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ON EIGENFUNCTIONS OF HILL'S EQUATION WITH SYMMETRIC DOUBLE WELL POTENTIAL

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ABSTRACT. Throughout this paper the asymptotic approximations for eigenfunctions of eigenvalue problems associated with Hill's equation satisfying periodic and semi-periodic boundary conditions are derived when the potential is symmetric double well. These approximations are used to determine the Green's functions of the related problems. Then, the obtained results are adapted to the Whittaker-Hill equation which has the symmetric double well potential and is widely investigated in the literature.

1. INTRODUCTION

Consider the Hill's equation

$$y'' + [\lambda - q(x)]y = 0, \quad x \in [0, a]$$
 (1)

under the periodic boundary conditions y(0) = y(a), y'(0) = y'(a), or the semiperiodic boundary conditions y(0) = -y(a), y'(0) = -y'(a). Here, λ is a real parameter and the potential q(x) is a real-valued, absolutely continuous and periodic function with period a such that

$$\int_0^a q(t)dt = 0.$$

The equation (1) is fundamental for the quantum mechanical treatment of atomic and molecular phenomena. This kind of equation was first used by Hill [21] in modelling of the moon motion. It also appears in the theory of particle orbits in linear accelerators and alternating gradient synchrotrons, because the field structures are periodic [10, 25, 32].

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The derivation of asymptotic formulae for eigenvalues and eigenfunctions of Hill's equation, when restrictive conditions were imposed on q, is of interest in its own right and has a long history. Exact solutions of differential equations are unfortunately rare in applied mathematics and physics. Asymptotical interpretation of the differential equations plays an important role in understanding the behaviour of such differential equations [5, 12, 27, 30, 31]. Motivation for studying eigenvalue and eigenfunction asymptotics has come from several different types of problems including instability intervals and gaps of eigenvalues [3,4,11,15,22,26], the derivation and properties of the Green's function [7–9, 13, 14, 23], inverse spectral theory and theory on reconstructing the potential function from knowledge of spectral data [16, 19], and the general theory of periodic potentials [2, 6, 18, 24, 28].

The main purpose of this paper is to determine asymptotic formulae for the eigenfunctions of the Hill's equation with q(x) being of a symmetric double well potential under the periodic and semi-periodic boundary conditions. We call q a double well potential, if there are points $x_1 < x_2 < x_3$ in [0, a] such that q is monotone decreasing on $[0, x_1]$ and $[x_2, x_3]$ and is monotone increasing elsewhere. In this work, it is assumed in particular that the potential function q is a continuous function on [0, a] which is symmetric on [0, a] as well as on $[0, \frac{a}{2}]$ and non-increasing on $[0, \frac{a}{4}]$, that is, $q(x) = q(a - x) = q(\frac{a}{2} - x)$, mathematically.

Denote by λ_n and μ_n (n = 0, 1, 2, ...) the periodic and semi-periodic eigenvalues of (1), respectively. These eigenvalues are interlaced in the following way:

$$\lambda_0 < \mu_0 \le \mu_1 < \lambda_1 \le \lambda_2 < \mu_2 \le \mu_3 < \dots \to \infty.$$

Başkaya [4] obtained the asymptotic approximations of the periodic and semiperiodic eigenvalues of (1) having symmetric double well potential such that, as $n \to \infty$

$$\begin{aligned} \lambda_{2n+1} &= \frac{4(n+1)^2 \pi^2}{a^2} \mp \frac{1}{(n+1)\pi} \Big| \int_0^{a/4} q'(t) \sin\left(\frac{4(n+1)\pi}{a}t\right) dt \Big| \\ &- \frac{a}{16(n+1)^2 \pi^2} [aq^2(a) + 2a \int_0^{a/4} q(t)q'(t) dt \\ &- 8 \int_0^{a/4} tq(t)q'(t) dt] + o(n^{-2}) \end{aligned}$$
(2)

