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Convergent Iteration Method for the Anharmonic Oscillator Schrödinger Eigenvalue Problem

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A new method is presented for solving the Schrödinger eigenvalue problem for anharmonic oscillators, using the Liouville transformation and a systematic iteration procedure. The Liouville transformation changes the potential V in the original eigenvalue equation to Q, which is highly singular. But, the singularity can be softened by rewriting the basic equation. We turn the equation into an integral equation and solve it by iteration. A simple criterion is established for the convergence of the iteration series. Our method is tested on the model of $2\mu x^2 + \lambda x^4$ potential ($\mu, \lambda > 0$) for the purpose of comparing it with the perturbation theory. Most remarkably, our method gives iteration series for the eigenfunctions $u_n(x)$, converging uniformly in x irrespective of the magnitude of λ, implying the convergence for the eigenvalues also, while the perturbation theory is known to give divergent series no matter how small λ is. Our method gives very good results for eigenvalues already at the first iteration, the better for the higher excited states.

KEYWORDS: Schrödinger eigenvalue problem, approximation method, Liouville transformation, convergent iteration, ($2\mu x^2 + \lambda x^4$)-potential

1. Introduction

There have been continued efforts to develop approximation methods for solving the Schrödinger eigenvalue problem for the anharmonic oscillator with potential $2\mu x^2 + \lambda x^4$: numerical solution[1)] by Milne's method;[2)] the perturbation method[3–6)] and the WKB method[7–9)] both with series diverging but asymptotic and Borel summable; the so-called variational Sturmian approximation;[10,11)] and asymptotic iteration method[12)] whose convergence has not been examined yet.

We would like to add one more method based on the Liouville transformation, which gives a *convergent* iteration series, at least to the model we consider as a touchstone. It is true that the eigenvalues can be obtained numerically by Milne's method easily and to an arbitrary degree of approximation, and then the eigenfunctions likewise by numerically solving Schrödinger equation for the eigenvalues so obtained, but it is certainly useful to have simple analytic expressions for the eigenfunctions to a good approximation.

We shall present our method in §2 for a one-dimensional Schrödinger equation with a potential $V(x)$ which grows to $+\infty$ as $x \to \pm\infty$, and is in addition assumed to be symmetric for the sake of simplicity. We use the Liouville transformation with singularities of the transformed potential softened significantly by rewriting the basic equation. We convert the equation to an integral equation, which we solve by iteration in §3, establishing in §4 a sufficient condition for its convergence, uniform in x. The eigenvalues are extracted from the eigenfunctions, so that the uniform convergence of the eigenfunctions implies the convergence for the eigenvalues.

The use of the Liouville transformation makes our eigenfunctions look like the ones in the WKB approximation, but it is different because firstly it is not an expansion in powers of $\hbar$, and moreover gives a convergent series at least for the models, one presented below and the others to be treated in the paper to follow, in contrast to the divergent one in the WKB approximation,[7,8)] and secondly it does not use asymptotic approximation in any sense in connecting the eigenfunctions at the turning points nor at the center of symmetry of the potential.

In §5, our method is applied to the case of $V(x) = 2\mu x^2 + \lambda x^4$ ($\mu, \lambda > 0$) for the sake of comparing it with the perturbation theory taking λx^4 as perturbation. We find that our method gives the better approximation to the eigenvalues already in the first approximation than the perturbation theory does except for the case of the ground state with very small λ. Our method gives the better approximation to the higher excited states. We shall establish moreover that our iteration series for the eigenfunctions $u_n(x)$ converge uniformy in x irrespective of the magnitude of λ, while the perturbation series is known to diverge[6)] and is only asymptotic for $\lambda \to 0$. Some discussions are given in the final section.

2. Liouville Transformation and the Connection Conditions

We present a new approximation method for solving the Schrödinger eigenvalue problem,

$$\left\{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right\}u(x) = Eu(x) \qquad (-\infty < x < \infty) \tag{2.1}$$

in one-dimension, in which the potential $V(x)$ is assumed, for the sake of simplicity, to be symmetric,

$$V(-x) = V(x), \tag{2.2}$$

bounded below, to grow to ∞ as $x \to \pm\infty$, and to have only two turning points, $x = \pm a$,

$$V(\pm a) = E, \tag{2.3}$$

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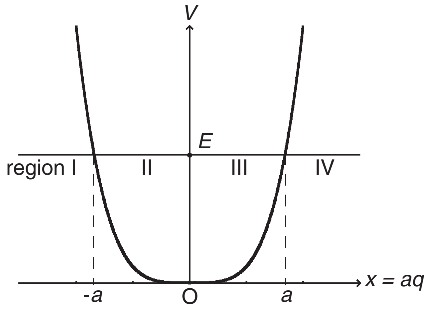

Fig. 1. The potential $V(x)$ and the regions of the x-axis.

for the energy eigenvalue E concerned. We divide the x-axis into four regions as shown in Fig. 1. The symmetry (2.2) of our potential allows us to restrict our attention to region I and II when studying the eigenvalue problem with the eigenfunctions being extended to region III and IV by its symmetry (even parity) or antisymmetry (odd parity).

We change the scale by

$$x = aq$$

for $u(x) = u_l(q; E)$ with the suffix l distinguishing the regions (l = I, II). Then eq. (2.1) becomes

$$\left\{\frac{d^2}{dq^2} \mp \kappa(E)^2 w(q; E)\right\} u_l(q; E) = 0, \tag{2.4}$$

where

$$w(q; E) = \left|\frac{V(a(E)q)}{E} - 1\right|, \tag{2.5}$$

$$\kappa(E) = \left(\frac{2ma(E)^2}{\hbar^2} E\right)^{1/2}. \tag{2.6}$$

Here and in the following also, the upper sign is for region I and the lower sign for region II. Since the scale a depends on E by eq. (2.3), it is denoted by $a(E)$ in eqs. (2.5) and (2.6). The parameter E may be suppressed when there is no danger of confusion.

2.1 *Liouville transformation*

The Liouville transformation[13] is defined as $u \mapsto \Lambda$ and $q \mapsto \xi$ by

$$u_l(q; E) = w(q; E)^{-1/4} \Lambda_l(\xi; E) \tag{2.7}$$

and

$$\xi(q; E) = \kappa(E)\zeta(q; E),$$
$$\zeta(q; E) = \mp \int_{-1}^{q} w(q'; E)^{1/2}\, dq'. \tag{2.8}$$

Then, eq. (2.4) becomes

$$\left(\frac{d^2}{d\xi^2} \mp 1\right)\Lambda_l(\xi; E) = \frac{1}{\kappa(E)^2} Q(q; E)\Lambda_l(\xi; E), \tag{2.9}$$

where

$$Q(q; E) = -\frac{5}{16}\frac{1}{w(q; E)^3}\left(\frac{dw(q; E)}{dq}\right)^2 + \frac{1}{4}\frac{1}{w(q; E)^2}\frac{d^2 w(q; E)}{dq^2}. \tag{2.10}$$

The function (2.10) in our basic equation (2.9) is singular at the turning point $q = -1$, or the boundary between region I and II where $w(q; E) = 0$. We shall show that this singularity can be softened significantly[14] by adding $(5/36)(1/\zeta^2)$ to $Q(q; E)$.

To show this, we examine the behavior of $Q(q; E)$ in the neighborhood of the turning point $q = -1$ using the Taylor expansion,

$$1 - \frac{V(aq)}{E} = a_1(q+1) + a_2(q+1)^2 + a_3(q+1)^3 + \cdots.$$

The coefficients a_i depend on E, though suppressed. We have

$$w(q; E) = \mp\{a_1(q+1) + a_2(q+1)^2 + a_3(q+1)^3 + \cdots\}, \tag{2.11}$$

which leads to

$$Q(q; E) = \pm\left\{\frac{5}{16a_1}\frac{1}{(q+1)^3} - \frac{3a_2}{16a_1^2}\frac{1}{(q+1)^2} + \frac{-9a_1a_3 + 6a_2^2}{16a_1^3}\frac{1}{q+1} + \cdots\right\}. \tag{2.12}$$

On the other hand

$$\zeta = \pm\int_q^{-1} w(q'; E)^{1/2}\, dq'$$
$$= \frac{2a_1^{1/2}}{3}\{\mp(q+1)\}^{3/2}\left(1 + \frac{3a_2}{10a_1}(q+1) + \frac{12a_1a_3 - 3a_2^2}{56a_1^2}(q+1)^2 + \cdots\right) \tag{2.13}$$

and therefore

$$\frac{5}{36}\frac{1}{\zeta(q; E)^2} = \pm\left\{-\frac{5}{16a_1}\frac{1}{(q+1)^3} + \frac{3a_2}{16a_1^2}\frac{1}{(q+1)^2} + \frac{75a_1a_3 - 66a_2^2}{560a_1^3}\frac{1}{q+1} + \cdots\right\}. \tag{2.14}$$

Adding eqs. (2.12) and (2.14), we get

$$\tilde{Q}(q; E) := Q(q; E) + \frac{5}{36}\frac{1}{\zeta(q; E)^2}$$
$$= \pm\frac{-15a_1a_3 + 9a_2^2}{35a_1^3}\frac{1}{q+1} + \cdots, \tag{2.15}$$

which is now free from the first two singularities in the curly bracket in eq. (2.12), but still has the singularity of order $1/(q+1)$.

