# Duality in perturbation theory and the quantum adiabatic approximation

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Duality is considered for the perturbation theory by deriving, given a series solution in a small parameter, its dual series with the development parameter being the inverse of the other. A dual symmetry in perturbation theory is identified. It is then shown that the dual to the Dyson series in quantum mechanics is given by a recently devised series having the adiabatic approximation as leading order. A simple application of this result is given by rederiving a theorem for strongly perturbed quantum systems. [S1050-2947(98)01311-0]

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A known result of fluid mechanics [1], given the Navier-Stokes equation in the absence of any forcing

$$\frac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}-\nu\nabla^2\mathbf{u}+\nabla p=0, \tag{1}$$

where $\nu$ is the viscosity, $p$ the pressure, and $\mathbf{u}$ the velocity field, is that, by fixing the zeroth-order solution through the Eulerian part as [2]

$$\frac{\partial \mathbf{u}_0}{\partial t}+(\mathbf{u}_0\cdot\nabla)\mathbf{u}_0=0, \tag{2}$$

one obtains a perturbation series for a large Reynolds number Re while, taking at the leading order the equation

$$\frac{\partial \mathbf{w}_0}{\partial t}-\nu\nabla^2\mathbf{w}_0=0, \tag{3}$$

one obtains a perturbation series for small Re. So far, this was the only case in perturbation theory, as applied to physics, with an equation generating both a small perturbation series and its strong perturbation counterpart.

Duality in perturbation theory should then be understood in the sense that, for a given differential equation, one has the possibility to derive perturbation series in both a small development parameter and its inverse, giving in this way the possibility to study a solution in different regions of the parameter space. However, it should be said that the method could not be of absolutely general usefulness as some limitations can appear for the computation of both the leading and higher orders. In addition, there exist situations where better approximations are known, as I will show. However, it is easy to realize that many problems in physics can get new insight from this approach, so it is worthwhile to exploit it.

A natural question, in the light of the above-defined duality in perturbation theory, is what should be the dual to the well-known Dyson series for the Schrödinger equation. The answer to this question is the main aim of this paper. In fact, the existence of this possibility gives a technique to analyze quantum systems in different regions of their parameter space.

Quite recently I showed that solutions for the Schrödinger equation, in time-dependent problems, can be obtained when a strong perturbation is applied to a quantum system [3]. This approach seems to indicate that, at the leading order, an adiabatic approximation should be used [4]. On a different line of research, Mostafazadeh [5] was able to show that a series exists, for the Schrödinger equation, with a well-defined development parameter, having the adiabatic approximation as leading order. Using duality in perturbation theory, the above different research lines can be merged, as I am going to show, giving us the main result of this paper. In fact, the series derived by Mostafazadeh is dual to the Dyson series. Then the theory of strong perturbations in quantum mechanics can be proved to be dual to the standard small perturbation theory.

In order to show how a dual series can be obtained in a simple case, let us consider the model given by the differential equation

$$\ddot{x}=f_0(x)+\lambda f_1(x), \tag{4}$$

where the overdots mean derivation with respect to the time and $\lambda$ is an ordering parameter. It is a well-known matter that, when $\lambda\to 0$, a solution series of the form $x\sim x_0+\lambda x_1+\lambda^2 x_2+O(\lambda^3)$ can be obtained. However, as for the Navier-Stokes equations, we are free to choose at the leading order, as an unperturbed equation, $\ddot{x}_0=\lambda f_1(x_0)$. To show that this choice gives a dual perturbation series, I rescale the time variable in Eq. (4) as $t\to\sqrt{\lambda}t=\tau$. One gets

$$\lambda\ddot{x}=f_0(x)+\lambda f_1(x), \tag{5}$$

where now the overdots mean derivation with respect to $\tau$. It is quite easy to verify that the series

$$x=x_0+\frac{1}{\lambda}x_1+\frac{1}{\lambda^2}x_2+O\left(\frac{1}{\lambda^3}\right) \tag{6}$$

is a solution of Eq. (5) when

$$\begin{aligned}\ddot{x}_0&=f_1(x_0),\\ \ddot{x}_1&=f_1'(x_0)x_1+f_0(x_0),\\ \ddot{x}_2&=f_0'(x_0)x_1+f_1'(x_0)x_2+\frac{1}{2}f_1''(x_0)x_1^2,\\ &\vdots\end{aligned} \tag{7}$$

In analogy with the results in quantum mechanics [3], I take the above as the dual method to small perturbation theory to

 

obtain a dual perturbation series to a given one. It is important to note that the above result is true independently of one's ability to solve the leading-order equations.

