

I. WIGNER FUNCTION FOR ANHARMONIC OSCILLATOR

We consider Hamiltonian of a harmonic oscillator perturbed by a polynomial potential,

$$H = \frac{1}{2} \sum_{i=1}^N \left(p_i^2 + \omega_i^2 q_i^2 \right) + \lambda \sum_{\{k_i\}} f_{\{k_i\}} q_1^{k_1} q_2^{k_2} q_1^{k_1} \dots q_N^{k_N}, \quad (1)$$

where summation is performed over N -component multi-indexes $\{k_i\}$. Here, we restrict ourselves to cubic anharmonic terms with $k_1 + k_2 + \dots + k_N = 3$, although this method could be extended in principle to higher anharmonic corrections. In (1), λ is a small perturbation parameter.

The perturbed Wigner-function is expanded in powers of λ ,

$$\rho(\vec{p}, \vec{q}) = \rho_0(\vec{p}, \vec{q}) + \lambda \rho_1(\vec{p}, \vec{q}) + O(\lambda^2), \quad (2)$$

where

$$\rho_0(\vec{p}, \vec{q}) = \exp \left(- \sum_{i=1}^N \left(\frac{p_i^2}{\omega_i} + \omega_i q_i^2 \right) \right) \quad (3)$$

is the harmonic-oscillator Wigner function, and $\rho_1(\vec{p}, \vec{q})$ is the first anharmonic correction to be determined here.

To develop perturbation theory for the ground state wave function $\Psi(\vec{q})$, it is convenient to rewrite the Scrodinger equation in terms of the function $S(\vec{q}) = -\ln \Psi(\vec{q})$ []:

$$-\frac{1}{2} \sum_{i=1}^N \left(\frac{\partial S}{\partial q_i} \right)^2 + \frac{1}{2} \sum_{i=1}^N \frac{\partial^2 S}{\partial q_i^2} + V(\vec{q}) - E = 0 \quad (4)$$

Without the second sum, Eq. (4) reduces to Hamilton - Jacobi equation for action of a classical particle moving in a potential $E - V(\vec{q})$. In such a quasiclassical limit, perturbation theory for $S(\vec{q})$ is easily developed []. More general quantum case which is considered here is still solvable analytically, but resulting corrections have more monomial terms.

Let us expand quantities entering Eq. (4) in powers of λ :

$$S(\vec{q}) = S_0(\vec{q}) + \lambda S_1(\vec{q}) + O(\lambda^2), \quad (5)$$

$$V(\vec{q}) = V_0(\vec{q}) + \lambda V_1(\vec{q}) + O(\lambda^2), \quad (6)$$

$$E = E_0 + \lambda E_1 + O(\lambda^2). \quad (7)$$

Zero-order terms are:

$$S_0(\vec{q}) = \frac{1}{2} \sum_{i=1}^N \omega_i q_i^2 \quad (8)$$

$$V_0(\vec{q}) = \frac{1}{2} \sum_{i=1}^N \omega_i^2 q_i^2 \quad (9)$$

$$E_0 = \frac{1}{2} \sum_{i=1}^N \omega_i. \quad (10)$$

First-order correction to the potential, see Eq. (1), is

$$V_1(\vec{q}) = \sum_{k_1+k_2+\dots+k_N=3} f_{\{k_i\}} q_1^{k_1} q_2^{k_2} q_1^{k_1} \dots q_N^{k_2}. \quad (11)$$

Expansions (5) are substituted into Eq. (4), and the left hand side is expanded in λ . In the first order in λ , Eq. (4) is equivalent to

$$-\sum_{i=1}^N \frac{\partial S_0}{\partial q_i} \frac{\partial S_1}{\partial q_i} + \frac{1}{2} \sum_{i=1}^N \frac{\partial^2 S_1}{\partial q_i^2} + V_1(\vec{q}) - E_1 = 0 \quad (12)$$

which is a linear equation in respect to a number E_1 and a function $S_1(\vec{q})$.

Let us suppose that $S_1(\vec{q})$ is a polynomial

$$S_1(\vec{q}) = \sum_{\{k_i\}} s_{\{k_i\}} q_1^{k_1} q_2^{k_2} q_1^{k_1} \dots q_N^{k_2}. \quad (13)$$

Then Eq. (12) is equivalent to a set of linear equations in respect to coefficients $s_{\{k_i\}}$ and E_1 ,

$$\sum_{i=1}^N \left[-k_i \omega_i s_{\{k_i\}} + \frac{1}{2} (k_i + 1)(k_i + 2) s_{\{k_1, k_2, \dots, k_i+2, \dots, k_N\}} \right] + f_{\{k_i\}} - \delta(\{k_i\}, \{0\}) E_1 = 0, \quad (14)$$

where coefficients are supposed to be zero if one of indexes is negative.