2.2 *Integral equations*

Using $\tilde{Q}(q; E)$ in eq. (2.15) with softened singularity, we rewrite eq. (2.9) as

$$\left(\frac{d^2}{d\xi^2} \mp 1 + \frac{5}{36}\frac{1}{\xi^2}\right)\Lambda_l(\xi; E) = \frac{1}{\kappa(E)^2}\tilde{Q}(q; E)\Lambda_l(\xi; E), \tag{2.16}$$

which is the basic equation we are going to solve under the boundary condition,

$$\Lambda_{\rm I}(\xi; E) \to 0 \quad \text{as} \quad \xi \to \infty, \tag{2.17}$$

and smooth connections of $u_{\rm I}(q; E)$ and $u_{\rm II}(q; E)$ at their boundary, $q = -1$, and $u_{\rm II}(q; E)$ and $u_{\rm III}(q; E)$ at $q = 0$.

Put

$$\Lambda_l(\xi;E) = \xi^{1/2} Z_l(\xi;E).$$

Then, eq. (2.16) becomes

$$\left(\frac{d^2}{d\xi^2} + \frac{1}{\xi}\frac{d}{d\xi} \mp 1 - \frac{1}{3^2}\frac{1}{\xi^2}\right) Z_l(\xi;E) = \frac{1}{\kappa(E)^2}\tilde{Q}(q;E) Z_l(\xi;E). \quad (2.18)$$

If $\tilde{Q}$ were 0, then this would be the equation for the Bessel function of order $\pm 1/3$, its solutions being

$$Z_{\mathrm{I}}(\xi) = \begin{cases} K_{1/3}(\xi) \\ I_{1/3}(\xi) \end{cases} \quad \text{in region I,}$$

$$Z_{\mathrm{II}}(\xi) = \begin{cases} J_{1/3}(\xi) \\ J_{-1/3}(\xi) \end{cases} \quad \text{in region II.}$$

We convert the differential equation (2.18) into integral equation in the respective regions.

(a) Region I

For region I, taking the boundary condition (2.17) into account, we have

$$\Lambda_{\mathrm{I}}(\xi;E) = \xi^{1/2} K_{1/3}(\xi) + \frac{1}{\kappa(E)^2}\int_0^\infty G_{\mathrm{I}}(\xi,\xi')\tilde{Q}(q';E)\Lambda_{\mathrm{I}}(\xi';E)\, d\xi', \quad (2.19)$$

where the Green function is given by

$$G_{\mathrm{I}}(\xi,\xi') = -(\xi\xi')^{1/2}\{K_{1/3}(\xi) I_{1/3}(\xi')\theta(\xi-\xi') + I_{1/3}(\xi) K_{1/3}(\xi')\theta(\xi'-\xi)\} \quad (2.20)$$

and

$$\int_0^\infty \cdots d\xi' = \int_{-\infty}^{-1} \cdots \kappa(E) w(q';E)^{1/2}\, dq'$$

with $\xi' = \xi(q';E)$ defined by eq. (2.8). In terms of q', the integral (2.19) converges at the turning point, due to the Jacobian $w(q';E)^{1/2}$ canceling the singularity of $\tilde{Q}(q';E)$ partially.

(b) Region II

For region II also, we have the integral equation,

$$\Lambda_{\mathrm{II}}(\xi;E) = \xi^{1/2}\{A(E) J_{1/3}(\xi) + B(E) J_{-1/3}(\xi)\} + \frac{1}{\kappa(E)^2}\int_0^{\xi(0;E)} G_{\mathrm{II}}(\xi,\xi')\tilde{Q}(q';E)\Lambda_{\mathrm{II}}(\xi';E)\, d\xi'. \quad (2.21)$$

The upper limit $\xi(0;E)$ of the integral in eq. (2.21) is defined by eq. (2.8) with $q = 0$, so that

$$\int_0^{\xi(0;E)} \cdots d\xi' = \int_{-1}^{0} \cdots \kappa(E) w(q';E)^{1/2}\, dq'$$

with the integral converging at the turning point as above due to $w(q';E)^{1/2}$.

We have candidates for the Green function,

$$G_{\mathrm{II}}^{\mathrm{A}}(\xi,\xi') = -\frac{\pi}{\sqrt{3}}(\xi\xi')^{1/2}\{J_{-1/3}(\xi) J_{1/3}(\xi')\theta(\xi-\xi') + J_{1/3}(\xi) J_{-1/3}(\xi')\theta(\xi'-\xi)\}, \quad (2.22)$$

$$G_{\mathrm{II}}^{\mathrm{B}}(\xi,\xi') = \frac{\pi}{\sqrt{3}}(\xi\xi')^{1/2}\{J_{1/3}(\xi) J_{-1/3}(\xi')\theta(\xi-\xi') + J_{-1/3}(\xi) J_{1/3}(\xi')\theta(\xi'-\xi)\}, \quad (2.23)$$

and their linear combinations,

$$G_{\mathrm{II}}^{\alpha}(\xi,\xi') = \alpha G_{\mathrm{II}}^{\mathrm{A}}(\xi,\xi') + (1-\alpha) G_{\mathrm{II}}^{\mathrm{B}}(\xi,\xi') \quad (0 \le \alpha \le 1), \quad (2.24)$$

all of which must give the same Λ_{II} as long as eqs. (2.19) and (2.21) give the solutions (2.7) connected smoothly at $q = -1$ and 0.

We choose here $G_{\mathrm{II}}(\xi,\xi') = G_{\mathrm{II}}^{\mathrm{A}}(\xi,\xi')$ as the Green function in region II.

Remark. We shall show in the paper to follow that, in the case of $V(x) = \lambda x^{2k}$, the maximum of $2k$ for the iteration to converge depends on the choice of the Green function in region II.

2.3 Connection conditions

The coefficients $A(E)$ and $B(E)$ in eq. (2.21) are determined by the condition that the solutions $u_l(q;E) = N w(q;E)^{-1/4}\Lambda_l(\xi;E)$ in the regions $l = \mathrm{I}$ and II are connected smoothly at their boundary $\xi = 0$ $(q = -1)$, where N is the normalization constant.

The energy eigenvalue E is determined by the condition that the solutions $u_l(q;E)$ in the regions $l = \mathrm{II}$ and III are connected smoothly at their boundary $\xi = \xi(0;E)$ $(q = 0)$, or equivalently, due to our symmetry assumption (2.2), by

$$\frac{d}{dq}\{w(q;E)^{-1/4}\Lambda_{\mathrm{II}}(\xi;E)\}\Big|_{\xi=\xi(0;E)} = 0 \quad \text{(even state)},$$
$$w(q;E)^{-1/4}\Lambda_{\mathrm{II}}(\xi;E)\Big|_{\xi=\xi(0;E)} = 0 \quad \text{(odd state)}, \quad (2.25)$$

where the even states are the states of even parity with symmetric eigenfunctions, $u(-q;E) = u(q;E)$, and the odd states of odd parity with antisymmetric eigenfunctions, $u(-q;E) = -u(q;E)$.

But, we have

$$\frac{dw(q;E)}{dq}\Big|_{\xi=\xi(0;E)} = 0,$$

because $dV(x)/dx = 0$ at $x = 0$ by our symmetry assumption (2.2) on $V(x)$, so that the connection condition (2.25) for the even states becomes

$$\frac{d\Lambda_{\mathrm{II}}(\xi;E)}{d\xi} = 0 \quad (2.26)$$

at $\xi = \xi(0;E)$, while for the odd states,

$$\Lambda_{\mathrm{II}}(\xi;E) = 0 \quad (2.27)$$

at $\xi = \xi(0;E)$. Thus, order the solutions ξ of eqs. (2.26) and (2.27) according to their magnitudes, and call them $\gamma_n(E)$ $(n = 0, 1, \ldots)$. Then, we get the equation, $\xi(0;E) = \gamma_n(E)$, for the energy eigenvalue $E = E_n$, that is,

$$\kappa(E)\int_{-1}^{0}\left\{1 - \frac{V(a(E)q)}{E}\right\}^{1/2} dq = \gamma_n(E). \quad (2.28)$$

We call eq. (2.28) the eigenvalue formula.

3. Iteration

We construct the solutions $\Lambda_l(\xi;E)$ to eqs. (2.19) and (2.21) by iteration,

$$\Lambda_l(\xi;E) = \lim_{\nu\to\infty}\Lambda_l^{(\nu)}(\xi;E) \quad \text{with}$$

$$\Lambda_l^{(\nu)}(\xi;E)=\sum_{\sigma=0}^{\nu}\lambda_l^{(\sigma)}(\xi;E), \tag{3.1}$$

which are determined, in the respective regions, successively by

$$\lambda_l^{(\sigma+1)}(\xi;E)=\frac{1}{\kappa(E)^2}\int_{\Xi_l}G_l(\xi,\xi')\,\tilde{Q}(q';E)\,\lambda_l^{(\sigma)}(\xi';E)\,\mathrm{d}\xi' \quad (l=\mathrm{I},\mathrm{II};\sigma=0,1,\ldots) \tag{3.2}$$

with G_I for region I given by eq. (2.20) and $G_\mathrm{II}=G_\mathrm{II}^\mathrm{A}$ for region II by eq. (2.22). The domains of integrations are

$$\Xi_l=\begin{cases}[0,\infty) & (l=\mathrm{I})\\ [0,\xi(0;E)] & (l=\mathrm{II}).\end{cases}$$

The convergence of the infinite series (3.1) will be examined in §4.