We see that the arbitrariness in the choice of the leading-order equation gives rise to a symmetry. In fact, setting $\lambda = 1$ in Eq. (4), there is no longer a reason to see any difference between the perturbation and the unperturbed system in the same way as happens in fluid mechanics. This means that the series given by the small perturbation theory can be derived from the one given by the dual method and vice versa by simply interchanging $f_0(x) \leftrightarrow f_1(x)$. That is a symmetry of the perturbation theory whose meaning can be really understood only after the introduction of the dual series. Actually, the general solution of Eq. (4) can be written, for the one-dimensional case, as

$$t - t_0 = \int_{x_0}^{x} dx' \frac{1}{\sqrt{2}\sqrt{E + \int_{x_0}^{x'} f_0(x'')dx'' + \int_{x_0}^{x'} f_1(x'')dx''}}, \tag{8}$$

with $E$ a motion constant. It is easily seen that both the series expansions, for small $f_0$ or $f_1$, can be straightforwardly obtained. What is interesting is that the small parameter in a case is the inverse of the development parameter in the other. From the discussion above it should be clear that both series can have the same problems as secularities or divergent terms.

A more interesting example is given by the Duffing equation

$$\ddot{x} + \omega_0^2 x + \beta x^3 = f_0 \cos(\omega t). \tag{9}$$

By setting $\tau = \omega_0 t$, $\nu = \omega/\omega_0$, $\xi = (\omega_0^2/f_0)x$, and $\lambda = \beta f_0^2/\omega_0^6$, one gets the rescaled equation

$$\ddot{\xi} + \xi + \lambda \xi^3 = \cos(\nu\tau), \tag{10}$$

where the overdots mean derivation with respect to $\tau$ and $\lambda$ is just a parameter measuring the strength of the nonlinearity. Equation (10) is generally considered, analytically, only for small $\lambda$, but what happens in the limit of a very strong nonlinearity? Duality can be applied and one easily realizes that, for large values of the parameter $\lambda$, the quantity $\epsilon = \frac{1}{2}\dot{\xi}^2 + \lambda \frac{1}{4}\xi^4$ tends to be a constant of motion. This is due to the result that the perturbation completely drives the system. So we have regular periodic motion in the considered limit. This example shows that, although the leading-order equation can be easy to solve, going to higher orders could be very involved.

A class of important problems arises from the Schrödinger equation that I consider in the one-dimensional form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0(x)\psi + \lambda V_1(x)\psi = E\psi, \tag{11}$$

where $\lambda \to \infty$. One could apply immediately the symmetry between the dual and small perturbation theories discussed so far and use without difficulty the Rayleigh-Schrödinger approximation scheme. While that is a correct approach, I will show how the dual method works in this case. So let us set $\xi = \sqrt{\lambda}x$, $\psi = \psi_0 + (1/\lambda)\psi_1 + O(1/\lambda^2)$, and $E = \lambda E_0 + E_1 + O(1/\lambda)$. This yields the equations

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_0}{d\xi^2} + V_1(\epsilon\xi)\psi_0 = E_0\psi_0,$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{d\xi^2} + V_1(\epsilon\xi)\psi_1 + V_0\psi_0 = E_1\psi_0 + E_0\psi_1, \tag{12}$$

$$\vdots$$

where $\epsilon = 1/\sqrt{\lambda}$. At the leading order we get a well-known equation, that is, a second-order differential equation with a slowly varying coefficient due to the perturbation. In this case we can apply the WKB approximation [6]. Thus the dual method yields in this case a solution that is a combination of both Rayleigh-Schrödinger and semiclassical methods.

There are several problems where the above approximation can be applied. A well-known example is given by the anharmonic oscillator that has a large body of literature [7] and is a model that any approximation scheme should address. The Hamiltonian can be cast in the form

$$H = \frac{p^2}{2} + \frac{1}{2}q^2 + \frac{\lambda}{4}q^4. \tag{13}$$

The method I discussed so far gives an unambiguous answer to this problem, i.e., the leading-order approximation, when the anharmonicity is very strong, can be obtained by solving the equation

$$\left(\frac{p^2}{2} + \frac{\lambda}{4}q^4\right)\psi_0(q) = E\psi_0(q). \tag{14}$$

The quartic oscillator is well known in the literature [8]. So we can compare our method with numerical results. To leading order of the WKB approximation of the energy levels, normalized in unit of $[(\hbar^2/2)\sqrt{\lambda/4}]^{2/3}$, the agreement is within 18% with the true value of the ground-state energy for the anharmonic oscillator. That agreement improves for higher excited states. However, we know from Symanzick scaling that the quartic oscillator is the right approximation for energy levels of the anharmonic oscillator when $\lambda \to \infty$ [9]. Often, the use of semiclassical eigenfunctions can be too involved and better approximation schemes, such as those given in Ref. [7], can improve the situation. Duality, as applied in perturbation theory, yields anyway a definite answer.

