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Converging approximations for the calculation of the energy in terms of Planck's constant (*)

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Résumé. — Afin de calculer l'énergie quand $\hbar$ est petit, on développe le second membre de l'équation de Brillouin-Wigner en fonction d'une constante de couplage λ . Les hiérarchies en $\hbar$ et λ se correspondent. Les approximants de Padé du développement du second membre convergent.

Abstract. — In order to calculate the energy when $\hbar$ is small, we expand the right-hand side of the Brillouin-Wigner equation in terms of a coupling constant λ . Both hierarchies in $\hbar$ and λ are connected. The Padé approximants of the right-hand side converge.

The present letter intends to show how the Brillouin-Wigner perturbation theory, combined with Padé approximants, can provide the calculation of eigenenergies of a quantum system with a converging and regular algorithm when Planck's constant vanishes.

For this purpose the unperturbed Hamiltonian $\mathcal{H}_0$ of the system under study is chosen as that of a harmonic oscillator. The unperturbed ground state and energy are labelled Φ_0 and ε_0 , respectively. The total Hamiltonian $\mathcal{H}$ is split into $\mathcal{H}_0$ and a perturbation λV , with $\lambda = 1$ in the physical case. The true eigenenergies E_n of the system are the solutions of the Brillouin-Wigner equation

$$E(\lambda) = \varepsilon_0 + F(E, \lambda), \quad \lambda = 1 \quad (1)$$

$$F(E, \lambda) \equiv \left\langle \Phi_0 \left| \lambda V + \lambda V \frac{Q}{E - \mathcal{H}_0 - \lambda Q V Q} \lambda V \right| \Phi_0 \right\rangle$$

$$= \sum_{k=1}^{\infty} \lambda^k \left\langle \Phi_0 \left| V \left(\frac{Q}{E - \mathcal{H}_0} V \right)^{k-1} \right| \Phi_0 \right\rangle \quad (2)$$

where $Q \equiv 1 - |\Phi_0\rangle\langle\Phi_0|$. Let M be a positive integer. By means of those terms of degree lower or equal to $2M$ of the perturbation expansion of F , eq. (2), with respect to λ , one can construct a Padé

approximant $[M/M]$ of F , $F_M(E, \lambda)$. If one replaces eq. (1) by the approximate equation

$$E(\lambda) = \varepsilon_0 + F_M(E, \lambda) \quad (3)$$

the solutions E_{nM} of this equation are approximations of the exact eigenvalues E_n .

When V is positive semi-definite it can be shown [1] that the values E_{nM} make an increasing sequence of lower bounds to E_n , which converge when $M \rightarrow \infty$. It is also trivial to show that they make a decreasing sequence of upper bounds when V is negative semi-definite. In both cases the main part of the proof is the reconstruction by bounds [2, 3], of the generalized Stieltjes function F by means of its Padé approximants with respect to λ . Regularization techniques [3] are available if necessary.

An interesting feature of the algorithm described by eq. (3) is the dependence of F_M upon $\hbar$. As a matter of fact, it is often possible to choose the splitting of a given $\mathcal{H}$ into $\mathcal{H}_0$ and V in such a way that the k th order term of the perturbation expansion described by eq. (2) is regular when $\hbar \rightarrow 0$ and, not only contains λ^k , but also $\hbar^k$ as a factor. The algorithm thus appears to be, in that sense, a semi-classical algorithm for the calculation of F , or F_M , and finally of E_n , in terms of a hierarchy of powers of $\hbar$.

This assertion can be first proved, for an illustrative example, in the case of a one-dimensional harmonic

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oscillator. Let μ be its mass and ω its frequency. One chooses

$$\mathcal{H}_0 = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{1}{2} \mu \omega_0^2 r^2, \quad \text{with } \omega_0 > \omega \quad (4)$$

and thus the perturbation

$$V = \frac{1}{2} \mu (\omega^2 - \omega_0^2) r^2 \quad (5)$$

is negative semi-definite. It is then trivial to check that any matrix element of V between eigenstates of $\mathcal{H}_0$ brings in a factor $\hbar$. The presence of $\hbar$ in the energy denominators due to $Q/(E - \mathcal{H}_0)$ does not change the global factor $\hbar^k$ which appears in the k th order term of the expansion, eq. (2).