and

In Section 2, the eigenfunctions of (1) corresponding to the eigenvalues, λ_n and μ_n , given by (2) and (3) are investigated. By using the estimates on the eigenfunctions, the Green's function asymptotics related to the Hill's equation are derived in Section 3. Here, the method developed by Fulton [20] is followed. In Section 4, the obtained results for the eigenfunctions and Green's functions are adapted to the Whittaker-Hill equation

$$\frac{d^2\psi}{dz^2} + [\lambda + 2k\cos(2z) + 2l\cos(4z)]\psi = 0$$

where λ, k, l are real. This equation arises after separating the wave equation using paraboloidal coordinates [1] and is equivalent to a time-independent Schrödinger equation,

$$-\alpha \frac{d^2\psi}{d\theta^2} + V(\theta)\psi = \varepsilon\psi,$$

that describes the internal rotational (torsinal) problem of a given molecular system around a dihedral angle $\theta = 2z$. $\varepsilon = \alpha \lambda/4$ is the energy eigenvalue of the eigenfunction $\psi = \psi(\theta)$ and $V(\theta) = V_1 \cos(\theta) + V_2 \cos(2\theta)$ is a period 2π function representing a symmetric periodic double well potential with $V_1 = -\alpha k/2$ and $V_2 = -\alpha l/2$ (see [29]).

The following results obtained in [18] will be used to determine the eigenfunctions.

Let $\phi_1(x,\lambda)$ and $\phi_2(x,\lambda)$ be the linearly independent solutions of (1) with the initial conditions

$$\phi_1(0,\lambda) = 1, \quad \phi_1'(0,\lambda) = 0, \quad \phi_2(0,\lambda) = 0, \quad \phi_2'(0,\lambda) = 1.$$
 (4)

Theorem 1. [18, §4.3] Assume that $\phi_1(x, \lambda)$ and $\phi_2(x, \lambda)$ are the solutions of (1) satisfying (4). Let q(x) be an absolutely continuous function. Then, as $\lambda \to \infty$,

$$\phi_1(x,\lambda) = \cos(x\sqrt{\lambda}) + \frac{1}{2}\lambda^{-\frac{1}{2}}Q(x)\sin(x\sqrt{\lambda}) + \frac{1}{4}\lambda^{-1}\left\{q(x) - q(0) - \frac{1}{2}Q^2(x)\right\}$$
$$\times \cos(x\sqrt{\lambda}) + o(\lambda^{-1}),$$

$$\phi_{2}(x,\lambda) = \lambda^{-\frac{1}{2}} \sin(x\sqrt{\lambda}) - \frac{1}{2}\lambda^{-1}Q(x)\cos(x\sqrt{\lambda}) + \frac{1}{4}\lambda^{-\frac{3}{2}} \left\{ q(x) + q(0) - \frac{1}{2}Q^{2}(x) \right\} \sin(x\sqrt{\lambda}) + o(\lambda^{-\frac{3}{2}})$$

where

$$Q(x) = \int_0^x q(t)dt.$$
 (5)

2. Asymptotics of Eigenfunctions

In this section we obtain the asymptotic approximations for eigenfunctions of (1) satisfying the periodic and semi-periodic boundary conditions.

Before, we prove the following lemma for q(x) being of a symmetric double well potential.

Lemma 1. If q(x) is a symmetric double well potential on [0, a], then

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$$\int_{0}^{x} q(t)dt = xq(x) + \frac{a}{2} \left[q\left(\frac{a}{2}\right) - q\left(\frac{a}{4}\right) \right] - \int_{a/4}^{a/2} tq'(t)dt - \int_{a/4}^{x} tq'(t)dt.$$
(6)