The 0th order solutions, $\Lambda_l^{(0)}(\xi;E)=\lambda_l^{(0)}(\xi;E)$, are obtained by putting $\tilde{Q}=0$ in eqs. (2.19) and (2.21),

$$\Lambda_\mathrm{I}^{(0)}(\xi;E)=\xi^{1/2}K_{1/3}(\xi),$$
$$\Lambda_\mathrm{II}^{(0)}(\xi;E)=\xi^{1/2}\{A(E)J_{1/3}(\xi)+B(E)J_{-1/3}(\xi)\}. \tag{3.3}$$

The coefficients, $A(E)=A^{(\nu)}(E)$ and $B(E)=B^{(\nu)}(E)$ in eqs. (2.21) and (3.3), vary with the order ν at which the iteration is approximately terminated, because these coefficients are determined by connecting the approximate eigenfunctions,

$$u_l^{(\nu)}(q;E)=N^{(\nu)}w(q;E)^{-1/4}\Lambda_l^{(\nu)}(\xi,E)$$

in region I and region II smoothly at their boundary $\xi=0$ ($q=-1$). The energy eigenvalues, $E=E_n^{(\nu)}$, are determined by eq. (2.28) with $\gamma_n(E)=\gamma_n^{(\nu)}(E)$, the approximate zeros of (2.26) or (2.27) for $\Lambda_\mathrm{II}(\xi;E)=\Lambda_\mathrm{II}^{(\nu)}(\xi;E)$. The coefficient $N^{(\nu)}$ is determined by normalization of the eigenfunction,

$$2\int_{-\infty}^{-a}|u_\mathrm{I}^{(\nu)}(x;E^{(\nu)})|^2\,\mathrm{d}x+2\int_{-a}^{0}|u_\mathrm{II}^{(\nu)}(x;E^{(\nu)})|^2\,\mathrm{d}x=1 \quad (x=aq).$$

3.1 0th order approximation

If we terminate the iteration at the 0th order $\nu=0$, the approximate eigenfunctions in region I and II are given by eq. (3.3),

$$u_\mathrm{I}^{(0)}(q;E)=N^{(0)}\{w(q;E)\}^{-1/4}\xi^{1/2}K_{1/3}(\xi),$$
$$u_\mathrm{II}^{(0)}(q;E)=N^{(0)}\{w(q;E)\}^{-1/4}\xi^{1/2}\{A^{(0)}(E)J_{1/3}(\xi)+B^{(0)}(E)J_{-1/3}(\xi)\}. \tag{3.4}$$

3.1.1 Connection at $q=-1$ to determine $A^{(0)}(E)$ and $B^{(0)}(E)$

We have to connect $u_\mathrm{I}^{(0)}(q;E)$ in region I and $u_\mathrm{II}^{(0)}(q;E)$ in region II smoothly at $q=-1$ by adjusting $A^{(0)}(E)$ and $B^{(0)}(E)$.

(a) Region I

In the neighborhood of $q=-1$, we put

$$q=-1-z \quad (0\le z\ll 1). \tag{3.5}$$

From eq. (2.11), we get

$$w(q;E)^{-1/4}=(a_1z)^{-1/4}\left(1+\frac{a_2}{4a_1}z+\cdots\right), \tag{3.6}$$

and from eq. (2.13)

$$\xi(q;E)^{1/2}=\sqrt{\frac{2}{3}}\kappa(E)^{1/2}a_1^{1/4}z^{3/4}\left(1-\frac{3a_2}{20a_1}z+\cdots\right). \tag{3.7}$$

Since

$$K_{1/3}(\xi)=\frac{\pi}{\sqrt{3}\Gamma(2/3)}\left(\frac{\sqrt{a_1}\kappa(E)}{3}\right)^{-1/3}z^{-1/2}\left(1+\frac{a_2}{10a_1}z\right)-\frac{\pi}{\sqrt{3}\Gamma(4/3)}\left(\frac{\sqrt{a_1}\kappa(E)}{3}\right)^{1/3}z^{1/2}+O(z^{3/2}), \tag{3.8}$$

the eigenfunction (3.4) in region I behaves as a function of $z=-(1+q)$ as

$$u_\mathrm{I}^{(0)}(q;E)\sim N^{(0)}\kappa(E)^{1/2}\sqrt{\frac{2}{3}}\left(1+\frac{a_2}{10a_1}z\right)\times\left\{\frac{\pi}{\sqrt{3}\Gamma(2/3)}\left(\frac{\sqrt{a_1}\kappa(E)}{3}\right)^{-1/3}\left(1+\frac{a_2}{10a_1}z\right)-\frac{\pi}{\sqrt{3}\Gamma(4/3)}\left(\frac{\sqrt{a_1}\kappa(E)}{3}\right)^{1/3}z+O(z^2)\right\}. \tag{3.9}$$

(b) Region II

In the neighborhood of $q=-1$, we put

$$q=-1+z \quad (0\le z\ll 1). \tag{3.10}$$

Since

$$w(q;E)^{-1/4}=(a_1z)^{-1/4}\left(1-\frac{a_2}{4a_1}z+\cdots\right), \tag{3.11}$$

$$\xi(q;E)^{1/2}=\sqrt{\frac{2}{3}}\kappa(E)^{1/2}a_1^{1/4}z^{3/4}\left(1+\frac{3a_2}{20a_1}z+\cdots\right), \tag{3.12}$$

and

$$J_{\pm 1/3}(\xi)=\left(\frac{\xi}{2}\right)^{\pm 1/3}\left\{\frac{1}{\Gamma(1\pm 1/3)}+O(\xi^2)\right\}, \tag{3.13}$$

the eigenfunction (3.4) in region II behaves as

$$u_\mathrm{II}^{(0)}(q;E)\sim N^{(0)}\kappa(E)^{1/2}\sqrt{\frac{2}{3}}\left(1-\frac{a_2}{10a_1}z\right)\times\left\{\frac{B^{(0)}(E)}{\Gamma(2/3)}\left(\frac{\sqrt{a_1}\kappa(E)}{3}\right)^{-1/3}\left(1-\frac{a_2}{10a_1}z\right)+\frac{A^{(0)}(E)}{\Gamma(4/3)}\left(\frac{\sqrt{a_1}\kappa(E)}{3}\right)^{1/3}z+O(z^2)\right\}. \tag{3.14}$$

Note the difference in sign of z between eqs. (3.5) and (3.10). Then the smooth connection of eqs. (3.9) and (3.14) as function of q requires that

$$A^{(0)}(E)=B^{(0)}(E)=\frac{\pi}{\sqrt{3}}, \tag{3.15}$$

irrespective of E.

3.1.2 Connection at $q=0$ to determine $E_n^{(0)}$

Smooth connection of the eigenfunctions in region II and III at $q=0$ determines the 0th order approximation of the eigenvalues $E=E_n^{(0)}$.

(a) Even states

Equation (2.26) on (3.3) with (3.15) becomes

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\{\xi^{1/2}J_{1/3}(\xi)+\xi^{1/2}J_{-1/3}(\xi)\}=0,$$

or equivalently

$$\{J_{1/3}(\xi)+6\xi J_{-2/3}(\xi)\}+\{J_{-1/3}(\xi)-6\xi J_{2/3}(\xi)\}=0 \quad (3.16)$$

by the formulas,

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\{\xi^{1/3}J_{1/3}(\xi)\}=\xi^{1/3}J_{-2/3}(\xi),$$
$$\frac{\mathrm{d}}{\mathrm{d}\xi}\{\xi^{1/3}J_{-1/3}(\xi)\}=-\xi^{1/3}J_{2/3}(\xi).$$

The jth zero of eq. (3.16), $\gamma_n(E)$ ($n=2j$), is independent of E, so that it is written as $\gamma_{2j}^{(0)}$ with the superscript (0) indicating the 0th order approximation and the subscript $2j$ the order of the excited states. They are found to be

$$\gamma_0^{(0)}=0.880\ 167\ 1,$$
$$\gamma_2^{(0)}=3.945\ 062,$$
$$\gamma_4^{(0)}=7.078\ 484,\cdots. \quad (3.17)$$

These values, we note, are universally good for any potentials $V(x)$ and are independent of E in addition. [The higher order $\gamma_n^{(\nu)}$'s ($\nu\geq 1$) depend on E.] The corresponding energy eigenvalues $E=E_{2j}^{(0)}$ are given by eq. (2.28), the eigenvalue formula, with $\gamma_n(E)=\gamma_{2j}^{(0)}$.

