Theory of quantum resonance: A renormalization-group approach

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The standard perturbation theory for time-dependent problems in quantum mechanics is reconsidered through renormalization-group methods. This approach justifies *a posteriori* the theory of quantum resonance given by the multiple-scale analysis of the perturbation series applied to the coupled equations of wave-function amplitudes. The resonance equations for the leading-order amplitude probabilties are then obtained up to second order and a general method for the algorithmic computation of higher-order terms of the perturbation series is given. The three-level model in a monochromatic wave with two resonant states is discussed in the light of the present results. [S1050-2947(98)04607-1]

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Perturbation theory is a widely used tool in physics. However, it is a well-known matter that the solution series sometimes cannot exist or the terms of the series can have some troubles. A typical problem is given by the so-called secular terms or secularities. Such terms restrict or even prevent the applicability of the perturbative solution to a large number of interesting problems. Recently, a general approach has been devised by Chen, Oono, and Goldenfeld [1] to dispose of secularities in a perturbation series through a renormalization-group (RG) method. Based on that work, Kunihiro was able to reformulate the RG method by the mathematical theory of the envelopes [2]. Due to their generality, such methods also proved to be successfully applicable to the problem of the resummation of divergent series obtained through the Rayleigh-Schrödinger perturbation theory [3].

In Ref. [4] we gave an applications of the RG methods in quantum mechanics discussing two interesting problems of quantum optics. In that paper we derived a general rule for the application of RG methods to the operator formulation of problems in quantum mechanics. However, as we are going to show, general results can be obtained by applying the above rule to the coupled equations for the probability amplitudes of the wave function.

In Ref. [5] we proposed a theory of quantum resonance by perturbatively solving the equations for the probability amplitudes. In order to get rid of the secular terms we used a method of the multiple scales [6] that, to our knowledge, has never been applied before to the Schrödinger equation. So, although we were able to show, also numerically, the successful application of the above method, it was not at all clear why it should work in the way we applied it. In any case, it was possible to prove that the widely used rotating-wave approximation (RWA), as generally applied in quantum mechanics [7], is the leading-order approximation of the perturbation series for probability amplitudes. Using the RG methods, we are now able to justify the results of Ref. [5] and improve them by obtaining higher-order corrections to the RWA. In addition, we get in this way a clear understanding of the very good working of the RWA in quantum optics.

It should be said that, in the literature, other attempts to improve the RWA have been made. The widely used approach for that aim is the Floquet method [8]. However, one of our intents is to understand the role of the RWA in the framework of the standard perturbation theory. That question has never been discussed before apart from our early attempts in Ref. [5].

We consider the problem of a quantum system, with a discrete spectrum for the sake of simplicity, under the effect of a time-dependent perturbation $V(t)$. The coupled equations for the probability amplitudes are given by [7]

$$i\hbar \frac{da_m}{dt} = \epsilon \sum_n e^{-(i/\hbar)(E_n - E_m)t} \langle m|V(t)|n\rangle a_n , \tag{1}$$

with E_n the energy eigenvalue corresponding to the eigenstate $|n\rangle$ of the unpertubed Hamiltonian and a_n the probability amplitude to find the perturbed system in the nth eigenstate of it, while ϵ is just an ordering parameter introduced for convenience. The kind of perturbations that interest us are those having a Fourier series as

$$V_{mn}(t) = \langle m|V(t)|n\rangle = \sum_p v_{mn}^p e^{ip\omega t}, \tag{2}$$

so that Eq. (1) can be rewritten as

$$i\hbar \frac{da_m}{dt} = \epsilon \sum_{n,p} e^{-i\Omega_{nm}^p t} v_{mn}^p a_n , \tag{3}$$

with $\Omega_{nm}^p = (1/\hbar)(E_n - E_m) - p\omega$. We now consider the amplitude a_m as a function of both t and t_0, the latter being an arbitrary initial time. Taking $a_m(t,t_0) = a_m^{(0)}(t,t_0) + \epsilon a_m^{(1)}(t,t_0) + \epsilon^2 a_m^{(2)}(t,t_0) + O(\epsilon^3)$, the application of the perturbation theory gives