Proof. Using integration by parts and $q(x) = q(a - x) = q(\frac{a}{2} - x)$, it is obtained that

$$\int_{0}^{x} q(t)dt = tq(t)\Big|_{t=0}^{x} - \int_{0}^{x} tq'(t)dt$$

$$= xq(x) - \left[\int_{0}^{a/2} tq'(t)dt + \int_{a/2}^{x} tq'(t)dt\right]$$

$$= xq(x) - \left[-\int_{0}^{a/2} tq'(a-t)dt + \int_{a/2}^{x} tq'(t)dt\right]$$

$$= xq(x) - \int_{a}^{a/2} (a-t)q'(t)dt - \int_{a/2}^{x} tq'(t)dt$$

$$= xq(x) + a[q(t)]\Big|_{t=a/2}^{a} - \int_{a/2}^{a} tq'(t)dt - \int_{a/2}^{x} tq'(t)dt$$

$$= xq(x) + a\left[q(a) - q\left(\frac{a}{2}\right)\right] - \int_{a/2}^{a} tq'(t)dt - \int_{a/2}^{x} tq'(t)dt$$

$$= xq(x) - \int_{a/2}^{a} tq'(t)dt - \int_{a/2}^{x} tq'(t)dt$$

$$= xq(x) - \left[\int_{0}^{a/4} tq'(t)dt + \int_{a/4}^{a/2} tq'(t)dt\right] - \int_{a/2}^{x} tq'(t)dt$$

$$= xq(x) - \left[\int_{0}^{a/4} tq'\left(\frac{a}{2} - t\right)dt + \int_{a/4}^{a/2} tq'(t)dt\right] - \int_{a/2}^{x} tq'(t)dt$$

$$= xq(x) - \left[\int_{a/2}^{a/4} \left(\frac{a}{2} - t\right)q'(t)dt + \int_{a/4}^{a/2} tq'(t)dt\right] - \int_{a/2}^{x} tq'(t)dt$$

Theorem 2. Let q(x) be a symmetric double well potential on [0, a]. Then as $\lambda \to \infty$, for the solutions of (1) with the initial conditions (4), we have

$$\phi_{1}(x,\lambda) = \cos(x\sqrt{\lambda}) + \frac{1}{2}\lambda^{-\frac{1}{2}} \{xq(x) + \frac{a}{2} \left[q\left(\frac{a}{2}\right) - q\left(\frac{a}{4}\right)\right] - \int_{a/4}^{a/2} tq'(t)dt$$
$$- \int_{a/4}^{x} tq'(t)dt \} \sin(x\sqrt{\lambda}) + \frac{1}{4}\lambda^{-1} \{q(x) - q(0) - \frac{1}{2} [xq(x) + \frac{a}{2} [q\left(\frac{a}{2}\right) - q\left(\frac{a}{4}\right)] - \int_{a/4}^{a/2} tq'(t)dt - \int_{a/4}^{x} tq'(t)dt]^{2} \} \cos(x\sqrt{\lambda}) + o(\lambda^{-1}),$$
(7)

$$\phi_{2}(x,\lambda) = \lambda^{-\frac{1}{2}} \sin(x\sqrt{\lambda}) - \frac{1}{2}\lambda^{-1} \{xq(x) + \frac{a}{2} \left[q\left(\frac{a}{2}\right) - q\left(\frac{a}{4}\right)\right] - \int_{a/4}^{+} tq'(t)dt - \int_{a/4}^{x} tq'(t)dt\} \cos(x\sqrt{\lambda}) + \frac{1}{4}\lambda^{-\frac{3}{2}} \{q(x) + q(0) - \frac{1}{2}[xq(x) + \frac{a}{2}[q\left(\frac{a}{2}\right) - q\left(\frac{a}{4}\right)] - \int_{a/4}^{a/2} tq'(t)dt - \int_{a/4}^{x} tq'(t)dt]^{2} \sin(x\sqrt{\lambda}) + o(\lambda^{-\frac{3}{2}}).$$
(8)

Proof. If we use Theorem 1 and substitute (6) in (5), the proof is done.