The situation is surely more interesting in time-dependent problems. By noting that the only meaningful quantities are transition probabilities between states of the unperturbed system, we have the initial conditions definitely fixed, breaking in this way the dual symmetry of the perturbation theory. In fact, in Ref. [3] I showed that the problem

$$[H_0 + \lambda V(t)]|\psi\rangle = i\hbar\partial_t|\psi\rangle \tag{15}$$

with $\partial_t = \partial/\partial t$ and $\lambda \to \infty$, using the above dual method, has the leading-order solution

$$|\psi\rangle \sim U(t)|n\rangle + O\left(\frac{1}{\lambda}\right), \tag{16}$$

with

$$\lambda V(t)U(t) = i\hbar\partial_t U(t) \tag{17}$$

and $H_0|n\rangle = E_n|n\rangle$. So the unperturbed solution fixes the initial condition as also happens in the small perturbation theory. However, in order to leave the dual symmetry untouched, one should physically consider also systems initially prepared with the eigenstates of the perturbation, but this is not the case for the computation of probability transitions. Then we can conclude that for the time-dependent perturbation theory as usually applied in quantum mechanics, the dual symmetry is broken due to the choice of the initial conditions.

By the methods discussed above, we can obtain the main result of the paper. Our aim is to show that the dual to the Dyson perturbation series, for the time-dependent Schrödinger equation, is given by the series obtained by Mostafazadeh [5] having the adiabatic approximation as leading order. So let us consider the Schrödinger equation $H(t)U = i\hbar\partial_t U$, $U$ being the time evolution operator. The Dyson series is the solution of that equation and can be written formally as

$$U(t) = \mathcal{T}\exp\left(-\frac{i}{\hbar}\int_0^t dt' H(t')\right), \tag{18}$$

with $\mathcal{T}$ the time-ordering operator. This is a compact form for the series development

$$U(t) = I - \frac{i}{\hbar}\int_0^t dt' H(t') + \left(-\frac{i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' H(t')H(t'') + \cdots. \tag{19}$$

A dual series to the one above is meant as a series having for development parameter its inverse, as discussed above. To obtain it, let us consider the case with the Hamiltonian $H$ being constant in time. Assuming, for the sake of simplicity, here and in the following that the Hamiltonian has a discrete spectrum, the solution to the time-dependent Schrödinger equation is easily obtained through the time evolution operator $U(t) = \Sigma_n e^{-(i/\hbar)E_n t}|n\rangle\langle n|$, with $H|n\rangle = E_n|n\rangle$, where the effect of the time derivative is simply $\partial_t U(t) = \Sigma_n[-(i/\hbar)E_n]e^{-(i/\hbar)E_n t}|n\rangle\langle n|$. Instead, for a time-dependent Hamiltonian $H(t)$, in the case of the adiabatic approximation we have $U_A(t) = \Sigma_n e^{i\alpha_n(t)}|n,t\rangle\langle n,0|$, where $\alpha_n(t) = \gamma_n(t) - (1/\hbar)\int_0^t dt' E_n(t')$ with $H(t)|n,t\rangle = E_n(t)|n,t\rangle$, so that $E_n(t)$ gives the dynamical part of the phase $\alpha_n(t)$ and $\gamma_n(t) = i\int_0^t dt'\langle n,t'|\partial_{t'}|n,t'\rangle$ the geometrical part. It is natural to ask how one can define a derivative $D_t$ to obtain the same result as for the time-independent case, that is, $D_t U_A(t) = \Sigma_n[-(i/\hbar)E_n(t)]e^{i\alpha_n(t)}|n,t\rangle\langle n,0|$. It is quite easy to verify that the following definition of $D_t$ has the required property

$$D_t = \partial_t + i\sum_{\substack{n,m \\ n\neq m}} \langle m,t|i\partial_t|n,t\rangle|m,t\rangle\langle n,t|, \tag{20}$$

so that the adiabatic approximation is exact for the equation

$$H(t)U_A(t) = i\hbar D_t U_A(t) \tag{21}$$

and it is easily verified that $iD_t|k,t\rangle = \dot{\gamma}_k(t)|k,t\rangle$. In this way, we are a step away from the sought result. In fact, let us introduce a generic perturbation $V(t)$ into Eq. (21), so that