$$a_m^{(0)}(t,t_0)=a_m(t_0), \tag{4}$$

$$a_m^{(1)}(t,t_0)=-\frac{i}{\hbar}\sum_{\substack{n,p\\ \Omega_{nm}^p=0}} v_{mn}^p a_n(t_0)(t-t_0)+\frac{1}{\hbar}\sum_{\substack{n,p\\ \Omega_{nm}^p\neq 0}}\frac{e^{-i\Omega_{nm}^p t}-e^{-i\Omega_{nm}^p t_0}}{\Omega_{nm}^p}v_{mn}^p a_n(t_0), \tag{5}$$

$$a_m^{(2)}(t,t_0)=-\frac{1}{2\hbar^2}(t-t_0)^2\sum_{\substack{n,p\\ \Omega_{nm}^p=0}}\sum_{\substack{n_1,p_1\\ \Omega_{n_1n}^{p_1}=0}} v_{mn}^p v_{nn_1}^{p_1} a_{n_1}(t_0)-\frac{i}{\hbar^2}(t-t_0)\sum_{\substack{n,p,n_1,p_1\\ \Omega_{nm}^p+\Omega_{n_1n}^{p_1}=0,\\ \Omega_{nm}^p\neq 0,\Omega_{n_1n}^{p_1}\neq 0}}\frac{v_{mn}^p v_{nn_1}^{p_1}}{\Omega_{n_1m}^{p_1}}a_{n_1}(t_0)-\frac{i}{\hbar^2}(t-t_0)$$
$$\times\sum_{\substack{n,p\\ \Omega_{nm}^p\neq 0}}\sum_{\substack{n_1,p_1\\ \Omega_{n_1n}^{p_1}=0}}\frac{v_{mn}^p v_{nn_1}^{p_1}}{\Omega_{nm}^p}a_{n_1}(t_0)e^{-i\Omega_{nm}^p t}+\frac{i}{\hbar^2}(t-t_0)\sum_{\substack{n,p\\ \Omega_{nm}^p=0}}\sum_{\substack{n_1,p_1\\ \Omega_{n_1n}^{p_1}\neq 0}}\frac{v_{mn}^p v_{nn_1}^{p_1}}{\Omega_{n_1m}^{p_1}}a_{n_1}(t_0)e^{-i\Omega_{nm}^p t_0}+\mathcal{I}. \tag{6}$$

By $\mathcal{I}$ we mean "irrelevant terms," that is, terms that have no effect on the arguments that follow.

Now we proceed using the rule introduced in Ref. [4] and dress all the phases in the exponentials by setting $-t_0=\phi(t_0)$, $\phi(t_0)$ being a renormalizable parameter to be determined by our method. We have

$$a_m^{(0)}(t,t_0)=a_m(t_0), \tag{7}$$

$$a_m^{(1)}(t,t_0)=-\frac{i}{\hbar}\sum_{\substack{n,p\\ \Omega_{nm}^p=0}} v_{mn}^p a_n(t_0)(t-t_0)+\frac{1}{\hbar}\sum_{\substack{n,p\\ \Omega_{nm}^p\neq 0}}\frac{e^{-i\Omega_{nm}^p t}-e^{i\Omega_{nm}^p\phi(t_0)}}{\Omega_{nm}^p}v_{mn}^p a_n(t_0), \tag{8}$$