Theorem 3. The eigenfunctions of the periodic problem having symmetric double well potential satisfy, as $n \to \infty$

$$\phi_1(x,n) = \cos\frac{2(n+1)\pi x}{a} + \frac{a}{4(n+1)\pi} \{xq(x) + \frac{a}{2} \left[q\left(\frac{a}{2}\right) - q\left(\frac{a}{4}\right)\right] \\ - \int_{a/4}^{a/2} tq'(t)dt - \int_{a/4}^x tq'(t)dt\} \sin\frac{2(n+1)\pi x}{a} + \frac{a^2}{16(n+1)^2\pi^2} \\ \times \{q(x) - q(0) - \frac{1}{2} [xq(x) + \frac{a}{2} \left[q\left(\frac{a}{2}\right) - q\left(\frac{a}{4}\right)\right] - \int_{a/4}^{a/2} tq'(t)dt \\ - \int_{a/4}^x tq'(t)dt]^2\} \cos\frac{2(n+1)\pi x}{a} + o(n^{-2}),$$

$$\begin{split} \phi_2(x,n) &= \frac{a}{2(n+1)\pi} \sin \frac{2(n+1)\pi x}{a} - \frac{a^2}{8(n+1)^2 \pi^2} \{ xq(x) + \frac{a}{2} \left[q\left(\frac{a}{2}\right) - q\left(\frac{a}{4}\right) \right] \\ &- \int_{a/4}^{a/2} tq'(t) dt - \int_{a/4}^{x} tq'(t) dt \} \cos \frac{2(n+1)\pi x}{a} + \frac{a^3}{32(n+1)^3 \pi^3} \\ &\times \{q(x) + q(0) - \frac{1}{2} [xq(x) + \frac{a}{2} \left[q\left(\frac{a}{2}\right) - q\left(\frac{a}{4}\right) \right] - \int_{a/4}^{a/2} tq'(t) dt \\ &- \int_{a/4}^{x} tq'(t) dt]^2 \} \sin \frac{2(n+1)\pi x}{a} + o(n^{-3}). \end{split}$$

Theorem 4. The eigenfunctions of the semi-periodic problem having symmetric double well potential satisfy, as $n \to \infty$

$$\begin{split} \phi_1(x,n) &= \cos \frac{(2n+1)\pi x}{a} + \frac{a}{2(2n+1)\pi} \{ xq(x) + \frac{a}{2} \left[q\left(\frac{a}{2}\right) - q\left(\frac{a}{4}\right) \right] \\ &- \int_{a/4}^{a/2} tq'(t) dt - \int_{a/4}^x tq'(t) dt \} \sin \frac{(2n+1)\pi x}{a} + \frac{a^2}{4(2n+1)^2 \pi^2} \\ &\times \{ q(x) - q(0) - \frac{1}{2} [xq(x) + \frac{a}{2} \left[q\left(\frac{a}{2}\right) - q\left(\frac{a}{4}\right) \right] - \int_{a/4}^{a/2} tq'(t) dt \\ &- \int_{a/4}^x tq'(t) dt]^2 \} \cos \frac{(2n+1)\pi x}{a} + o(n^{-2}), \end{split}$$

$$\phi_2(x,n) &= \frac{a}{(2n+1)\pi} \sin \frac{(2n+1)\pi x}{a} - \frac{a^2}{2(2n+1)^2 \pi^2} \{ xq(x) + \frac{a}{2} [q\left(\frac{a}{2}\right) \\ &- q\left(\frac{a}{4}\right)] - \int_{a/4}^{a/2} tq'(t) dt - \int_{a/4}^x tq'(t) dt \} \cos \frac{(2n+1)\pi x}{a} \\ &+ \frac{a^3}{4(2n+1)^3 \pi^3} \{ q(x) + q(0) - \frac{1}{2} [xq(x) + \frac{a}{2} \left[q\left(\frac{a}{2}\right) - q\left(\frac{a}{4}\right) \right] \\ &- \int_{a/4}^{a/2} tq'(t) dt - \int_{a/4}^x tq'(t) dt]^2 \} \sin \frac{(2n+1)\pi x}{a} + o(n^{-3}). \end{split}$$

To prove Theorem 3 and Theorem 4, the related eigenvalues given by (2) and (3) are substituted in Theorem 2.