A graphical solution of eq. (3) for the calculation of the ground state energy E_0 is given by figure 1 in the case where $\omega_0 = 2\omega$, with $M = 1$ and $M = 2$. One finds, as expected, a decreasing sequence $\varepsilon_0 = \hbar\omega$, $E_{01} = 0.549 \hbar\omega$, $E_{02} = 0.507 \hbar\omega$, in fast convergence towards $E_0 = 1/2 \hbar\omega$.

Fig. 1.

In the more general case of a one-dimensional particle with a local non-harmonic potential $\mathcal{V}(r)$ one assumes that $\mathcal{V}$ reaches an absolute minimum $\mathcal{V}_m$ at r_m and that its Taylor series around r_m converges. By means of the second derivative $\mathcal{V}_m''$ of $\mathcal{V}$ at r_m one defines the elementary length $l = [\hbar^2/(\mu\mathcal{V}_m'')]^{1/4}$ and a scaling length $l_0 = \alpha l$ with $0 < \alpha \leq 1$. The parameter α will remain temporarily fixed. One defines a scaling energy $e_0 = \hbar^2/(\mu l_0^2)$. The shift and scaling operations $r = r_m + l_0 \rho$ and $E = \mathcal{V}_m + e_0 \varepsilon$ reduce the Schrödinger equation into

$$\left[-\frac{1}{2} \frac{d^2}{d\rho^2} + \frac{1}{2} \alpha^4 \rho^2 + \frac{1}{6} \alpha^5 \frac{\mathcal{V}_m'''}{\mathcal{V}_m''} \rho^3 + \frac{1}{24} \alpha^6 \frac{\mathcal{V}_m^{(4)}}{\mathcal{V}_m''} \rho^4 + \dots - \varepsilon \right] \varphi(\rho) = 0. \quad (6)$$

As well as the quantities l , l_0 and e_0 , the dimensionless numbers $\mathcal{V}_m^{(p)} l^{p-2} / \mathcal{V}_m''$ derived from the derivatives of $\mathcal{V}$ at r_m of order $p > 2$ vanish when $\hbar \rightarrow 0$. For instance the coefficient of ρ^3 is of order $\hbar^{1/2}$. When multiplied by the scaling energy e_0 , which is of order $\hbar$, the contribution of the corresponding matrix element to the calculation of F is thus of order $\hbar^{3/2}$. More generally, any anharmonic term $\mathcal{V}_m^{(p)}(r - r_m)^p$ has matrix elements going like $\hbar^{p/2}$, thus of order $\hbar$ at least since $p > 2$.

If therefore one chooses

$$\mathcal{H}_0 = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \mathcal{V}_m + \frac{1}{2} \mathcal{V}_m'' \alpha^{-4} (r - r_m)^2, \quad (7)$$

$$V = \mathcal{V} - \mathcal{V}_m - \frac{1}{2} \mathcal{V}_m'' \alpha^{-4} (r - r_m)^2, \quad (8)$$

the k th order term with respect to V in the perturbative calculation of F does still contain a factor $\hbar^k$. This is however provided that the series of matrix elements induced by the Taylor series converges. The fast decay of harmonic oscillator wave functions when $|r| \rightarrow \infty$ should help [4] such a convergence in practical cases.

We need still to adjust α so that $V \leq 0$. If $\mathcal{V}_m''' = 0$, which is not unusual in practical cases, one may take $\alpha = 1$, with the benefit of matrix elements of V vanishing like $\hbar^2$. If $\mathcal{V}_m''' \neq 0$, there are often (see Fig. 2) values of $\alpha < 1$ for which $V \leq 0$, except when $\mathcal{V}$ rises too strongly somewhere.

Fig. 2.

It is trivial to generalize these considerations to the case of N particle in d dimensions. One can use a hyperspherical, Nd -dimensional formalism. This holds provided local $\mathcal{V}$, which now depends on Nd coordinates, has a unique absolute minimum. Kinematical degeneracies (translations, rotations) of this minimum would induce the breaking of symmetries by the choice of $\mathcal{H}_0$. Symmetry restauration is possible, however [5].

In conclusion one may by-pass the singularities [6] of an expansion of the energy in terms of $\hbar$, whose nature in $\exp\{1/\hbar\}$ has recently [7] been analysed, by an alternate expansion of the right-hand side of the Brillouin-Wigner equation. Convergence when

$\hbar \rightarrow 0$ is obtained by a positivity condition and the use of Padé approximants.

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