon - (\mathrm{i}\Gamma/2)$) eq. (2.3) can be written in the form

$$(E_\nu(z) - H_{qq})\,|\nu_q(z)\rangle = H_{qp}\,|\nu_p(z)\rangle$$

$$(z - H_{pp})\,|\nu_p(z)\rangle = H_{pq}\,|\nu_q(z)\rangle \qquad \left(z = \epsilon - \frac{\mathrm{i}\Gamma}{2}\right) \tag{2.11}$$

Let us assume H_{pq} small. Then there are two cases

(a) z does not in the limit of $H_{pq}\to 0$ coincide with the energy Z^0_β of the quasistable state φ_β:

$$H_{pp}\varphi_\beta = Z^0_\beta\varphi_\beta \quad Z^0_\beta = \epsilon^0_\beta - \frac{\mathrm{i}\Gamma^0_\beta}{2} \tag{2.12}$$

In order to keep the boundary condition of the decay (outgoing waves) we may write

$$|\nu_p(z)\rangle = G_p(z)H_{pq}\,|\nu_q(z)\rangle,$$

$$G^+_p(z) = \exp\left(-\frac{\mathrm{i}\Gamma}{2}\,\partial_\epsilon\right)\times\frac{1}{\epsilon - H_{pp} - \mathrm{i}\alpha} \tag{2.13}$$

For example in the (academic) case of the nonrelativistic free-single-particle Green function we obtain

$$G^+_p(n;z) = -\frac{m}{2\pi}\frac{e^{\mathrm{i}(\kappa - \mathrm{i}\gamma)n}}{n} \qquad n = |r - r|$$

$$\left(\kappa - \mathrm{i}\gamma = \left(2m\left(\epsilon - \frac{\mathrm{i}\Gamma}{2}\right)\right)^{1/2}\right) \tag{2.14}$$

From eq. (2.11) we have again the eigenvalue problem in the q space

$$(E_\nu(z) - \mathcal{H}_q(z))|\nu_q(z)\rangle = 0$$

$$\mathcal{H}_q(z) = H_{qq} + \Delta_q(z),\quad \Delta_q(z) = H_{qp}G_p(z)H_{pq} \tag{2.15}$$

It is easy to see that the solution of eq. (2.11) is connected to the solution of (2.3) by

$$|\nu_{p,q}(z)\rangle = \exp\left(-\frac{\mathrm{i}\Gamma}{2}\,\partial_\epsilon\right)|n_{p,q}(\epsilon);$$

$$E_\nu(z) = \exp\left(-\frac{\mathrm{i}\Gamma}{2}\,\partial_\epsilon\right)E_n(\epsilon) \tag{2.16}$$

An equation, similar to (2.15) is given by Fonda and Newton [5].

It should be mentioned that for $\epsilon_\nu < \epsilon_t$ the width $\Gamma_\nu = 0$. Indeed from (2.16) one can see that if $\mathrm{Im}\,E_n(\epsilon) = 0$ the trivial solution is simply $\Gamma_\nu = 0$ (in the region $\epsilon < \epsilon_t$ only the stable states exist).

(b) z tends towards Z^0_β from eq. (2.12) for $H_{pq}\to 0$. In this case we may write

$$(z_\beta - H_{qq})\,|\beta_p\rangle = H_{qp}\,|\beta_p\rangle$$

$$(z_\beta - H_{pp})\,|\beta_p\rangle = H_{pq}\,|\beta_q\rangle \tag{2.17}$$

From the first of these equations we have

$$|\beta_q\rangle = (z_\beta - H_{qq})^{-1}H_{qp}|\beta_p\rangle \tag{2.18}$$

By substituting this eq. into (2.18) we obtain

$$(z_\beta - H_p(z_\beta))\,|\beta_p\rangle = 0$$

$$H_p(z) = H_{pp} + \Delta_p(z);\quad \Delta_p(z) = H_{pq}(z - H_{qq})^{-1}H_{qp} \tag{2.19}$$

Thus looking at the different regions of z (i) and (iii) we may conclude that the general solution of the coupled equations (2.11) with the decay boundary has the real discrete ($\mathrm{Im}\,z_\nu = -(\Gamma_\nu/2) = 0$ when $\mathrm{Re}\,z_\nu < \epsilon_t$) and complex eigenvalues $\Gamma_\nu > 0$ when $\mathrm{Re}\,z_\nu > \epsilon_t$

$$|\nu\rangle \equiv (|\nu_p(z)\rangle + |\nu_q(z)\rangle)_{z=\epsilon_\nu - (\mathrm{i}\Gamma_\nu/2)} \tag{2.20}$$

where

$$\Gamma_\nu = \frac{\langle\nu|J_R|\nu\rangle}{\langle\nu|\nu\rangle} \tag{2.21}$$

