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On Quasiclassical Quantization

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A method of calculating the energy levels in a quasiclassical quantization is presented for the one-dimensional case. The value of the levels is obtained in the form of in expansion $\hbar$. Under certain assumptions on the form of the potential energy $U(x)$, this expansion can be obtained in a general form. Computations are carried out for a potential energy having a minimum and rising on either side of the minimum, i.e., of an oscillator type.

As is well known, in the quasiclassical method for the solution of the problems of quantum mechanics, the wave equation ψ is written in the form

$$\psi = e^{i\sigma/\hbar}. \tag{1}$$

Making this formal substitution in the Schrödinger equation

$$\Delta\psi + (2\mu/\hbar^2)(E - U) = 0, \tag{2}$$

we obtain an equation for the function σ:

$$(\nabla\sigma)^2 + (\hbar/i)\Delta\sigma = 2\mu(E - U). \tag{3}$$

The formal solution of Eq. (3) is written in the form of a power series in $\hbar$:

$$\sigma = \sigma_0 + (\hbar/i)\sigma_1 + (\hbar/i)^2\sigma_2 + \ldots \tag{4}$$

Substituting (4) in (3), we ultimately get, for the one-dimensional case,

$$\sigma_0' = p;\ \sigma_1' = -p'/2p;\ \sigma_2' = p''/4p^2 - 3p'^2/8p^3; \tag{5}$$
$$\sigma_3' = -p'''/8p^3 + 3p''p'/4p^4 - 3p'^3/4p^5;$$
$$\sigma_4' = p^{(IV)}/16p^4 - 5p'''p'/8p^5 - 13p''^2/32p^5 + 99p''p'^2/32p^6 - 297p'^4/128p^7;\ldots,$$

where $p = \sqrt{2\mu(E-U)}$ is the classical momentum.

For real p, the quantities $\sigma_0', \sigma_1', \ldots$ and $\sigma_0, \sigma_1, \ldots$ are real, and the quantity σ can be uniquely divided into two components which define the phase and modulus of the wave function:

$$\psi = \exp\{\sigma_1 - \hbar^2\sigma_3 + \hbar^4\sigma_5 - \ldots\} \times \exp\{i(\sigma_0/\hbar - \hbar\sigma_2 + \hbar^3\sigma_4 - \ldots)\}. \tag{6}$$

Another linearly independent solution of the Schrödinger equation is obtained by substituting $i \to -i$ in Eq. (6). For imaginary p, all the expressions in the exponent are real.

Let $x = a$ be a turning point, i.e., $U(a) = E$. Let us find the phase of the wave function for $x > a$, considering that, in this region, $E > U(x)$, and in the region $x < a$, $E < U(x)$, and the modulus of the wave function decreases with decreasing x. Solving the Schrödinger equation exactly in the neighborhood of the turning point, where the potential energy can be approximated by a linear function of the coordinate x, and joining the exact solution with the quasiclassical one, we obtain an expression for the phase, as is usually done. The exact solution of the Schrödinger equation with a linear potential which satisfies the conditions set forth above has the form (except for a constant multiplier)

$$\psi = \begin{cases} \sqrt{|\xi|}\left[I_{-1/3}\left(\frac{2}{3}|\xi|^{3/2}\right) + I_{1/3}\left(\frac{2}{3}|\xi|^{3/2}\right)\right], & x < 0; \\ \sqrt{\xi}\left[J_{-1/3}\left(\frac{2}{3}\xi^{3/2}\right) + J_{1/3}\left(\frac{2}{3}\xi^{3/2}\right)\right], & x > 0, \end{cases}$$

$$\xi = \alpha x/\hbar^{3/2},\quad \alpha = \sqrt{2\mu(-\partial U/\partial x)_a}.$$

Its asymptotic expansion for $\hbar \to 0$ can be written for $x > 0$ in the form*

$$\frac{3}{\sqrt{\pi}} \frac{1}{\xi^{1/4}} \exp\left\{-\frac{5}{64}\frac{1}{\xi^3} + \frac{565}{2048}\frac{1}{\xi^6} - \ldots\right\} \sin\left(\frac{2}{3}\xi^{3/2} + \frac{\pi}{4} - \frac{5}{48}\frac{1}{\xi^{3/2}} + \frac{1105}{9216}\frac{1}{\xi^{9/2}} - \ldots\right). \tag{7}$$

The phase of $\frac{2}{3}\frac{\alpha x^{3/2}}{\hbar} + \frac{\pi}{4} - \frac{5}{48}\frac{\hbar}{\alpha x^{3/2}} + \frac{1105}{9216}\frac{\hbar^3}{\alpha^3 x^{9/2}}$ must be joined with the phase of the function

$$\exp\{\sigma_1 - \hbar^2\sigma_3 + \hbar^4\sigma_5 - \ldots\} \times \sin\left(\frac{\sigma_0}{\hbar} - \hbar\sigma_2 + \hbar^3\sigma_4 - \ldots + \text{const}\right) \tag{8}$$

close to $x = a$, determining the unknown constant in this case.

