

QUASI-CLASSICAL WAVE FUNCTION OF A SYSTEM WITH MANY DEGREES OF FREEDOM

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An approximate expression is presented for the quasi-classical wave function of a system with many degrees of freedom. The result obtained is valid in a broader range than is perturbation theory.

A quasi-classical solution of the Schrödinger equation can be obtained only for the one-dimensional problem. When the number of degrees of freedom is large, a solution is possible only if the variables separate. Yet, it is precisely for the non-separating variables that the quasi-classical approximation is of special interest, since it is impossible to solve the corresponding classical problem. In this case, some information can be obtained with the aid of perturbation theory. The condition under which the latter is applicable is, as is well known, the inequality $(V/E)(ka) \ll 1$, where V is the perturbation, E the energy of the system, k the wave vector, and a the dimension of the classically admissible region of motion. In the present communication we calculate for a system with many degrees of freedom a quasi-classical wave function which is valid under less stringent requirements.

Let a system with N degrees of freedom have a discrete spectrum and let it be described by a Hamiltonian $H_0 + V$. It is assumed that the variables in H_0 are separable, so that the wave functions $\Psi^0_{(n_k)}$ of the unperturbed system are known; n_k is the set of quantum numbers ($k = 1, \dots, N$). We assume the quasi-classical condition $n_k \gg 1$ to be satisfied. The unperturbed system goes over in the classical limit to a system with a Hamiltonian H_0 , which carries out a finite motion over all the degrees of freedom. Such a system is characterized by a set of frequencies ω_k and action variables I_k . Its energy is $E = E(I_k)$. In order to write down the Schrödinger equation in the action and angle variable representation (φ -representation), it is necessary to replace I_k by the operator $i^{-1}\partial/\partial\varphi_k$. We obtain

$$E\left(\frac{1}{i}\frac{\partial}{\partial\varphi_k}\right)\Psi^0_{(n_k)} = E_{(n_k)}\Psi^0_{(n_k)}. \tag{1}$$

We write down the perturbed equation in the

form

$$E\left(\frac{1}{i}\frac{\partial}{\partial\varphi_k}\right)U_{(n_k)}\Psi^0_{(n_k)} + V\left(\varphi_k, \frac{1}{i}\frac{\partial}{\partial\varphi_k}\right)U_{(n_k)}\Psi^0_{(n_k)} = [E_{(n_k)}^0 + \Delta_{(n_k)}]U_{(n_k)}\Psi^0_{(n_k)}, \tag{2}$$

where $U_{(n_k)}\Psi^0_{(n_k)}$ is the perturbed wave function and $\Delta_{(n_k)}$ is the shift in the level characterized by the numbers n_k (we are considering the nondegenerate case). In the quasi-classical approximation we can replace $i^{-1}\partial/\partial\varphi_k$ in $V(\varphi_k, i^{-1}\partial/\partial\varphi_k)$ by n_k , since $i^{-1}\partial/\partial\varphi_k \sim n_k$, and the noncommutativity of φ_k and $\partial/\partial\varphi_k$ is of the order of unity.

We are interested in the correction to the wave function corresponding to the n_k level. We expand $E(\hat{I}_k)$ in powers of $(\hat{I}_k - n_k)$ and confine ourselves to the linear term. The error resulting from this is best estimated by comparing the final result with the known expression for the quasi-classical wave function of the one-dimensional problem, as will be done below. We thus obtain

$$\sum_k \frac{1}{i}\omega_k \partial U_{(n_k)}\Psi^0_{(n_k)}/\partial\varphi_k + V(\varphi_k, n_k)U_{(n_k)}\Psi^0_{(n_k)} = [E_{(n_k)}^0 + \Delta_{(n_k)}]U_{(n_k)}\Psi^0_{(n_k)}. \tag{3}$$

Inasmuch as $\Psi^0_{(n_k)}$ is a solution of (3) when $V = \Delta = 0$, $U_{(n_k)}$ satisfies the equation¹⁾

$$\sum_k \omega_k \partial U_{(n_k)}/\partial\varphi_k = i[\Delta_{(n_k)} - V(\varphi_k, n_k)]U_{(n_k)}. \tag{4}$$

We write its solution in the form

¹⁾An equation similar to (4) can be obtained with the aid of perturbation theory of classical mechanics, by writing Ψ in the form $\exp(iS)$, where S is the classical action. The difference in this case lies in the absence of the term with Δ in the right half. The calculation of the level shift thus constitutes a separate problem.