$$a_m^{(2)}(t,t_0)=-\frac{1}{2\hbar^2}(t-t_0)^2\sum_{\substack{n,p\\ \Omega_{nm}^p=0}}\sum_{\substack{n_1,p_1\\ \Omega_{n_1n}^{p_1}=0}} v_{mn}^p v_{nn_1}^{p_1} a_{n_1}(t_0)-\frac{i}{\hbar^2}(t-t_0)\sum_{\substack{n,p,n_1,p_1\\ \Omega_{nm}^p+\Omega_{n_1n}^{p_1}=0,\\ \Omega_{nm}^p\neq 0,\ \Omega_{n_1n}^{p_1}\neq 0}}\frac{v_{mn}^p v_{nn_1}^{p_1}}{\Omega_{n_1m}^{p_1}}a_{n_1}(t_0)-\frac{i}{\hbar^2}(t-t_0)$$
$$\times\sum_{\substack{n,p\\ \Omega_{nm}^p\neq 0}}\sum_{\substack{n_1,p_1\\ \Omega_{n_1n}^{p_1}=0}}\frac{v_{mn}^p v_{nn_1}^{p_1}}{\Omega_{nm}^p}a_{n_1}(t_0)e^{-i\Omega_{nm}^p t}+\frac{i}{\hbar^2}(t-t_0)\sum_{\substack{n,p\\ \Omega_{nm}^p=0}}\sum_{\substack{n_1,p_1\\ \Omega_{n_1n}^{p_1}\neq 0}}\frac{v_{mn}^p v_{nn_1}^{p_1}}{\Omega_{n_1m}^{p_1}}a_{n_1}(t_0)e^{i\Omega_{nm}^p\phi(t_0)}+\mathcal{I}. \tag{9}$$

Then we impose the renormalization-group condition

$$\left.\frac{da_m(t,t_0)}{dt_0}\right|_{t_0=t}=0,$$

using the above equations for computing a_m, and the following set of equations is obtained:

$$i\hbar\frac{d\overline{a}_m}{dt}=\epsilon\sum_{\substack{n,p\\ \Omega_{nm}^p=0}} v_{mn}^p\overline{a}_n(t)+\epsilon^2\Bigg[\sum_{\substack{n,p,n_1,p_1\\ \Omega_{nm}^p+\Omega_{n_1n}^{p_1}=0,\\ \Omega_{nm}^p\neq 0,\ \Omega_{n_1n}^{p_1}\neq 0}}\frac{v_{mn}^p v_{nn_1}^{p_1}}{\hbar\Omega_{n_1m}^{p_1}}\overline{a}_{n_1}(t)+\sum_{\substack{n,p\\ \Omega_{nm}^p\neq 0}}\sum_{\substack{n_1,p_1\\ \Omega_{n_1n}^{p_1}=0}}\frac{v_{mn}^p v_{nn1}^{p_1}}{\hbar\Omega_{nm}^p}\overline{a}_{n_1}(t)e^{i\Omega_{nm}^p\phi(t)}$$
$$-\sum_{\substack{n,p\\ \Omega_{nm}^p=0}}\sum_{\substack{n_1,p_1\\ \Omega_{n_1n}^{p_1}\neq 0}}\frac{v_{mn}^p v_{nn_1}^{p_1}}{\hbar\Omega_{n_1m}^{p_1}}\overline{a}_{n_1}(t)e^{i\Omega_{n_1n}^{p_1}\phi(t)}\Bigg]+O(\epsilon^3), \tag{10}$$

$$\frac{d\phi(t)}{dt}=O(\epsilon^2), \tag{11}$$

having put the bar over the amplitudes to remember that these are the leading-order approximants to the true solutions and use has been made of the first-order equations

$$i\hbar\frac{d\overline{a}_m}{dt}=\epsilon\sum_{\substack{n,p\\ \Omega^p_{nm}=0}} v^p_{mn}\overline{a}_n(t)+O(\epsilon^2). \tag{12}$$

So we conclude that, at arbitrary t_0, we get a dependence from the initial time also into the resonance equation (10). Then the determination of the theory at $t_0=0$ can be simply realized, with $\phi(t)=\phi(t_0)=-t_0$, by taking $\phi(t)=0$ at the end of the computation. From the above equations, at a general initial time we can realize that when the perturbation is turned on adiabatically by a small exponential $e^{\delta t_0}$, with $\delta\to 0^+$, multiplying the terms dependent on ϕ in Eq. (10), in the limit $t_0\to-\infty$, the resonance equations of Ref. [5] are obtained.