We also have asymptotic formulae for the derivatives of $\phi_1(x, \lambda)$ and $\phi_2(x, \lambda)$. We will use them in calculation of the Green's functions.

Lemma 2. Consider the equation (1) having symmetric double well potential. As $\lambda \to \infty$, for the derivatives of its solutions, $\phi_1(x,\lambda)$ and $\phi_2(x,\lambda)$ which satisfy (4), we have

$$\begin{split} \phi_1'(x,\lambda) &= -\lambda^{\frac{1}{2}} \sin(x\sqrt{\lambda}) + \frac{1}{2} \{ xq(x) + \frac{a}{2} \left[q\left(\frac{a}{2}\right) - q\left(\frac{a}{4}\right) \right] - \int_{a/4}^{a/2} tq'(t) dt \\ &- \int_{a/4}^x tq'(t) dt \} \cos(x\sqrt{\lambda}) + \frac{1}{4} \lambda^{-\frac{1}{2}} \{ q(x) + q(0) + \frac{1}{2} [xq(x) + \frac{a}{2} [q\left(\frac{a}{2}\right) \\ &- q\left(\frac{a}{4}\right)] - \int_{a/4}^{a/2} tq'(t) dt - \int_{a/4}^x tq'(t) dt]^2 \} \sin(x\sqrt{\lambda}) + o(\lambda^{-\frac{1}{2}}), \end{split}$$
(9)
$$\phi_2'(x,\lambda) &= \cos(x\sqrt{\lambda}) + \frac{1}{2} \lambda^{-\frac{1}{2}} \{ xq(x) + \frac{a}{2} \left[q\left(\frac{a}{2}\right) - q\left(\frac{a}{4}\right) \right] - \int_{a/4}^{a/2} tq'(t) dt \end{split}$$

$$-\int_{a/4}^{x} tq'(t)dt \sin(x\sqrt{\lambda}) - \frac{1}{4}\lambda^{-1} \{q(x) - q(0) + \frac{1}{2}[xq(x) + \frac{a}{2}[q\left(\frac{a}{2}\right) - q\left(\frac{a}{4}\right)] - \int_{a/4}^{a/2} tq'(t)dt - \int_{a/4}^{x} tq'(t)dt]^{2} \cos(x\sqrt{\lambda}) + o(\lambda^{-1}).$$
(10)

Proof. Here, the proof of (9) will be shown. The proof of (10) is similar to that. If q(x) is a piecewise continuous function, then, as $\lambda \to \infty$,

$$\phi_1(x,\lambda) = \cos(x\sqrt{\lambda}) + \lambda^{-\frac{1}{2}} \int_0^x \sin\{(x-t)\sqrt{\lambda}\}q(t)\cos(t\sqrt{\lambda})dt + \lambda^{-1} \int_0^x \sin\{(x-t)\sqrt{\lambda}\}q(t)dt \int_0^t \sin\{(t-u)\sqrt{\lambda}\}q(u)\cos(u\sqrt{\lambda})du + O(\lambda^{-\frac{3}{2}})$$
(11)

(see [18, §4.3]). The usual variation of constants formula [17, §2.5] gives

$$\phi_1(x,\lambda) = \cos(x\sqrt{\lambda}) + \lambda^{-\frac{1}{2}} \int_0^x \sin\{(x-t)\sqrt{\lambda}\}q(t)\phi_1(t,\lambda)dt.$$

If we arrange this formula, one can write

$$\phi_1(x,\lambda) = \cos(x\sqrt{\lambda}) + \lambda^{-\frac{1}{2}} \{\sin(x\sqrt{\lambda}) \int_0^x \cos(t\sqrt{\lambda})q(t)\phi_1(t,\lambda)dt - \cos(x\sqrt{\lambda}) \int_0^x \sin(t\sqrt{\lambda})q(t)\phi_1(t,\lambda)dt\}.$$
(12)