At the point $x = a$, the momentum p vanishes; if x is considered as a complex variable, then for $p(x)$, the point $x = a$ is a branch point in which $p(x)$ is a double-valued function. The functions $\sigma_0', \sigma_2', \sigma_4', \ldots$ are also double-valued from the branch point for $x = a$, as is evident from Eq. (5).

To obtain the functions $\sigma_0, \sigma_2, \sigma_4, \ldots$, it is appropriate to carry out the transformation from ordinary to contour integration, since the functions $\sigma_2', \sigma_4', \ldots$ go to infinity for $x = a$. We make a cut in the complex plane x, going to the right from the point $x = a$; on the bottom side of the cut, let the square root take the positive sign, and on the upper side, the negative sign. Then the integral over x reduces to one-half the integral over the loop in which we go around from the point x on the upper side of the cut surrounding the point $x = a$ and proceed to the point x on the lower side of the cut.

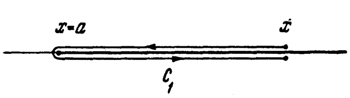

FIG. 1

* The series in the exponent and in the sine argument are determined identically. Upon expansion of the exponent and the sine in powers of $\xi^{-3/2}$, we obtain an asymptotic expansion in a series in the usual form, keeping all successive terms of the expansion up to terms of that order which they have in the exponent and in the sine argument.

For such a determination of the functions σ_0, $\sigma_2, \sigma_4, \ldots$, we have

$$\sigma_0 = \tfrac{1}{2}\int_{C_1} \sigma_0'\,dx; \qquad \sigma_2 = \tfrac{1}{2}\int_{C_1} \sigma_2'\,dx; \quad \sigma_4 = \tfrac{1}{2}\int_{C_1} \sigma_4'\,dx, \ldots \tag{9}$$

Comparing (6), (7) and (9), for x close to a, we obtain for the phase the value

$$\sigma_0/\hbar + \pi/4 - \hbar\sigma_2 + \hbar^3\sigma_4 - \ldots, \tag{10}$$

where the $\sigma_0, \sigma_2, \sigma_4, \ldots$ are determined by Eqs. (9).

We now consider a form of the potential energy $U(x)$ in which there are two turning points, $x = a$, $x = b$, where for $a < x < b$, $U(x) < E$, and in the rest of the region, $U(x) > E$. The wave function which vanishes for $x < a$ has (for $x > a$) the form (it can be considered real), except for a constant multiplier,

$$\exp\left\{\sigma_1 - \hbar^2\sigma_3 + \hbar^4\sigma_5 - \ldots\right\} \times \sin\left(\frac{\sigma_0}{\hbar} + \frac{\pi}{4} - \hbar\sigma_2 + \hbar^3\sigma_4 - \ldots\right), \tag{11}$$

where the $\sigma_0, \sigma_2, \sigma_4, \ldots$ are determined by Eqs. (9). The wave function which vanishes for $x > b$ has (for $x < b$) the form

$$\exp\{\sigma_1 - \hbar^2\sigma_3 + \hbar^4\sigma_5 - \ldots\} \times \sin\left(\frac{s_0}{\hbar} + \frac{\pi}{4} - \hbar s_2 + \hbar^3 s_4 - \ldots\right), \tag{12}$$

where the $s_0, s_2, s_4, \ldots$ are determined by

$$s_0 = \tfrac{1}{2}\int_{C_2} \sigma_0'\,dx; \qquad s_2 = \tfrac{1}{2}\int_{C_2} \sigma_2'\,dx; \quad s_4 = \tfrac{1}{2}\int_{C_2} \sigma_4'\,dx, \ldots \tag{13}$$

The contour C_2 is a loop surrounding the point $x = b$ in a counter-clockwise direction, in which the cut is taken from the point $x = b$ to the left; on the lower side of the cut the square root is positive, on the upper side it is negative.