Since inhomogeneous part of Eq. (12), $V_1(\vec{q}) - E_1$, is a third degree polynomial, it may be shown that the solution is at most a third degree polynomial too,

$$\begin{aligned} S_1(\vec{q}) = & \sum_{k_1+k_2+\dots+k_N=1} A_{\{k_i\}} q_1^{k_1} q_2^{k_2} q_1^{k_1} \dots q_N^{k_2} + \sum_{k_1+k_2+\dots+k_N=2} B_{\{k_i\}} q_1^{k_1} q_2^{k_2} q_1^{k_1} \dots q_N^{k_2} \\ & + \sum_{k_1+k_2+\dots+k_N=3} C_{\{k_i\}} q_1^{k_1} q_2^{k_2} q_1^{k_1} \dots q_N^{k_2}. \end{aligned} \quad (15)$$

In (15), we split (13) in three homogeneous polynomials of the first, the second, and the third degrees. Now, recurrence relation (14) between polynomial coefficients reads

$$B_{\{2,0,0,\dots,0\}} + B_{\{0,2,0,\dots,0\}} + \dots + B_{\{0,0,0,\dots,2\}} - E_1 = 0 \quad (16)$$

$$\sum_{i=1}^N [-k_i \omega_i A_{\{k_i\}} + \frac{1}{2}(k_i + 1)(k_i + 2)C_{\{k_1, k_2, \dots, k_i+2, \dots, k_N\}}] = 0 \quad (17)$$

$$\sum_{i=1}^N k_i \omega_i B_{\{k_i\}} = 0 \quad (18)$$

$$-\sum_{i=1}^N k_i \omega_i C_{\{k_i\}} + f_{\{k_i\}} = 0 \quad (19)$$

It follows from (19) that

$$C_{\{k_i\}} = \left(\sum_{i=1}^N k_i \omega_i \right)^{-1} f_{\{k_i\}}. \quad (20)$$

It follows from (18) that $B_{\{k_i\}} = 0$, and from (16) that $E_1 = 0$. Finally, from (17)

$$A_{\{k_i\}} = \frac{1}{2} \left(\sum_{i=1}^N k_i \omega_i \right)^{-1} \sum_{i=1}^N (k_i + 1)(k_i + 2)C_{\{k_1, k_2, \dots, k_i+2, \dots, k_N\}}. \quad (21)$$

Since the perturbed wavefunction is $\Psi(\vec{q}) = [1 - \lambda S_1(\vec{q})] \exp(-S_0(\vec{q})) + O(\lambda^2)$, then $\rho_1(\vec{p}, \vec{q})$ is a contribution to Wigner transform from integration of the function, $-2S_1(\vec{q} + \vec{\eta}/2) \exp(-S_0(\vec{q} + \vec{\eta}/2)) \exp(-S_0(\vec{q} - \vec{\eta}/2))$. Substituting there expansion (15), we finally find

$$\begin{aligned} \rho_1(\vec{p}, \vec{q}) = & - \sum_{k_1+k_2+\dots+k_N=1} A_{\{k_i\}} F_{k_1, \omega_1}(p_1, q_1) F_{k_2, \omega_2}(p_2, q_2) \dots F_{k_N, \omega_N}(p_N, q_N) \\ & - \sum_{k_1+k_2+\dots+k_N=3} C_{\{k_i\}} F_{k_1, \omega_1}(p_1, q_1) F_{k_2, \omega_2}(p_2, q_2) \dots F_{k_N, \omega_N}(p_N, q_N). \end{aligned} \quad (22)$$

where

$$F_{k, \omega}(p, q) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\eta (q + \eta/2)^k \exp\left(-\frac{\omega}{2}(q + \eta/2)^2 - \frac{\omega}{2}(q - \eta/2)^2\right) \cos(p\eta). \quad (23)$$

It can be expressed analitically as

$$\begin{aligned} F_{0, \omega}(p, q) &= \frac{2}{\sqrt{\pi\omega}} \exp\left(-\frac{p^2}{\omega} - \omega q^2\right), \\ F_{1, \omega}(p, q) &= \frac{2q}{\sqrt{\pi\omega}} \exp\left(-\frac{p^2}{\omega} - \omega q^2\right), \end{aligned}$$

$$\begin{aligned}
F_{2,\omega}(p, q) &= \frac{\omega - 2p^2 + 2\omega^2 q^2}{\sqrt{\pi\omega\omega^2}} \exp\left(-\frac{p^2}{\omega} - \omega q^2\right), \\
F_{3,\omega}(p, q) &= \frac{q(3\omega - 6p^2 + 2\omega^2 q^2)}{\sqrt{\pi\omega\omega^2}} \exp\left(-\frac{p^2}{\omega} - \omega q^2\right).
\end{aligned} \tag{24}$$

Indexes higher than 3 don't enter (22).

Final result of this section is given by Eq. (22), (24), (20), and (21).