It is obtained by differentiating (12) with respect to x and substituting $\phi_1(t, \lambda)$ from (11) in the integral that

$$\begin{split} \phi_1'(x,\lambda) &= -\lambda^{\frac{1}{2}} \sin(x\sqrt{\lambda}) + \lambda^{-\frac{1}{2}} \{\lambda^{\frac{1}{2}} \cos(x\sqrt{\lambda}) \int_0^x \cos(t\sqrt{\lambda})q(t)\phi_1(t,\lambda)dt \\ &+ \lambda^{\frac{1}{2}} \sin(x\sqrt{\lambda}) \int_0^x \sin(t\sqrt{\lambda})q(t)\phi_1(t,\lambda)dt \} \\ &= -\lambda^{\frac{1}{2}} \sin(x\sqrt{\lambda}) + \int_0^x \cos\{(x-t)\sqrt{\lambda}\}q(t)\phi_1(t,\lambda)dt \\ &= -\lambda^{\frac{1}{2}} \sin(x\sqrt{\lambda}) + \int_0^x \cos\{(x-t)\sqrt{\lambda}\}q(t)\cos(t\sqrt{\lambda})dt \\ &+ \lambda^{-\frac{1}{2}} \int_0^x \cos\{(x-t)\sqrt{\lambda}\}q(t)dt \int_0^t \sin\{(t-u)\sqrt{\lambda}\}q(u)\cos(u\sqrt{\lambda})du \\ &+ O(\lambda^{-1}). \end{split}$$
(13)

If differentiability conditions are imposed on q(x), (13) can be made more precise. Assume that q(x) is absolutely continuous. This implies that q'(x) exists almost everywhere and is integrable. Under these conditions, let consider the second term

on the right of (13). We have

$$\begin{split} \int_{0}^{x} \cos\{(x-t)\sqrt{\lambda}\}q(t)\cos(t\sqrt{\lambda})dt \\ &= \frac{1}{2}\int_{0}^{x} \left[\cos(x\sqrt{\lambda}) + \cos\{(x-2t)\sqrt{\lambda}\}\right]q(t)dt \\ &= \frac{1}{2}Q(x)\cos(x\sqrt{\lambda}) + \frac{1}{2}\int_{0}^{x}\cos\{(x-2t)\sqrt{\lambda}\}q(t)dt \\ &= \frac{1}{2}Q(x)\cos(x\sqrt{\lambda}) + \frac{1}{2}[-\frac{1}{2}\lambda^{-\frac{1}{2}}q(t)\sin\{(x-2t)\sqrt{\lambda}\}\Big|_{t=0}^{x} \\ &\quad + \frac{1}{2}\lambda^{-\frac{1}{2}}\int_{0}^{x}q'(t)\sin\{(x-2t)\sqrt{\lambda}\}dt] \\ &= \frac{1}{2}Q(x)\cos(x\sqrt{\lambda}) + \frac{1}{4}\lambda^{-\frac{1}{2}}\left[q(x) + q(0)\right]\sin(x\sqrt{\lambda}) \\ &\quad + \frac{1}{4}\lambda^{-\frac{1}{2}}\int_{0}^{x}q'(t)\sin\{(x-2t)\sqrt{\lambda}\}dt. \end{split}$$

The right-hand integral on the last equality is o(1) as $\lambda \to \infty$ by the Riemann-Lebesgue Lemma. So,

$$\int_0^x \cos\{(x-t)\sqrt{\lambda}\}q(t)\cos(t\sqrt{\lambda})dt = \frac{1}{2}Q(x)\cos(x\sqrt{\lambda}) + \frac{1}{4}\lambda^{-\frac{1}{2}}\left[q(x) + q(0)\right] \\ \times \sin(x\sqrt{\lambda}) + o(\lambda^{-\frac{1}{2}}).$$
(14)