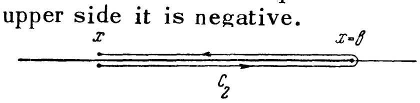

FIG. 2

The wave function of the energy level must vanish for $x < a$ and $x > b$; the decompositions (11) and (12) represent one and the same function; therefore, the phases determined by Eqs.(11) and (12) must in total give an integral multiple of π, which leads to the condition

$$\oint_C \sigma_0' dx - \hbar^2 \oint_C \sigma_2' dx + \hbar^4 \oint_C \sigma_4' dx - \ldots = (n + 1/2)\, 2\pi\hbar, \tag{14}$$

where the σ_0', σ_2', σ_4', ... are determined by Eqs. (5), $n = 0, 1, 2, \ldots$, and the closed integration contour C surrounds the points $x = a$ and $x = b$ in the counter-clockwise direction. The condition (14) is the exact quantization rule of Bohr.

FIG. 3

The quantities σ_0', σ_2', σ_4', ... entering into (14) are equal, according to Eq. (5), to the following:

$$\sigma_0' = \sqrt{2\mu(E-U)}; \tag{15}$$

$$\sigma_2' = -U''/8\sqrt{2\mu}(E-U)^{3/2} - 5U'^2/32\sqrt{2\mu}(E-U)^{5/2};$$

$$\sigma_4' = -U^{(IV)}/32(2\mu)^{3/2}(E-U)^{5/2} - 7U'''U'/32(2\mu)^{3/2}(E-U)^{7/2} - 19U''^2/128(2\mu)^{3/2}(E-U)^{7/2} - 221U''U'^2/256(2\mu)^{3/2}(E-U)^{9/2} - 1105U'^4/2048(2\mu)^{3/2}(E-U)^{11/2}, \ldots$$

We carry out the integration in Eq. (14) in the general form under the supposition that the potential energy $U(x)$ at a certain point has a minimum, and at points $x = a$ and $x = b$, $U(a) = U(b) = E$. We locate the origin of the coordinates at $U(x)$ so that $U(0) = 0$, $U'(0) = 0$. We displace the contour of integration C which surrounds the points $x = a$ and $x = b$ in the complex plane x so that the condition $E < |U(x)|$ is satisfied on it, which permits us to expand the function (15) in a series in E. This can be accomplished in each case if the singular points of the function $\sqrt{E - U(x)}$ are sufficiently far from the points $x = a$, $x = b$.

Thus, over the entire path of integration, cut longitudinally by the method described above, we have

$$\sigma_0' = i\sqrt{2\mu U}\sqrt{1 - \frac{E}{U}} \tag{16}$$

$$= i\sqrt{2\mu U}\left\{1 - \frac{1}{2}\frac{E}{U} - \frac{1}{2\cdot 4}\left(\frac{E}{U}\right)^2 - \frac{1\cdot 3}{2\cdot 4\cdot 6}\left(\frac{E}{U}\right)^3 - \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6\cdot 8}\left(\frac{E}{U}\right)^4 - \ldots\right\};$$

$$\sigma_2' = -\frac{iU''}{8\sqrt{2\mu}U^{3/2}}\left\{1 + \frac{3}{2}\frac{E}{U} + \frac{3\cdot 5}{2\cdot 4}\left(\frac{E}{U}\right)^2 + \ldots\right\} + \frac{5}{32}\frac{iU'^2}{\sqrt{2\mu}U^{5/2}}\left\{1 + \frac{5}{2}\frac{E}{U} + \frac{5\cdot 7}{2\cdot 4}\left(\frac{E}{U}\right)^2 + \ldots\right\};$$

$$\sigma_4' = \frac{iU^{(IV)}}{32(2\mu)^{3/2}U^{5/2}} - \frac{7}{32}\frac{iU'''U'}{(2\mu)^{3/2}U^{7/2}} - \frac{19}{128}\frac{iU''^2}{(2\mu)^{3/2}U^{7/2}} + \frac{221}{256}\frac{iU''U'^2}{(2\mu)^{3/2}U^{9/2}} - \frac{1105}{2048}\frac{iU'^4}{(2\mu)^{3/2}U^{11/2}} + \ldots,$$

Substituting (16) in (14), we obtain an equation for E, the solution of which is to be sought in the form of a series in $\hbar$:

$$E = \hbar E_1 + \hbar^2 E_2 + \hbar^3 E_3 + \ldots \tag{17}$$

Then the equation takes the form

$$i\oint_C dx\left\{\sqrt{2\mu U} + \hbar\left(-\frac{1}{2}\frac{\sqrt{2\mu}E_1}{U^{1/2}}\right) + \hbar^2\left(-\frac{\sqrt{2\mu}E_2}{2U^{1/2}} - \frac{\sqrt{2\mu}E_1^2}{8U^{3/2}} + \frac{U''}{8\sqrt{2\mu}U^{3/2}} - \frac{5U'}{32\sqrt{2\mu}U^{5/2}}\right) + \hbar^3\left(-\frac{\sqrt{2\mu}E_3}{2U^{1/2}} - \frac{\sqrt{2\mu}E_1E_2}{4U^{3/2}} - \frac{\sqrt{2\mu}E_1^3}{16U^{5/2}} + \frac{3U''E_1}{16\sqrt{2\mu}U^{5/2}} - \frac{25U'^2E_1}{64\sqrt{2\mu}U^{7/2}}\right)\right.$$