$$[H(t) + V(t)]U(t) = i\hbar D_t U(t). \tag{22}$$

In this form the duality principle of perturbation theory can be applied. Having $V(t)$ as the unperturbed Hamiltonian and $H(t)$ as the perturbation, we get no physical meaningful results from the leading-order equation $V(t)U^{(0)}(t) = i\hbar D_t U^{(0)}(t)$ unless we choose $V(t) = H(t)$ or

$$V(t) = -\sum_{\substack{n,m \\ n\neq m}} \langle m,t|i\hbar\partial_t|n,t\rangle|m,t\rangle\langle n,t|.$$

The latter is the interesting case giving trivially the standard Dyson series. So when we take $H(t)$ as the unperturbed Hamiltonian and $V(t)$ as the perturbation, we have at the leading order

$$H(t)U^{(0)}(t) = i\hbar D_t U^{(0)}(t), \tag{23}$$

but this is nothing other than Eq. (21) and then $U^{(0)}(t) = U_A(t)$ (i.e., at the leading order we have the adiabatic approximation). To complete the identification with the Mostafazadeh result, we have that the higher-order corrections are computed solving the equation

$$H'(t)U'(t) = i\hbar\partial_t U'(t), \tag{24}$$

where

$$H'(t) = U_A^\dagger(t)V(t)U_A(t) = -\sum_{n,m,n\neq m} e^{-i[\alpha_m(t)-\alpha_n(t)]}\langle m,t|i\hbar\partial_t|n,t\rangle|m,0\rangle\langle n,0|, \tag{25}$$

as given in Ref. [5]. Then one obtains [5]

$$U(t) = U_A(t)\mathcal{T}\exp\left(-\frac{i}{\hbar}\int_0^t dt' H'(t')\right), \tag{26}$$

which completes the proof. No adiabatic hypothesis entered into this argument, as it should be.

As an application of that result, a theorem recently derived by me and, in a rigourous way but in a different context, Joye [4] can be obtained for the theory of the strong perturbations in quantum mechanics [3]. In fact, it was proved that, for a quantum system described by the Schrödinger equation $[H_0 + \lambda V(t)]|\psi\rangle = i\hbar\partial_t|\psi\rangle$, in the limit $\lambda \to \infty$, the adiabatic approximation, using the eigenstates of the perturbation $V(t)$, is a good approximation for $|\psi\rangle$. So considering the perturbed system in the interaction picture gives the Hamiltonian $H_I(t) = U^{(0)\dagger}(t)\lambda V(t)U^{(0)}(t)$, where $H_0 U^{(0)}(t) = i\hbar\partial_t U^{(0)}(t)$. Then the result obtained for the

Dyson series by duality can be directly applied to $H_I(t)$. We obtain for a small $\lambda$ (otherwise we miss convergence) the Dyson series

$$U_I(t)=I-\frac{i}{\hbar}\int_0^t dt' H_I(t') + \left(-\frac{i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' H_I(t')H_I(t'')+\cdots \tag{27}$$

and, for a large $\lambda$, the Mostafazadeh result applied to $H_I(t)$ having at the leading order the adiabatic approximation, as it should be. It must be noticed that, in the latter case, the eigenstates to be considered are those of the perturbation. In fact, we have $U^{(0)\dagger}(t)V(t)U^{(0)}(t)|k,t\rangle_I=v_k^I(t)|k,t\rangle_I$, but this is equivalent to $V(t)[U^{(0)}(t)|k,t\rangle_I]=v_k^I(t)[U^{(0)}(t)|k,t\rangle_I]$. Then $v_k^I$ is an eigenvalue of $V(t)$ and $U^{(0)}(t)|k,t\rangle_I$ differs just by a time-dependent phase factor from the corresponding eigenstate of the perturbation. As a by-product, we get the confirmation that higher-order corrections are those computed by the method of strong perturbation theory as given in [4].

In summary, I introduced the duality principle in perturbation theory for differential equations. A dual method with respect to the theory of small perturbation is yielded and a dual symmetry between the two methods arises from the freedom in the choice of what the perturbation is. The use of duality shows that, for the time-dependent Schrödinger equation, the dual series to the Dyson one is given by a perturbation series computed recently by Mostafazadeh, with a well-defined development parameter, having the adiabatic approximation as leading order. This enriches the possibility to analyze quantum systems in completely different regions of their parameter space.


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