(b) Odd states

Equation (2.27) on (3.3) with (3.15) is

$$J_{1/3}(\xi)+J_{-1/3}(\xi)=0,$$

whose jth zero $\xi=\gamma_n^{(0)}$ ($n=2j+1$) are given by

$$\gamma_1^{(0)}=2.383\ 447,$$
$$\gamma_3^{(0)}=5.510\ 196,$$
$$\gamma_5^{(0)}=8.647\ 358,\cdots. \quad (3.18)$$

These values are again universally good for any potentials $V(x)$ and are independent of E. They determine the energy eigenvalues $E=E_{2j+1}^{(0)}$ by eq. (2.28), the eigenvalue formula, with $\gamma_n(E)=\gamma_{2j+1}^{(0)}$.

3.2 1st order approximation

We push the approximation one step further.

3.2.1 Wave functions to the first order

We terminate the iteration series (3.1) at the first order $\nu=1$.

(a) Region I

The first order contribution,

$$\lambda_{\mathrm{I}}^{(1)}(\xi;E)=\frac{1}{\kappa(E)^2}\int_0^\infty G_{\mathrm{I}}(\xi,\xi')\,\tilde{Q}(q';E)\,\xi'^{1/2}K_{1/3}(\xi')\,\mathrm{d}\xi',$$

from eq. (3.2) with $\sigma=0$ gives the approximate eigenfunction in region I,

$$u_{\mathrm{I}}^{(1)}(q;E)=N^{(1)}w(q;E)^{-1/4}\xi^{1/2}\{K_{1/3}(\xi)\varphi(\xi)+I_{1/3}(\xi)\psi(\xi)\} \quad (3.19)$$

with

$$\varphi(\xi)=1-\frac{1}{\kappa(E)^2}\int_0^\xi \xi' I_{1/3}(\xi')\,K_{1/3}(\xi')\,\tilde{Q}(q';E)\,\mathrm{d}\xi',$$
$$\psi(\xi)=-\frac{1}{\kappa(E)^2}\int_\xi^\infty \xi'\{K_{1/3}(\xi')\}^2\tilde{Q}(q';E)\,\mathrm{d}\xi'. \quad (3.20)$$

The integrations here can be carried out in terms of q' using the relation (2.8). To evaluate the integrals, we have to rely on numerical calculations. Though the singularity of $\tilde{Q}$ mentioned in §2 is suppressed partially by the Jacobian $\mathrm{d}\xi=\kappa w^{1/2}\mathrm{d}q$ to make the integral converge, special attention is paid to treat it by the double exponential formula.[15)] We shall not repeat these remarks which apply to the similar integrals to follow.

(b) Region II

The first order contribution,

$$\lambda_{\mathrm{II}}^{(1)}(\xi;E)=\frac{1}{\kappa(E)^2}\int_0^{\xi(0;E)} G_{\mathrm{II}}(\xi,\xi')\,\tilde{Q}(q';E)\,\xi'^{1/2}\times\{A(E)J_{1/3}(\xi')+B(E)J_{-1/3}(\xi')\}\,\mathrm{d}\xi',$$

from eq. (3.2) with $\sigma=0$ gives the first order approximation for the eigenfunction in region II [the series (3.1) terminated at $\nu=1$],

$$u_{\mathrm{II}}^{(1)}(q;E)=N^{(1)}w(q;E)^{-1/4}\xi^{1/2}\times[A^{(1)}(E)\{J_{1/3}(\xi)\varphi_1(\xi)+J_{-1/3}(\xi)\varphi_2(\xi)\}+B^{(1)}(E)\{J_{1/3}(\xi)\psi_1(\xi)+J_{-1/3}(\xi)\psi_2(\xi)\}], \quad (3.21)$$

where

$$\varphi_1(\xi)=1-\frac{1}{\kappa(E)^2}\frac{\pi}{\sqrt{3}}\int_\xi^{\xi(0;E)}\xi' J_{1/3}(\xi')J_{-1/3}(\xi')\tilde{Q}(q';E)\,\mathrm{d}\xi',$$
$$\varphi_2(\xi)=-\frac{1}{\kappa(E)^2}\frac{\pi}{\sqrt{3}}\int_0^\xi \xi'\{J_{1/3}(\xi')\}^2\tilde{Q}(q';E)\,\mathrm{d}\xi',$$
$$\psi_1(\xi)=-\frac{1}{\kappa(E)^2}\frac{\pi}{\sqrt{3}}\int_\xi^{\xi(0;E)}\xi'\{J_{-1/3}(\xi')\}^2\tilde{Q}(q';E)\,\mathrm{d}\xi',$$
$$\psi_2(\xi)=1-\frac{1}{\kappa(E)^2}\frac{\pi}{\sqrt{3}}\int_0^\xi \xi' J_{1/3}(\xi')J_{-1/3}(\xi')\tilde{Q}(q';E)\,\mathrm{d}\xi' \quad (3.22)$$

with $\xi(0;E)$ given by eq. (2.8).

3.2.2 Connection at $q=-1$ to determine $A^{(1)}(E)$ and $B^{(1)}(E)$

To connect the wave functions, (3.19) and (3.21), smoothly at $q=-1$, we have to know their behavior around $q=-1$ up to the 1st order in $z=\mp(q+1)$. For this purpose, we have only to take the 0th order terms of φ, ψ, φ_1, φ_2, ψ_1, and ψ_2:

$$\varphi(\xi)\sim 1,\quad \psi(\xi)\sim-\frac{\pi}{\sqrt{3}}C_1(E),$$
$$\varphi_1(\xi)\sim 1-C_2(E),\quad \varphi_2(\xi)\sim 0,$$
$$\psi_1(\xi)\sim -C_3(E),\quad \psi_2(\xi)\sim 1, \quad (3.23)$$

where

$$C_1(E)=\frac{1}{\kappa(E)^2}\frac{\sqrt{3}}{\pi}\int_0^\infty \xi\{K_{1/3}(\xi)\}^2\tilde{Q}(q;E)\,\mathrm{d}\xi,$$
$$C_2(E)=\frac{1}{\kappa(E)^2}\frac{\pi}{\sqrt{3}}\int_0^{\xi(0;E)}\xi J_{1/3}(\xi)J_{-1/3}(\xi)\tilde{Q}(q;E)\,\mathrm{d}\xi,$$

$$C_3(E) = \frac{1}{\kappa(E)^2}\frac{\pi}{\sqrt{3}}\int_0^{\xi(0;E)} \xi\{J_{-1/3}(\xi)\}^2\tilde{Q}(q;E)\,d\xi. \quad (3.24)$$

In fact, in the case of the first term in the bracket in eq. (3.19), for example,

$$\begin{aligned} \xi' &= O(z'^{3/2}), \quad I_{1/3}(\xi') = O(z'^{1/2}), \\ K_{1/3}(\xi') &= O(z'^{-1/2}), \quad \tilde{Q} = O(z'^{-1}), \end{aligned} \quad (3.25)$$

so that eq. (3.20) gives $\varphi = 1 + O(z^2)$, whose $O(z^2)$ term can be discarded when multiplied by $w^{-1/4}\xi^{1/2}K_{1/3}(\xi) = O(1)$. The case of the second term in the bracket in eq. (3.19) is a little different: Equations (3.20) and (3.25) give $\psi = -(\pi/\sqrt{3})C_1(E) + O(z)$, whose $O(z)$ term can again be discarded because it is multiplied by $w^{-1/4}\xi^{1/2}I_{1/2}(\xi) = O(z)$. Similar arguments apply to the terms in eq. (3.23).

Using eqs. (3.6), (3.7), (3.8), and (3.23), we obtain

$$\begin{aligned} u_{\mathrm{I}}^{(1)}(q;E) \sim N^{(1)}\sqrt{2}\left(\frac{\kappa(E)}{3a_1}\right)^{1/6} & \\ \times \Bigg[\frac{1}{\Gamma(2/3)}\frac{\pi}{\sqrt{3}}\left(1 - \frac{a_2}{5a_1}(q+1)\right) & \\ + \frac{1}{\Gamma(4/3)}\left(\frac{\sqrt{a_1}\kappa(E)}{3}\right)^{2/3} & \\ \times \frac{\pi}{\sqrt{3}}[1 + C_1(E)](q+1)\Bigg], & \end{aligned} \quad (3.26)$$

and

$$\begin{aligned} u_{\mathrm{II}}^{(1)}(q;E) \sim N^{(1)}\sqrt{2}\left(\frac{\kappa(E)}{3a_1}\right)^{1/6} & \\ \times \Bigg[\frac{1}{\Gamma(2/3)}B^{(1)}(E)\left(1 - \frac{a_2}{5a_1}(q+1)\right) & \\ + \frac{1}{\Gamma(4/3)}\left(\frac{\sqrt{a_1}\kappa(E)}{3}\right)^{2/3} & \\ \times \{A^{(1)}(E)[1 - C_2(E)] - C_3(E)B^{(1)}(E)\}(q+1)\Bigg] & \end{aligned} \quad (3.27)$$

using eqs. (3.11), (3.12), and (3.13) instead. Then the smooth connection of these functions at $q = -1$ requires that

$$\begin{aligned} A^{(1)}(E) &= \frac{\pi}{\sqrt{3}}\frac{1 + C_1(E) + C_3(E)}{1 - C_2(E)}, \\ B^{(1)}(E) &= \frac{\pi}{\sqrt{3}}. \end{aligned} \quad (3.28)$$

3.2.3 *Connection at $q = 0$ to determine $E_n^{(1)}$*

Connecting the eigenfunctions in region II and III smoothly at their boundary, $q = 0$, determines the 1st order approximation of the energy eigenvalues $E_n^{(1)}$.