Since the states $|\nu\rangle$ satisfy an eigenvalue equation (2.11) for the same Hamiltonian as that of the Schrödinger equation for $|a(t)\rangle$, an expansion of $|a(t)\rangle$ in terms of the $|\nu\rangle$ (even if these are not the usual Schrödinger eigenstates) will have time independent coefficients, when we let the $|\nu\rangle$ vectors have the time dependence given by

$$|\nu(t)\rangle = |\nu\rangle \cdot \exp\left(-\mathrm{i}\left(\epsilon_\nu - \frac{\mathrm{i}\Gamma_\nu}{2}\right)t\right)$$

$$(|\nu\rangle \equiv |\nu(0)\rangle) \tag{2.22}$$

So we write – *formally*, postponing the question of the validity (i.e. convergence etc.) of the expansion

$$|a(t)\rangle = \sum_\nu c_\nu |\nu\rangle \exp\left(-\mathrm{i}\left(\epsilon_\nu - \frac{\mathrm{i}\Gamma_\nu}{2}\right)t\right) \tag{2.23}$$

We shall now assume, that the q space consists of a finite number of vectors only, N_q. This is obviously the case with the space of nuclear shell model states. For Coulomb bound states, it means that the potential must be treated in a screening approximation or that high lying bound states must be included in p-space; this is also necessary for our introduction of R, since the radius of the Rydberg states goes to infinity as n^2. We see, that in the limit of $H_{pq} \to 0$, we have N_q linear independent vectors $|\nu_q\rangle$, and that if H_{pq} is increased (numerically) in a continuous way, within certain limits this must still be the case with the $|\nu_q\rangle$ belonging to eigenvalues of type (a), except for very special cases, which could be avoided by a negligibly small change of H.

These $|\nu_q\rangle$ (for finite H_{pq}) are in general not orthogonal, but together with the solutions of

$$(H_q^* - E_\nu^*)|\tilde{\nu}_q\rangle = 0 \tag{2.24}$$

they form a biorthogonal system

$$\langle\tilde{\nu}_q'|\nu_q\rangle = 0, \quad \nu' \neq \nu \tag{2.25}$$

With the proper normalization of the $|\nu_q\rangle$ we therefore have the completeness relation in q-space

$$\sum_{\nu=0}^{N_q} n_\nu |\nu_q\rangle\langle\tilde{\nu}_q| = q \quad n_\nu = \langle\tilde{\nu}_q|\nu_q\rangle^{-1} \tag{2.26}$$

3. Time dependent description and conclusions

We can now write (2.23) ($t = 0$)

$$|a(0)\rangle = |a\rangle = q|a\rangle = \sum c_\nu q|\nu\rangle =$$

$$\sum_\nu^{N_q} c_\nu|\nu_q\rangle = \sum_\nu^{N_q} n_\nu|\nu_q\rangle\langle\tilde{\nu}_q|a\rangle \equiv \sum_\nu^{N_q} n_\nu|\nu\rangle\langle\tilde{\nu}|a\rangle$$

$$(|\tilde{\nu}_q\rangle = q|\tilde{\nu}\rangle) \tag{3.1}$$

where we have used (2.26) and (2.2).

The probability of finding the system in the initial state $|a\rangle$ at time t (non-decay probability) is by (2.22) given by

$$|\langle a|a(t)\rangle|^2 = \sum_{\nu,\nu'}^{N_q} \langle a|\nu\rangle\langle\tilde{\nu}|a\rangle\langle a|\tilde{\nu}'\rangle\langle\nu'|a\rangle \times$$

$$\exp\left(-\mathrm{i}\left(\epsilon_\nu - \epsilon_{\nu'} - \frac{i}{2}(\Gamma_\nu + \Gamma_{\nu'})\right)t\right) n_\nu n_{\nu'} \tag{3.2}$$

Since the Hamiltonian H contains all fields responsible for the interactions (electromagnetic mesonic etc.) the only stable state may be the ground state $\nu = 0$ of the system with the same number N of particles as in the initial state $|a\rangle$. If such a state exists eq. (3.2) can be written in the form

$$|\langle a|a(t)\rangle|^2 = |\langle 0|a\rangle|^4$$

$$+ 2|\langle 0|a\rangle|^2 \sum_{\nu'\neq 0} \mathrm{Re}\,(\langle a|\nu\rangle\langle\tilde{\nu}|a\rangle\, \mathrm{e}^{-\mathrm{i}\epsilon_\nu t}) \times$$

$$\exp\left(-\frac{\mathrm{i}\Gamma_\nu}{2}t\right) n_\nu$$

$$+ \sum_{\nu,\nu'\neq 0} \langle a|\nu\rangle\langle\tilde{\nu}|a\rangle\langle a|\tilde{\nu}'\rangle\langle\nu'|a\rangle \times$$

$$\exp\left(-\mathrm{i}\left(\epsilon_\nu - \epsilon_{\nu'} - \frac{i}{2}(\Gamma_\nu + \Gamma_{\nu'})\right)t\right) n_\nu n_{\nu'} \tag{3.3}$$

Thus in general the non-decay probability contains a constant term (if the ground state of N particles exists), purely exponentially decaying terms ($\nu = \nu'$ in the third sum) and terms with both decaying and oscillating factors. If the ground state $|0\rangle$ for the considered system of N particles does not exist we have only the sum of decaying and oscillating terms.