$$U_{(n_k)} = \exp\left(\frac{i\Delta_{(n_k)}}{N} \sum_k \frac{\Phi_k}{\omega_k}\right) \exp\left[i \int_0^{t_0} V(\varphi_k + \omega_k t) dt\right], \quad (5)$$

where t_0 is the root of the equation $V_k(\varphi_k + \omega_k t_0) = 0$. The function $V(\varphi_k)$, specified in the region $0 \leq \varphi_k \leq 2\pi$, is continued analytically in all of φ_k space, and the root t_0 can, in particular, be complex.

The expression for $\Delta_{(n_k)}$ can be readily obtained by considering the two equations

$$\begin{aligned} (H_0 + V) U\Psi_{(n_k)}^0 &= [E_{(n_k)}^0 + \Delta_{(n_k)}] U\Psi_{(n_k)}^0, \\ H_0\Psi_{(n_k)}^0 &= E_{(n_k)}^0 \Psi_{(n_k)}^0. \end{aligned} \quad (6)$$

Multiplying from the left by $\overline{\Psi_{(n_k)}^0}$ and integrating, we get

$$\Delta_{(n_k)} = \langle n_k | UV | n_k \rangle / \langle n_k | U | n_k \rangle. \quad (7)$$

The matrix elements in (7) are taken over by the unperturbed wave functions. Formulas (5) and (7) solve our problem in the φ -representation.

The transition to the x -representation is made in accordance with the well-known formulas for unitary transformations. We present the result only. The transition matrix $f_{\varphi_k}(x_k)$ is

$$f_{\varphi_k}(x_k) = \sum_{n_1 \dots n_N} \Psi_{n_k}^0(\varphi_k) \Psi_{n_k}^0(x_k). \quad (8)$$

The perturbed wave function in the x -representation is

$$\Psi_{(n_k)}(x_k) = \int U_{n_k}(\varphi_k) \Psi_{n_k}^0(\varphi_k) f_{\varphi_k}(x_k) d\varphi_1 \dots d\varphi_N. \quad (9)$$

The function $V(\varphi_k, n_k)$ is determined by its Fourier components

$$\{V(\varphi_k, n_k)\}_{m_k} = \langle n_k - m_k | V | n_k \rangle, \quad (10)$$

where the matrix element is taken over the unperturbed wave functions in the x -representation. Formula (10) corresponds to the well known expression for matrix elements calculated with quasi-classical wave functions.

To estimate the applicability limits of the obtained results we consider the one-dimensional case. Formula (5) then assumes the form

$$U_n(\varphi) = \exp\left\{\frac{i}{\omega} \int_0^{\varphi} [\Delta - V(\varphi')] d\varphi'\right\}. \quad (11)$$

On the other hand, there exists an 'exact' quasi-classical function

$$\begin{aligned} \Psi_n(x) &= U_n(x) \Psi_n^0(x) \\ &= \{2[E_n + \Delta_n - U(x) - V(x)]\}^{-1/2} \\ &\times \exp\left\{i \int_{x_0}^x \sqrt{2[E_n + \Delta_n - U(x) - V(x)]} + \gamma_n\right\}. \end{aligned} \quad (12)$$

Taking into account the relation

$$\varphi = \omega t = \omega \int_{x_0}^x \frac{dx}{\sqrt{2[E - U(x)]}}, \quad (13)$$

we verify that formula (11) gives the first term in the expansion of the square root in the exponent of (12) in powers of $(\Delta_n - V)/(E_n - U) \sim V/E$.

The condition for the validity of this approximation is

$$(V/E)(ka)^{1/2} \ll 1, \quad ka \sim n. \quad (14)$$

It is necessary to put in the pre-exponential factor $V = \Delta = 0$, which corresponds to the condition

$$V/E \ll 1. \quad (15)$$

Finally, we disregarded in the derivation the displacement δa of the cusp (in the multi-dimensional case—the caustic). Its order of magnitude is $\delta a = aV/E$. This neglect is valid if δa is much smaller than the distance from the cusp, at which the quasi-classical solution is 'pieced together' with the solution of the Airy equation. This leads to the inequality

$$(V/E)(ka)^{3/2} \ll 1. \quad (16)$$

The limitation (16) is the strongest of the three and determines the limits of applicability of the results obtained.

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