(a) Even states

The connection condition at $q = 0$, eq. (2.26) as applied to the 1st order correction, permits simplification at $\xi = \xi(0;E)$,

$$\begin{aligned} &\frac{d}{d\xi}\Bigg\{J_{-1/3}(\xi)\int_0^{\xi}\xi' J_{1/3}(\xi')Z(\xi')\tilde{Q}(q';E)\,d\xi' \\ &\quad + J_{1/3}(\xi)\int_{\xi}^{\xi(0;E)}\xi' J_{-1/3}(\xi')Z(\xi')\tilde{Q}(q';E)\,d\xi'\Bigg\} \\ &= \frac{dJ_{-1/3}(\xi)}{d\xi}\int_0^{\xi(0;E)}\xi' J_{1/3}(\xi')Z(\xi')\tilde{Q}(q';E)\,d\xi' \\ &\qquad (Z(\xi') = J_{\pm 1/3}(\xi')), \end{aligned}$$

reducing eq. (2.26) to

$$\begin{aligned} &A^{(1)}(E)\{J_{1/3}(\xi) + 6\xi J_{-2/3}(\xi)\} \\ &\quad + \{-C_4(E)\,A^{(1)}(E) + (1 - C_2(E))B^{(1)}(E)\} \\ &\quad \times \{J_{-1/3}(\xi) - 6\xi J_{2/3}(\xi)\} = 0, \end{aligned} \quad (3.29)$$

where

$$C_4(E) = \frac{1}{\kappa(E)^2}\frac{\pi}{\sqrt{3}}\int_0^{\xi(0;E)}\xi\{J_{1/3}(\xi)\}^2\tilde{Q}(q;E)\,d\xi.$$

The jth zero of eq. (3.29) gives $\gamma_{2j}^{(1)}(E)$ to be used for the right-hand side of eq. (2.28), the eigenvalue formula, to determine the $(2j)$th eigenvalues $E_{2j}^{(1)}$.

(b) Odd states

For the odd states, eq. (2.27) as applied to $\Lambda_{\mathrm{II}}^{(1)}$ is reduced to

$$\begin{aligned} &A^{(1)}(E)J_{1/3}(\xi) + \{-C_4(E)\,A^{(1)}(E) \\ &\quad + (1 - C_2(E))B^{(1)}(E)\}J_{-1/3}(\xi) = 0, \end{aligned} \quad (3.30)$$

and its jth zero, $\gamma_{2j+1}^{(1)}(E)$, determines the $(2j+1)$th eigenvalue $E_{2j+1}^{(1)}$ from eq. (2.28) also.

In a similar way, we can push the iteration to the higher order.

4. Convergence Condition for the Iteration

We now discuss the convergence of the series (3.1) generated by the iteration (3.2). If it converges uniformly in ξ, the energy eigenvalues as obtained by connecting the approximate wave functions for region II and III converge also.

4.1 *Convergence rate*

Recall eq. (3.2) for the iteration,

$$\begin{aligned} \lambda_l^{(\sigma+1)}(\xi;E_n) = \frac{1}{\kappa(E)}\int_{D_l} & G_l(\xi,\xi')\tilde{Q}(q';E_n) \\ & \times \lambda_l^{(\sigma)}(\xi';E_n)w(q';E_n)^{1/2}\,dq' \end{aligned} \quad (4.1)$$

with

$$D_{\mathrm{I}} = (-\infty,-1), \quad \xi(q;E_n) = \kappa(E_n)\int_q^{-1} w(q';E_n)^{1/2}\,dq',$$

$$D_{\mathrm{II}} = (-1,0), \quad \xi(q;E_n) = \kappa(E_n)\int_{-1}^{q} w(q';E_n)^{1/2}\,dq'.$$

Take the absolute value of (4.1) and pull $\lambda_l^{(\sigma)}$ out of the integral by taking its supremum,

$$\begin{aligned} |\lambda_l^{(\sigma+1)}(\xi;E_n)| \le \sup_{q''\in D_l}|\lambda_l^{(\sigma)}(\xi'';E_n)|\frac{1}{\kappa(E_n)} & \\ \times \int_{D_l}|G_l(\xi,\xi')|\,|\tilde{Q}(q';E_n)|w(q';E_n)^{1/2}\,dq'. & \end{aligned}$$

Take the supremum of both sides again to obtain

$$\sup_{q\in D_l}|\lambda_l^{(\sigma+1)}(\xi;E_n)| \le r_{nl}\cdot\sup_{q\in D_l}|\lambda_l^{(\sigma)}(\xi;E_n)| \quad (4.2)$$

with

$$r_{nl} = \frac{1}{\kappa(E_n)}\sup_{q\in D_l}\int_{D_l}|G_l(\xi,\xi')|\,|\tilde{Q}(q';E_n)|w(q';E_n)^{1/2}\,dq', \quad (4.3)$$

which we call the convergence rate. If $r_{nl} < 1$, then the inequality (4.2) proves that the series (3.1) converges uniformly in ξ.

4.2 *Quick estimate*

For the purpose of quick estimates of the convergence rate (4.3), we replace $|G_l(\xi,\xi')|$ by its upper bound c_l and pull it out of the integral,

$$r_{nl} \le r'_{nl} := \frac{c_l}{\kappa(E_n)} \int_{D_l} |\tilde{Q}(q'; E_n)| w(q'; E_n)^{1/2}\, dq'. \qquad (4.4)$$

Let us prove

$$|G_{\rm I}(\xi,\xi')| \le 0.723, \quad |G_{\rm II}(\xi,\xi')| \le 1.362,$$

so that $c_{\rm I} = 0.723$ and $c_{\rm II} = 1.362$.

(a) Region I

The Green function in region I is given by eq. (2.20), where $K_{1/3}$ is related to the Hankel function by

$$K_{1/3}(\xi) = \frac{\pi i}{2} e^{\pi i/6} H^{(1)}_{1/3}(i\xi). \qquad (4.5)$$

Using Heine's formula,

$$H^{(1)}_{1/3}(i\xi) = \frac{2}{\pi i} e^{-\pi i/6} \int_0^\infty e^{-\xi\cosh t} \cosh(t/3)\, dt,$$

and replacing $\cosh(t/3)$ by $\cosh(t/2)$, we obtain

$$0 < K_{1/3}(\xi) < \int_0^\infty e^{-\xi\cosh t} \cosh(t/2)\, dt.$$

By the change of the variable of integration, $\sqrt{2\xi}\sinh(t/2) = u$, therefore

$$0 < K_{1/3}(\xi) < \frac{\sqrt{2}e^{-\xi}}{\sqrt{\xi}} \int_0^\infty e^{-u^2}\, du$$
$$= \sqrt{\frac{\pi}{2}} \frac{1}{\sqrt{\xi}} e^{-\xi} = 1.254 \frac{1}{\sqrt{\xi}} e^{-\xi}. \qquad (4.6)$$

To find a bound for

$$I_{1/3}(\xi) = \frac{e^{-\pi i/6}}{2} \{H^{(1)}_{1/3}(i\xi) + H^{(2)}_{1/3}(i\xi)\} \qquad (4.7)$$

in $G_{\rm I}(\xi,\xi')$, we obtain, on the one hand,

$$|H^{(1)}_{1/3}(i\xi)| = \frac{2}{\pi} K_{1/3}(\xi) < 0.799 \frac{1}{\sqrt{\xi}} e^{-\xi} \qquad (4.8)$$

by eqs. (4.5) and (4.6). For $H^{(2)}_{1/3}(i\xi)$ on the other, we use Hankel's formula,

$$H^{(2)}_{1/3}(i\xi) = \frac{2ie^{5\pi i/12}e^{\xi}}{\sqrt{\pi}\Gamma(5/6)(2i\xi)^{1/3}} \int_C \{iz(z-2\xi)\}^{-1/6} e^{-z}\, dz,$$

in place of Heine's, where the contour C goes along the upper side of the half-line $z = te^{\pi i/4}$ from $t = \infty$ to 0, turns around 0 counterclockwise and then goes to infinity along the lower side of the same half-line. Since $|z - 2\xi| > \sqrt{2}\xi$ for all $z \in C$,

$$\left|\int_C \{z(z-2\xi)\}^{-1/6} e^{-z}\, dz\right|$$
$$< 2^{-1/12}\xi^{-1/6} \int_0^\infty t^{-1/6} e^{-t/\sqrt{2}} |e^{-\pi i/3} - 1|\, dt$$
$$= 2^{1/3}\xi^{-1/6}\Gamma(5/6),$$

so that

$$|H^{(2)}_{1/3}(i\xi)| < \frac{2}{\sqrt{\pi}} \frac{e^{\xi}}{\sqrt{\xi}} = 1.129 \frac{e^{\xi}}{\sqrt{\xi}}. \qquad (4.9)$$

Putting inequalities (4.8) and (4.9) into eq. (4.7), we obtain

$$0 < I_{1/3}(\xi) < (0.400e^{-2\xi} + 0.565) \frac{e^{\xi}}{\sqrt{\xi}},$$

hence

$$0 < I_{1/3}(\xi) < (0.400e^{-2c} + 0.565) \frac{e^{\xi}}{\sqrt{\xi}} \ (\xi > c) \qquad (4.10)$$

for any $c > 0$.