The time-dependence of the probability (3.3) is general and independent of the choice of the initial state $|a\rangle$. It is obvious that $|a\rangle$ cannot be stable if $|a\rangle \neq |0\rangle$.

The observation of details of the time-dependence of the confined system is complicated in experiments. Therefore usually only some decaying channels can be measured in time. In order to give the general scheme we consider the simple case of the decay in one channel.

Suppose that the system of N nonrelativistic interacting fermions has no ground state but there is a stable state $|\lambda\rangle$ for the system of $N-1$ fermions. Therefore the initial state $|a\rangle$ will emit one particle and turn into the state $|\lambda\rangle$. Using the commutation relations for Fermi field operators and eq. (2.20) we may write

$$\left(\epsilon_\nu - \frac{i}{2}\Gamma_\nu - H - T_\mathbf{r} - U_\mathbf{r}\right)\psi_\mathbf{r}|\nu\rangle = 0, \quad T_\mathbf{r} = -\frac{1}{2m}\nabla_\mathbf{r}^2 \tag{3.4}$$

Let us assume that $V_\mathbf{r}$ is a mean one-particle potential. For the one particle "wave-function" (overlap-function) $\psi_\nu(r) = \langle\lambda|\psi_\mathbf{r}|\nu\rangle$ we have from eq. (3.4)

$$\left(E_\nu - \frac{i}{2}\Gamma_\nu - T_\mathbf{r} - V_\mathbf{r}\right)\psi_\nu(\mathbf{r}) = \langle\lambda|\delta U_\mathbf{r}\psi_\mathbf{r}|\nu\rangle,$$

$$\delta U_\mathbf{r} = U_\mathbf{r} - V_\mathbf{r}, \quad E_\nu = \epsilon_\nu - \epsilon_\lambda, \quad H|\lambda\rangle = \epsilon_\lambda|\lambda\rangle$$

According to the decay boundary condition we may write

$$\psi_\nu(\mathbf{r}) = \exp\left(-\frac{\mathrm{i}\Gamma_\nu}{2}\partial_{E_\nu}\right)\frac{1}{E_\nu - T_\mathbf{r} - V_\mathbf{r} + \mathrm{i}\alpha}\langle\lambda|\delta U_\mathbf{r}|\nu\rangle \tag{3.5}$$

From (3.5) we obtain the amplitude of finding the system of

$N-1$ particles in the stable state $|\lambda\rangle$ and one particle at the point $\mathbf{r}$ at time t

$$\psi_a(\mathbf{r},t) = \sum_\nu \exp\left(-\frac{i\Gamma_\nu}{2}\,\partial_{E_\nu}\right)\frac{e^{-iE_\nu t}}{E_\nu - T_\mathbf{r} - V_\mathbf{r} + i\alpha}\times$$

$$\langle\lambda|\delta U_\mathbf{r}\psi_\mathbf{r}|\nu\rangle\langle\tilde{\nu}|a\rangle \qquad (3.6)$$

For large $r \gg R_a$ (R_a is the characteristic size of the volume Ω_a) (3.6) has the form

$$\psi_a(\mathbf{r},t) = \sum_\nu \frac{1}{r} f_\nu(\mathbf{n}) \exp\left(i(x_\nu - i\gamma_\nu)r - i\left(E_\nu - \frac{i}{2}\Gamma_\nu\right)t\right),$$

$$\mathbf{n} = \frac{r}{|r|},\ \kappa - i\gamma = \left(2m\left(E - \frac{i}{2}\Gamma\right)\right)^{1/2} \qquad (3.7)$$

Using the completeness at time $t = 0$ one can obtain

$$\psi_a(\mathbf{r}, t=0) = \langle\lambda|\psi_\mathbf{r}|a\rangle = 0 \quad r > R \qquad (3.8)$$

(Remember that in the state $|a\rangle$ all particles are confined in the volume Ω_a). Therefore the exponential dependence on r in (3.7) that each term of the sum is proportional to $e^{\gamma_\nu r}$ does not mean divergence of $\psi_a(\mathbf{r},t)$. The physical meaning of the t- and r-dependence of $\psi_a(\mathbf{r}, t)$ are well known from the one particle decay theory [5]. We may consider different decays (electromagnetic, two particles etc.) by using the same method of commutation relations and equations of motion for different field operators.

The general form (3.3) of the probability describes any decay of any system of particles but in practice some details of the time-dependence can be observed only in molecular and atomic experiments (e.g. the oscillations of the probability).

The detailed behaviour of decaying states has been discussed by many authors, see particularly the review of Fonda, Ghirardi and Rimini [1] and references in that, especially [7]. The present work adds little to this discussion. Our aim has rather been to point at a common framework, which could be useful for a general understanding of the concept of decaying states of resonances. Particularly the (limited) freedom of choice of p- and q-spaces seems to correspond well to a limited freedom in the description of a decaying state. The condition, that H_{pq} is small is the main feature of the division into p- and q-spaces, and it corresponds to our mind to a necessary condition for the introduction of the *concept* of decaying states.

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