$$+ \hbar^4\left(-\frac{\sqrt{2\mu}E_4}{2U^{1/2}} - \frac{\sqrt{2\mu}E_1E_3}{4U^{3/2}} - \frac{\sqrt{2\mu}E_2^2}{8U^{3/2}} - \frac{3\sqrt{2\mu}E_1^2E_2}{16U^{5/2}} - \frac{5\sqrt{2\mu}E_1^4}{128U^{7/2}} + \frac{3U''E_2}{16\sqrt{2\mu}U^{5/2}} + \frac{15U''E_1^2}{64\sqrt{2\mu}U^{7/2}} - \frac{25U'^2E_2}{64\sqrt{2\mu}U^{7/2}} - \frac{175U'^2E_1^2}{256\sqrt{2\mu}U^{9/2}} + \frac{U^{(IV)}}{32(2\mu)^{3/2}U^{5/2}} - \frac{7U'''U'}{32(2\mu)^{3/2}U^{7/2}} - \frac{19U''^2}{128(2\mu)^{3/2}U^{7/2}} + \frac{221U''U'^2}{256(2\mu)^{3/2}U^{9/2}}\right.$$

$$\left.\left. - \frac{1105U'^4}{2048(2\mu)^{3/2}U^{11/2}}\right) + \ldots\right\} = \left(n + \frac{1}{2}\right)2\pi\hbar.$$

Equating terms with equal powers of $\hbar$, we can, term by term, find the coefficients of the series (17). The term without $\hbar$ is identically equal to zero, since the integrand $+\sqrt{U(x)}$ is a single-valued function which has no singularities inside the contour C [we recall that $U(0) = 0$, $U'(0)=0$].

The terms for $\hbar$ give

$$-i\frac{\sqrt{2\mu}E_1}{2}\oint_C \frac{dx}{\sqrt{U}} = \left(n+\frac{1}{2}\right)2\pi.$$

The function under the integral, $1/+\sqrt{U(x)}$, is a single-valued function having one pole within the contour C (at $x = 0$) with residue

$$\sqrt{2/U''(0)},$$

therefore,

$$E_1 = \sqrt{U''(0)/\mu}\,(n + {}^1/_2). \tag{18}$$

Equating to zero the terms in $\hbar^2$, we take it into consideration that each of the components in the integrand is single-valued inside the contour C and has a single pole at $x = 0$ with a corresponding residue. Computing these residues and using E_1 from (18), we obtain

$$E_2 = \frac{1}{\mu}\left[\frac{(n+{}^1/_2)^2}{16}\left(\frac{U^{(\mathrm{IV})}(0)}{U''(0)} - \frac{5U'''^2(0)}{3U''^2(0)}\right) + \frac{1}{64}\left(\frac{U^{(\mathrm{IV})}(0)}{U''(0)} - \frac{7U'''^2(0)}{9U''^2(0)}\right)\right]. \tag{19}$$

Additional coefficients in the expansion (17) are computed in similar fashion. Thus,

$$E_3 = \frac{\hbar^3}{\mu^{3/2}\sqrt{U''(0)}}\left\{\frac{\left(n+\frac{1}{2}\right)^3}{288}\left(\frac{U^{(\mathrm{VI})}(0)}{U''(0)} - \frac{17U^{(\mathrm{IV})2}(0)}{8U''^2(0)} - \frac{7U^{(\mathrm{V})}(0)\,U'''(0)}{U''^2(0)} + \frac{75U^{(\mathrm{IV})}(0)\,U'''^2(0)}{4U''^3(0)} - \frac{235U'''^4(0)}{24U''^4(0)}\right)\right.$$
$$\left. + \frac{5}{1152}\left(n+\frac{1}{2}\right)\left(\frac{U^{(\mathrm{VI})}(0)}{U''(0)} - \frac{67U^{(\mathrm{IV})2}(0)}{40U''^2(0)} - \frac{19U^{(\mathrm{V})}(0)\,U'''(0)}{5U''^2(0)} - \frac{153U^{(\mathrm{IV})}(0)\,U'''^2(0)}{20U''^3(0)} - \frac{77U'''^4(0)}{24U''^4(0)}\right)\right\}. \tag{20}$$

The term E_1 corresponds to a harmonic oscillator, while the subsequent terms are determined by the departure from harmonicity.

Equations (17)-(20) give a better approximation for small n, i.e., for the lower levels.

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