For $0 < \xi < c$, we use the Taylor expansion of $(2/\xi)^{1/3} I_{1/3}(\xi)$, whose terms are all positive, showing that it is monotone increasing. Hence

$$\left(\frac{2}{\xi}\right)^{1/3} I_{1/3}(\xi) < \left(\frac{2}{c}\right)^{1/3} I_{1/3}(c).$$

Applying the inequality,

$$\xi^{1/3} \le 0.374 \frac{e^{\xi}}{\sqrt{\xi}},$$

we obtain

$$I_{1/3}(\xi) < \frac{0.374\, I_{1/3}(c)}{c^{1/3}} \frac{e^{\xi}}{\sqrt{\xi}} \quad (0 < \xi < c). \qquad (4.11)$$

The coefficients of $e^{\xi}/\sqrt{\xi}$ in eqs. (4.10) and (4.11) are close to each other at $c = 1.8$. In fact, that for the former is 0.576 and 0.573 for the latter, so that we obtain

$$0 < I_{1/3}(\xi) < 0.576 \frac{e^{\xi}}{\sqrt{\xi}} \qquad (4.12)$$

for all $\xi > 0$.

By the inequalities (4.6) and (4.12),

$$|G_{\rm I}(\xi,\xi')| < 0.723\{e^{-\xi}e^{\xi'}\theta(\xi-\xi') + e^{\xi}e^{-\xi'}\theta(\xi'-\xi)\},$$

and hence

$$|G_{\rm I}(\xi,\xi')| < 0.723. \qquad (4.13)$$

Remark. We have confirmed (4.13) by estimating the coefficients corresponding to 1.254 in (4.6) and 0.576 in (4.12) by numerically evaluating $K_{1/3}(\xi)$ and $I_{1/3}(\xi)$. They turned out to be 1.2535 and 0.415, respectively, giving a stronger bound:

$$|G_{\rm I}(\xi,\xi')| < 0.521.$$

(b) Region II

The Green function in region II is given by eq. (2.22). We use Poisson's integral formula,[16]

$$J_\nu(z) = \frac{(z/2)^\nu}{\Gamma(1/2)\Gamma(\nu + (1/2))} \int_0^\pi e^{iz\cos\theta} \sin^{2\nu}\theta\, d\theta$$
$$(\mathrm{Re}\,\nu > -1/2),$$

to obtain

$$|J_\nu(\xi)| \le \frac{(\xi/2)^\nu}{\Gamma(\nu+1)} \le \frac{c^{\nu+1/2}}{2^\nu\Gamma(\nu+1)} \frac{1}{\sqrt{\xi}} \quad (0 < \xi \le c) \qquad (4.14)$$

for any $c > 0$. We shall determine the constant $c > 0$ later.

For $\xi > c$, we use the asymptotic expansion,[17)]

$$H_\nu^{(\iota)}(z) = \left(\frac{2}{\pi z}\right)^{1/2} \mathrm{e}^{\pm\mathrm{i}(z-\pi\nu/2-\pi/4)} \times \left\{\sum_{m=0}^{p-1} \frac{(1/2-\nu)_m \Gamma(\nu+m+1/2)}{m!\Gamma(\nu+1/2)(\pm 2iz)^m} + R_p^{(\iota)}\right\} \quad (\iota = 1, 2)$$

with $p = 1$,

$$H_\nu^{(\iota)}(z) = \left(\frac{2}{\pi z}\right)^{1/2} \mathrm{e}^{\pm\mathrm{i}(z-\pi\nu/2-\pi/4)}(1 + R_1^{(\iota)}),$$

where

$$|R_1^{(\iota)}| \le \frac{1/2-\nu}{2\xi\,\Gamma(\nu+1/2)} \int_0^\infty \mathrm{e}^{-u} u^{\nu+1/2}\,\mathrm{d}u = \frac{1/4-\nu^2}{2\xi} < \frac{1/4-\nu^2}{2c}.$$

Hence,

$$|J_\nu(\xi)| \le \max_{\iota=1,2} |H_\nu^{(\iota)}(\xi)| \le \left(\frac{2}{\pi}\right)^{1/2}\left(1 + \frac{1/4-\nu^2}{2c}\right)\frac{1}{\sqrt{\xi}} \quad (\xi > c). \qquad (4.15)$$

We determine c by equating the coefficients of $1/\sqrt{\xi}$ in (4.14) and (4.15) to obtain

$$\frac{c^{\nu+1/2}}{2^\nu \Gamma(\nu+1)} = \left(\frac{2}{\pi}\right)^{1/2}\left(1 + \frac{1/4-\nu^2}{2c}\right) = \begin{cases} 0.856 & \text{at } c = 0.956\ (\nu = 1/3) \\ 0.877 & \text{at } c = 0.701\ (\nu = -1/3) \end{cases}.$$

Then,

$$\left|\sqrt{\xi} J_\nu(\xi)\right| < \begin{cases} 0.856 & (\nu = 1/3) \\ 0.877 & (\nu = -1/3) \end{cases}$$

holds for all $\xi > 0$, and consequently

$$|G_{\mathrm{II}}(\xi,\xi')| < \frac{\pi}{\sqrt{3}} \times 0.856 \times 0.877 = 1.362 \qquad (4.16)$$

by eq. (2.22).

Remark. We have confirmed (4.16) in a way similar to the one for the previous Remark. We have found a stronger bound:

$$|G_{\mathrm{II}}(\xi,\xi')| < 1.161.$$

5. The Case of the Potential $V(x) = 2\mu x^2 + \lambda x^4$

We apply our method to calculate the eigenvalues of the Hamiltonian,

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + 2\mu x^2 + \lambda x^4 \quad (\mu, \lambda > 0), \qquad (5.1)$$

and to compare the results with those from the perturbation theory, which is known to give series divergent how small λ is.

5.1 Normal form of the equation

By putting $x = \alpha y$ with $\alpha^4 = \hbar^2/(4m\mu)$, the Schrödinger equation (2.1) for (5.1) is turned into a normal form,

$$\left\{-\frac{\mathrm{d}^2}{\mathrm{d}y^2} + y^2 + \epsilon y^4\right\}\tilde{u}(y) = \tilde{E}\tilde{u}(y),$$

where

$$E = \tilde{E}\cdot\hbar\sqrt{\frac{\mu}{m}}, \quad \lambda = \frac{4\sqrt{m\mu^3}}{\hbar}\epsilon.$$

Then, w and κ in (2.5) and (2.6) turn out to be

$$w(q;E) = \left|\frac{4\tilde{E}\epsilon}{\{(1+4\tilde{E}\epsilon)^{1/2}+1\}^2} q^4 + \frac{2}{(1+4\tilde{E}\epsilon)^{1/2}+1} q^2 - 1\right|, \qquad (5.2)$$

$$\kappa(E) = \left(\frac{2\tilde{E}^2}{(1+4\tilde{E}\epsilon)^{1/2}+1}\right)^{1/2}. \qquad (5.3)$$

5.2 Energy eigenvalues

5.2.1 0th order approximation

The integral on the left-hand side of the eigenvalue formula (2.28) becomes

$$\int_{-1}^{0}\left\{1 - \frac{4\tilde{E}\epsilon}{\{(1+4\tilde{E}\epsilon)^{1/2}+1\}^2} q^4 - \frac{2}{(1+4\tilde{E}\epsilon)^{1/2}+1} q^2\right\}^{1/2} \mathrm{d}q = -\frac{1}{3k\,(\tilde{E}\epsilon)^{1/2}}\,E\!\left(\frac{\pi}{2},k\right) + \frac{(1+4\tilde{E}\epsilon)^{1/2}+1}{6k\,(\tilde{E}\epsilon)^{1/2}}\,F\!\left(\frac{\pi}{2},k\right),$$

where

$$E(\varphi,k) = \int_0^\varphi \sqrt{1-k^2\sin^2\theta}\,\mathrm{d}\theta, \qquad F(\varphi,k) = \int_0^\varphi \frac{\mathrm{d}\theta}{\sqrt{1-k^2\sin^2\theta}}$$

are the Legendre–Jacobi elliptic integrals and

$$k^2 = \frac{2\tilde{E}\epsilon}{(1+4\tilde{E}\epsilon)^{1/2}\{(1+4\tilde{E}\epsilon)^{1/2}+1\}}.$$

Therefore, eq. (2.28) for the lowest order approximation of the ground-state energy $\tilde{E}_0^{(0)}$ turns out to be

$$\frac{(1+4\tilde{E}\epsilon)^{1/4}}{3\epsilon}\left\{-E\!\left(\frac{\pi}{2},k\right) + \frac{(1+4\tilde{E}\epsilon)^{1/2}+1}{2}\,F\!\left(\frac{\pi}{2},k\right)\right\} = 0.880\,167\,1 \qquad (5.4)$$

with the right-hand side given by eq. (3.17). The energy eigenvalues $\tilde{E}_0^{(0)}$ obtained by solving eq. (5.4) for $\epsilon = 0.01, 0.1, 1$ are given in Table I together with those in the 1st order approximation to be calculated below.