So, finally, the resonance equation at $t_0=0$ up to second order is

$$\begin{aligned}i\hbar\frac{d\overline{a}_m}{dt}=&\epsilon\sum_{\substack{n,p\\ \Omega^p_{nm}=0}} v^p_{mn}\overline{a}_n(t)\\ &+\epsilon^2\Bigg[\sum_{\substack{n,p,n_1,p_1\\ \Omega^p_{nm}+\Omega^{p_1}_{n_1n}=0,\\ \Omega^p_{nm}\neq 0,\ \Omega^{p_1}_{n_1n}\neq 0}}\frac{v^p_{mn}v^{p1}_{nn1}}{\hbar\Omega^{p1}_{n1m}}\overline{a}_{n1}(t)\\ &+\sum_{\substack{n,p\\ \Omega^p_{nm}\neq 0}}\sum_{\substack{n_1,p_1\\ \Omega^{p_1}_{n_1n}=0}}\frac{v^p_{mn}v^{p1}_{nn1}}{\hbar\Omega^p_{nm}}\overline{a}_{n1}(t)\\ &-\sum_{\substack{n,p\\ \Omega^p_{nm}=0}}\sum_{\substack{n_1,p_1\\ \Omega^{p_1}_{n_1n}\neq 0}}\frac{v^p_{mn}v^{p_1}_{nn_1}}{\hbar\Omega^{p_1}_{n_1m}}\overline{a}_{n_1}(t)\Bigg]+O(\epsilon^3).\end{aligned} \tag{13}$$

Equations (10), (11), and (13) are the main result of the paper as, the most general form of the resonance equations up to second order is obtained. These equations should be supplemented with the perturbation series, obtained through the computation of $a_m(t,t_0)|_{t_0=t}$, that, for the sake of simplicity, we write up to first order

$$a_m(t)=\overline{a}_m(t)+\epsilon\sum_{\substack{n,p\\ \Omega^p_{nm}\neq 0}}\frac{e^{-i\Omega^p_{nm}t}-1}{\hbar\Omega^p_{nm}}v^p_{mn}\overline{a}_n(t)+O(\epsilon^2). \tag{14}$$

From Eq. (13) it easily realized that second order corrections to the probability amplitudes at the leading order give rise to detunings.

In order to see how the above results are applied in practice, let us consider the following three-level model in a monochromatic wave of frequency ω, so that we have two resonant levels $\omega_{31}=\omega_3-\omega_1=\omega$, with $\omega_n=E_n/\hbar$ and E_n the energy of the nth unperturbed level. The exact equations of the model are

$$\begin{aligned}i\hbar\frac{da_1}{dt}=&a_2V_{12}(e^{-i(\omega_{21}-\omega)t}+e^{-i(\omega_{21}+\omega)t})\\ &+a_3V_{13}(1+e^{-2i\omega t}),\end{aligned} \tag{15}$$

$$\begin{aligned}i\hbar\frac{da_2}{dt}=&a_1V_{21}(e^{-i(\omega_{12}-\omega)t}+e^{-i(\omega_{12}+\omega)t})\\ &+a_3V_{23}(e^{-i(\omega_{32}-\omega)t}+e^{-i(\omega_{32}+\omega)t}),\end{aligned} \tag{16}$$

$$\begin{aligned}i\hbar\frac{da_3}{dt}=&a_2V_{32}(e^{-i(\omega_{23}-\omega)t}+e^{-i(\omega_{23}+\omega)t})\\ &+a_1V_{31}(1+e^{2i\omega t}).\end{aligned} \tag{17}$$