To get the energy $\tilde{E} = \tilde{E}_1^{(0)}$ of the first excited state, we have only to replace the right-hand side of (5.4) by 2.383 447 from eq. (3.18). The results for the same ϵ's are given in Table II together with the 1st order approximation.

5.2.2 1st order approximation

In contrast to the case of the 0th order, the right-hand side of the eigenvalue formula (5.4) is not constant but functions, $\gamma_n(E)$, of $\tilde{E}$ determined as the zeros of eqs. (3.29) or (3.30), which we calculate numerically.

The results $\tilde{E}_n^{(1)}$ for the ground and the 1st excited states are given in Tables I and II, and are compared with the results from perturbation theory and the exact ones by Milne's numerical method.[2)]

Table I. The energy eigenvalues $\tilde{E}_0^{(\nu)}$ for the ground state in the 0th ($\nu = 0$) and the 1st order ($\nu = 1$) approximation. Also listed for reference are $\tilde{E}_{0,\rm pert}^{(\nu)}$ obtained by the 0th and the 1st order perturbation theory, and $\tilde{E}_{0,\rm exact}$ by Milne's method. The figures in brackets are the relative errors, $|\tilde{E}_0^{(\nu)} - \tilde{E}_{0,\rm exact}|/\tilde{E}_{0,\rm exact}$.

	ϵ		
	0.01	0.1	1
$\tilde{E}_0^{(0)}$	1.125 336 (0.117 099)	1.164 504 (0.093 138)	1.426 228 (0.024 330)
$\tilde{E}_0^{(1)}$	1.014 169 (0.006 745)	1.070 058 (0.004 480)	1.392 577 (0.000 162)
$\tilde{E}_{0,\rm pert}^{(0)}$	1.000 000 (0.007 320)	1.000 000 (0.061 284)	1.000 000 (0.281 791)
$\tilde{E}_{0,\rm pert}^{(1)}$	1.007 500 (0.000 125)	1.075 000 (0.009 120)	1.750 000 (0.256 866)
$\tilde{E}_{0,\rm exact}$	1.007 374	1.065 285	1.392 352

Table II. The energy eigenvalues $\tilde{E}_1^{(\nu)}$ for the first excited state in the 0th and the 1st order approximation, and corresponding $\tilde{E}_{1,\rm pert}^{(\nu)}$ and $\tilde{E}_{1,\rm exact}$ for reference.

	ϵ		
	0.01	0.1	1
$\tilde{E}_1^{(0)}$	3.068 521 (0.010 537)	3.326 367 (0.005 895)	4.657 326 (0.001 831)
$\tilde{E}_1^{(1)}$	3.036 813 (0.000 095)	3.306 952 (0.000 024)	4.648 837 (0.000 005)
$\tilde{E}_{1,\rm pert}^{(0)}$	3.000 000 (0.012 029)	3.000 000 (0.092 798)	3.000 000 (0.354 674)
$\tilde{E}_{1,\rm pert}^{(1)}$	3.037 500 (0.000 321)	3.375 000 (0.020 602)	6.750 000 (0.451 984)
$\tilde{E}_{1,\rm exact}$	3.036 525	3.306 872	4.648 813

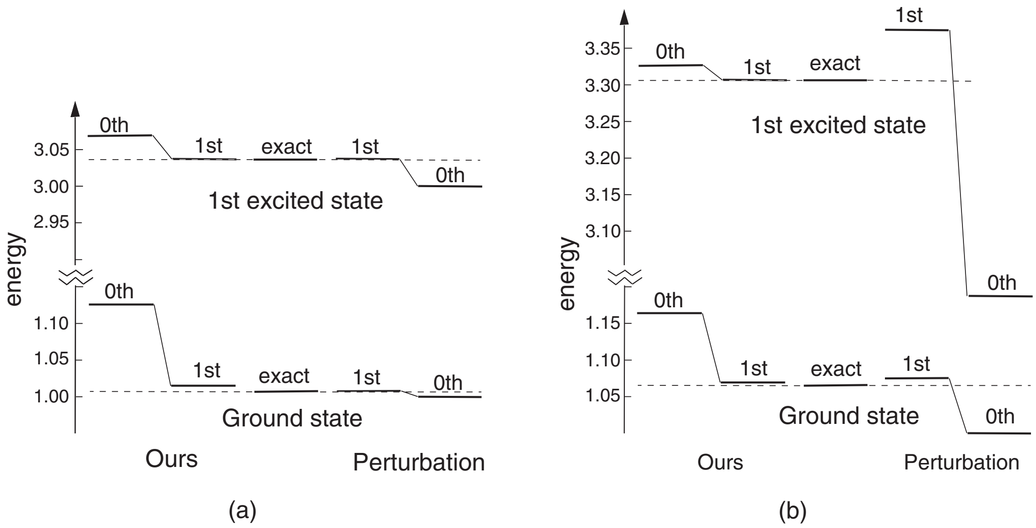

Fig. 2. The energy eigenvalues $\tilde{E}_n$ for the ground and the 1st excited states in the cases of (a) $\epsilon = 0.01$ and (b) $\epsilon = 0.1$. Comparison is made of our results, those by perturbation theory and the exact ones by Milne's numerical method.

Comparison is also made in Fig. 2 for the cases of (a) $\epsilon = 0.01$ and (b) $\epsilon = 0.1$, which shows how good our results are; the comparison favors our method the better for the larger ϵ, and in fact already for $\epsilon = 0.1$. For $\epsilon = 0.01$ in particular, our $E_0^{(0)}$ looks poorer than $E_{0,\rm pert}^{(0)}$, but they should not be compared to each other, because our $E_0^{(0)}$ is for $\tilde{Q} = 0$, or $Q = -(5/36)/\zeta^2$, and not for Q appropriate to $V = y^2 + \epsilon y^4$ with $\epsilon = 0$, for which V one calculates $E_{0,\rm pert}^{(0)}$. Our $E_n^{(\sigma)}$ approaches from different beginning at $\sigma = 0$ to the true E_n after $\tilde{Q}$ is fully incorporated.

Our approximation gets better as the higher the excited states we go. Moreover, we shall see in the next subsection that our iteration series (3.1) for the eigenfunctions $u_n(x)$ converge uniformly in x, irrespective of the magnitude of λ, while the perturbation series is known to diverge[3,5] how small λ is.

5.3 *Convergence proof for* $V(x) = 2\mu x^2 + \lambda x^4$

Let us prove the convergence of our iteration series (3.1) for the ground and the 1st excited states in the present case of the Hamiltonian (5.1) by showing that the convergence rate, r'_{nl} in eq. (4.4), are less than 1 significantly indeed for $n = 0, 1$ and $l = \mathrm{I, II}$.

To calculate the integral in eq. (4.4), we have to know the value of $\tilde{E}_n = \sqrt{m/\mu}E_n/\hbar$. We may use the approximate values for $\tilde{E}_n$ obtaind in the previous subsection. But, here let us proceed in other way by finding a region it belongs to, narrow enough for estimating r'_{nl}.

First, we consider the ground state, and find a lower bound of its energy eigenvalue. Since, for any $c > 0$,

$$2\mu x^2 + \lambda x^4 \geq 2\mu c x^2 - \frac{\mu^2}{\lambda}(c-1)^2 \qquad (5.5)$$

holds for all x, we consider the Hamiltonian of harmonic oscillator,

$$H' = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V'(x), \quad V'(x) = 2\mu c x^2 - \frac{\mu^2}{\lambda}(c-1)^2,$$

whose lowest energy eigenvalue is known,

$$E_0' = \hbar\sqrt{\frac{\mu}{m}}\sqrt{c} - \frac{\mu^2}{\lambda}(c-1)^2$$
$$= \frac{\hbar}{4\epsilon}\sqrt{\frac{\mu}{m}}\{4\epsilon\sqrt{c} - (c-1)^2\}. \tag{5.6}$$

Take the exact ground-state eigenfunction $u_0(x)$ (normalized) of our Hamiltonian H given in (5.1). Then

$$E_0 = \langle u_0, Hu_0\rangle > \langle u_0, H'u_0\rangle > E_0',$$

the middle inequality holding by (5.5) and the right-most one by the variation principle. We maximize E_0' in eq. (5.6) by varying c. The solution c_ϵ of $dE_0'/dc = 0$ or

$$c\sqrt{c} - \sqrt{c} - \epsilon = 0 \tag{5.7}$$

gives the maximum of E_0', so that we have the lower bound for E_0,

$$E_0 > \frac{3c_\epsilon + 1}{4\sqrt{c_\epsilon}}\hbar\sqrt{\frac{\mu}{m}}.$$

To find an upper bound, we take the ground-state eigenfunction,

$$v_0(x) = \left(\frac{2\sqrt{m\mu}}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{\sqrt{m\mu}}{\hbar}x^2\right),$$

of the harmonic oscillator

$$H'' = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V''(x), \quad V''(x) = 2\mu x^2.$$

Then, we obtain the upper bound,

$$E_0 < \langle v_0, Hv_0\rangle = \hbar\sqrt{\frac{\mu}{m}} + \lambda\langle x^4 v_0, v_0\rangle$$
$$= \left(1 + \frac{3}{4}\epsilon\right)\hbar\sqrt{\frac{\mu}{m}}.$$

Thus, in terms of $\tilde{E}_0 = E_0/\hbar\sqrt{\mu/m}$, we have

$$\frac{3c_\epsilon + 1}{4\sqrt{c_\epsilon}} < \tilde{E}_0 < 1 + \frac{3}{4}\epsilon, \tag{5.8}$$

where $c_\epsilon > 0$ is the solution of (5.7).