A RWA solution of the above equations was given in Ref. [9]. Instead, the corrected resonance equations up to second order, using Eq. (13), are

$$\begin{aligned}i\hbar\frac{d\overline{a}_1}{dt}&=V_{13}\overline{a}_3+\Delta_1\overline{a}_1,\\ i\hbar\frac{d\overline{a}_2}{dt}&=-(\Delta_1+\Delta_2)\overline{a}_2,\\ i\hbar\frac{d\overline{a}_3}{dt}&=V_{31}\overline{a}_1+\Delta_2\overline{a}_3,\end{aligned} \tag{18}$$

with

$$\Delta_1=\frac{|V_{13}|^2}{2\hbar\omega}-\frac{|V_{12}|^2}{\hbar}\frac{2\omega_{21}}{\omega_{21}^2-\omega^2}, \tag{19}$$

$$\Delta_2=-\frac{|V_{13}|^2}{2\hbar\omega}+\frac{|V_{32}|^2}{\hbar}\frac{2\omega_{32}}{\omega_{32}^2-\omega^2}, \tag{20}$$

the detunings originating from the perturbation. It should be said that, with respect to the solution of Ref. [5], we have here the right improvement of the RWA solution of Ref. [9]. In addition, the above resonance equations should be supplemented with the perturbation series that here we give up to first order,

$$\begin{aligned}a_1(t)=&\overline{a}_1(t)+\frac{1}{\hbar}V_{12}\left[\frac{e^{-i(\omega_{21}-\omega)t}-1}{\omega_{21}-\omega}\right.\\ &\left.+\frac{e^{-i(\omega_{21}+\omega)t}-1}{\omega_{21}+\omega}\right]\overline{a}_2(t)\\ &+V_{13}\frac{e^{-2i\omega t}-1}{2\hbar\omega}\overline{a}_3(t)+\cdots,\end{aligned}$$

$$a_2(t)=\overline{a}_2(t)+\frac{1}{\hbar}V_{21}\left[\frac{e^{-i(\omega_{12}-\omega)t}-1}{\omega_{12}-\omega}+\frac{e^{-i(\omega_{12}+\omega)t}-1}{\omega_{12}+\omega}\right]\overline{a}_1(t)+\frac{1}{\hbar}V_{23}\left[\frac{e^{-i(\omega_{32}-\omega)t}-1}{\omega_{32}-\omega}+\frac{e^{-i(\omega_{32}+\omega)t}-1}{\omega_{32}+\omega}\right]\overline{a}_3(t)+\cdots,$$

$$a_3(t)=\overline{a}_3(t)+\frac{1}{\hbar}V_{32}\left[\frac{e^{-i(\omega_{23}-\omega)t}-1}{\omega_{23}-\omega}+\frac{e^{-i(\omega_{23}+\omega)t}-1}{\omega_{23}+\omega}\right]\overline{a}_2(t)-V_{31}\frac{e^{2i\omega t}-1}{2\hbar\omega}\overline{a}_1(t)+\cdots. \tag{21}$$

We see that couplings between leading-order amplitudes can happen only by corrections to higher orders in the computation of the approximate solutions of the probability amplitudes. Again, this gives an insight of the fine working of the RWA.

It is realized without difficulty that Eqs. (18) and (21) give the resonance equations for the two-level model, by setting $V_{12}=V_{23}=0$, as computed in Ref. [5]. However, the equations for the two-level model for the leading-order amplitudes are structurally exact as odd higher-order corrections add terms to the Rabi frequency and even higher-order corrections add terms to the Bloch-Siegert shift. So we have the general form valid at any order for the leading-order amplitudes

$$i\frac{d\overline{a_1}}{dt}=\mathcal{R}\overline{a}_3+\Delta\overline{a}_1,\quad i\frac{d\overline{a_3}}{dt}=\mathcal{R}^*\overline{a}_1-\Delta\overline{a}_3, \tag{22}$$

with $\mathcal{R}$ the complex Rabi frequency and Δ the Bloch-Siegert shift to the resonance frequency. We conjecture that the same is true also for the three-level model discussed above, that is, Eqs. (18) should retain the same form at any order.

From the above discussion the ease of determining the physical meaning of the resonance equations appears to be clearly due to the choice to use the standard perturbation theory. The renormalization-group methods prove again to be a powerful method to improve a perturbation series. Due to the simplicity of the method it has been possible to build a general theory of the standard perturbation series in quantum mechanics, in which all the known phenomena of quantum resonance together give a very simple and unified picture.

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