The bounds for $\tilde{E}_1$ can be obtained similarly. Note that the variation principle says that $E_1 \le \langle u, Hu\rangle$ provided $u \perp u_0$. But, we know that the first excited state has an antisymmetric eigenfunction and such functions are orthogonal to u_0. Therefore, we can apply the variation principle to the 1st excited state by confining the test functions to be antisymmetric.

The bounds thus obtained for $\epsilon = 0.01, 0.1, 1$ are shown in Table III.

Let us explain the calculation of $r'_{0\mathrm{I}}$ in the case of $\epsilon = 0.01$ for example. For the lower bound $\tilde{E} = 1.0025$ in Table III, eqs. (5.2) and (5.3) give

$$w(q; E) = 0.009\,829\,q^4 + 0.990\,171\,q^2 - 1,$$
$$\kappa(E) = 0.997\,561.$$

Since the cancellation that happened in eq. (2.15) is too subtle for computer to perform the integration in eq. (4.4), we use the asymptotic formula due to eq. (2.15),

Table III. Upper and lower bounds for $\tilde{E}_0$ and $\tilde{E}_1$.

ϵ	Lower bound for $\tilde{E}_0$	Upper bound for $\tilde{E}_0$	ϵ	Lower bound for $\tilde{E}_1$	Upper bound for $\tilde{E}_1$
0.01	1.002 5	1.007 5	0.01	3.022 2	3.037 5
0.1	1.023 8	1.075 0	0.1	3.198 6	3.375 0
1	1.182 2	1.750 0	1	4.210 0	6.750 0

$$\tilde{Q}(q, E) \sim -0.030\,226\frac{1}{-1-q},$$

for $-1.01 < q < -1$. Then, we obtain

$$\frac{0.723}{0.997\,561}\int_{-\infty}^{-1.01}|\tilde{Q}(q; E)|w(q; E)^{1/2}\,dq = 0.051,$$
$$\frac{0.723}{0.997\,561}\int_{-1.01}^{-1}\frac{0.030\,226}{-1-q}w(q; E)^{1/2}\,dq = 0.004,$$

so that

$$r'_{0\mathrm{I}}(\tilde{E}) = 0.051 + 0.004 = 0.055 \tag{5.9}$$

for $\tilde{E} = 1.002\,5$. We have written unnecessarily large number of digits for $\kappa(E)$, just for identification.

In the same way, we calculate $r'_{nl}(\tilde{E})$ $(n = 0, 1)$ for the upper and lower bounds for $\epsilon = 0.01, 0.1, 1$ and $l = \mathrm{I}, \mathrm{II}$ with the results given in Table IV, showing that r'_{nl} is sufficiently small for the iteration series (3.1) to converge in all the cases.

Moreover, we plot $r'_{nl}(\tilde{E}_{n,\mathrm{exact}})$ $(n = 0, 1; l = \mathrm{I}, \mathrm{II})$ in Fig. 3 for an extended range of ϵ, that is, $0.001 < \epsilon < 20000$, where we have used $\tilde{E}_{n\,\mathrm{exact}}$ instead of its bounds. From these, we see that the convergence rate is far less than 1 for any $\epsilon > 0$ guaranteeing the convergence of (3.1) however large λ may be. As expected, r'_{nl} approaches to that for the monomial potential $V(x) = 2\mu x^2$ as $\epsilon \to 0$ and to that for $V(x) = \lambda x^4$ as $\epsilon \to \infty$.

Remark. For $V(x) = 2\mu x^2$,

$$r'_{0\mathrm{I}} = 0.060\,0, \quad r'_{0\mathrm{II}} = 0.240\,5,$$
$$r'_{1\mathrm{I}} = 0.020\,0, \quad r'_{1\mathrm{II}} = 0.080\,2,$$

and for $V(x) = \lambda x^4$,

$$r'_{0\mathrm{I}} = 0.103\,2, \quad r'_{0\mathrm{II}} = 0.203\,2,$$
$$r'_{1\mathrm{I}} = 0.039\,6, \quad r'_{1\mathrm{II}} = 0.078\,0.$$

The results show $r'_{1l} < r'_{0l}$ mainly due to $\kappa(E_1) > \kappa(E_0)$, indicating that our method gives better results for the excited state.

6. Discussion

We have proposed a new method for solving the Schrödinger eigenvalue problem for the anharmonic oscillator having the potential $V(x) \to \infty$ as $x \to \pm\infty$, which we assume for the sake of simplicity to be symmetric $V(-x) = V(x)$ and to have two turning points. We use the Liouville transformation and a systematic iteration procedure for eigenfunctions $u_n(x)$. A criterion has been established for convergence of the iteration uniform in x. The eigenvalues are extraced from the eigenfunctions so that the uniform convergence of the eigenfunctions implies the convergence of the eigenvalues in contrast to the divergence the perturbation theory gives no matter how small λ is.

Table IV. r'_{0l} and r'_{1l} for the upper and the lower bounds in Table III.

ϵ	$r'_{0\mathrm{I}}$ for lower bound	$r'_{0\mathrm{I}}$ for upper bound	$r'_{1\mathrm{I}}$ for lower bound	$r'_{1\mathrm{I}}$ for upper bound
0.01	0.055	0.055	0.017	0.017
0.1	0.047	0.044	0.017	0.017
1	0.074	0.058	0.033	0.024
ϵ	$r'_{0\mathrm{II}}$ for lower bound	$r'_{0\mathrm{II}}$ for upper bound	$r'_{1\mathrm{II}}$ for lower bound	$r'_{1\mathrm{II}}$ for upper bound
0.01	0.233	0.232	0.073	0.073
0.1	0.184	0.173	0.043	0.040
1	0.072	0.046	0.034	0.029

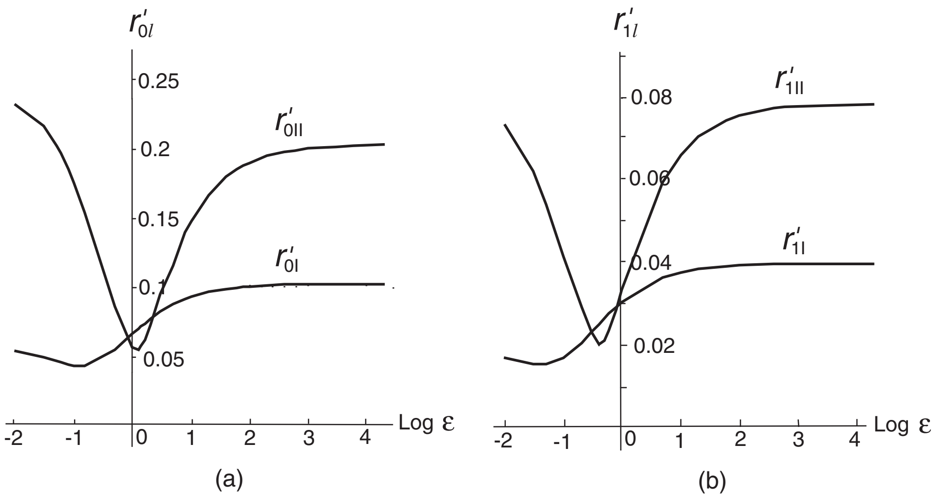

Fig. 3. r'_{0l} and r'_{1l} ($l = \mathrm{I}, \mathrm{II}$) as functions of ϵ. The difference in magnitudes between (a) r'_{0l} and (b) r'_{1l} is mainly due to the difference between $\kappa(E_0)$ and $\kappa(E_1)$.

For the purpose of comparing with the perturbation theory, we have applied our method to the case with the potential, $V(x) = 2\mu x^2 + \lambda x^4$ ($\lambda, \mu > 0$).

Our method gives a good approximation to the eigenvalues even in the first iteration, in fact better than the first order perturbation theory for the large λ, and in fact already for $\lambda > (4\sqrt{m\mu^3}/\hbar) \times 0.1$. The approximation by our method gets better, the higher the excited states we deal with (see Fig. 2 and Tables I and II). The uniform convergence of our iteration series is established irrespective of the magnitude of λ. It is remarkable that the speed of convergence is greater for some value of λ as shown in Fig. 3. It is true that our method is more complicated than the perturbation theory at least in the lower order of approximation. But, this is a price to pay for the convergent results.

Our method has a much wider applicability, as we show in the papers to follow.

There are two interesting problems we have left for future studies. One concerns those singularities of the energy eigenvalues as a function of λ, the coefficient of the x^4 term of the potential, whose existence is implied by the divergence of the perturbation series. The problem is to find out where the singularities are hidden in our converging series. The other problem is the choice available among different Green functions which we have noticed in §2.2. As we shall show in the paper to follow, they give equally good iteration solutions, but it is interesting that the convergence rates of the iteration are different depending on the Green functions we use. There are cases in which the iteration series converge with some of the Green functions but may not with others.

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