Also, from [18, §4.3]

$$\int_0^x \sin\{(x-t)\sqrt{\lambda}\}q(t)\cos(t\sqrt{\lambda})dt = \frac{1}{2}Q(x)\sin(x\sqrt{\lambda}) + \frac{1}{4}\lambda^{-\frac{1}{2}}\left[q(x) - q(0)\right] \\ \times \cos(x\sqrt{\lambda}) + o(\lambda^{-\frac{1}{2}}).$$
(15)

For the third term on the right of (13), together with (15) we find

$$\begin{split} \lambda^{-\frac{1}{2}} \int_{0}^{x} \cos\{(x-t)\sqrt{\lambda}\}q(t)dt \int_{0}^{t} \sin\{(t-u)\sqrt{\lambda}\}q(u)\cos(u\sqrt{\lambda})du \\ &= \frac{1}{2}\lambda^{-\frac{1}{2}} \int_{0}^{x} \cos\{(x-t)\sqrt{\lambda}\}q(t)Q(t)\sin(t\sqrt{\lambda})dt + O(\lambda^{-1}) \\ &= \frac{1}{4}\lambda^{-\frac{1}{2}} \int_{0}^{x} \left[\sin(x\sqrt{\lambda}) - \sin\{(x-2t)\sqrt{\lambda}\}\right]q(t)Q(t)dt + O(\lambda^{-1}) \\ &= \frac{1}{4}\lambda^{-\frac{1}{2}}\sin(x\sqrt{\lambda}) \left[\frac{Q^{2}(t)}{2}\right]\Big|_{t=0}^{x} + o(\lambda^{-\frac{1}{2}}) \\ &= \frac{1}{8}\lambda^{-\frac{1}{2}}Q^{2}(x)\sin(x\sqrt{\lambda}) + o(\lambda^{-\frac{1}{2}}), \end{split}$$
(16)

again by using the Riemann-Lebesgue Lemma. From (14) and (16), it is obtained that

$$\phi_1'(x,\lambda) = -\lambda^{\frac{1}{2}} \sin(x\sqrt{\lambda}) + \frac{1}{2}Q(x)\cos(x\sqrt{\lambda}) + \frac{1}{4}\lambda^{-\frac{1}{2}} \left\{ q(x) + q(0) + \frac{1}{2}Q^2(x) \right\} \\ \times \sin(x\sqrt{\lambda}) + o(\lambda^{-\frac{1}{2}}).$$
(17)

Using (6) in (5) and substituting this in (17) prove (9).

3. Asymptotics of Green's Functions

In this section, we aim to improve asymptotic formulae for Green's functions of the periodic and semi-periodic problems with symmetric double well potential. The Green's function $G(x, \zeta, \lambda)$ is given by

$$G(x,\zeta,\lambda) = \begin{cases} \frac{\phi_1(\zeta,\lambda)\phi_2(x,\lambda)}{w(\lambda)}, & 0 \le \zeta \le x \le a\\ \frac{\phi_1(x,\lambda)\phi_2(\zeta,\lambda)}{w(\lambda)}, & 0 \le x \le \zeta \le a \end{cases}$$
(18)

(see [20]). Here, $\phi_1(x, \lambda)$ and $\phi_2(x, \lambda)$ are linearly independent solutions of (1) satisfying (4). And, we define $w(\lambda)$ as follows

$$w(\lambda) := \phi_1(x,\lambda)\phi_2'(x,\lambda) - \phi_1'(x,\lambda)\phi_2(x,\lambda).$$
(19)

It is known as the Wronskian function of $\phi_1(x,\lambda)$ and $\phi_2(x,\lambda)$.

Theorem 5. Suppose that the equation (1) has the symmetric double well potential and its independent solutions, $\phi_1(x, \lambda)$ and $\phi_2(x, \lambda)$ satisfy the initial conditions (4). Then, the Green's function of the problem is, as $\lambda \to \infty$

$$\begin{split} G(x,\zeta,\lambda) &= \lambda^{-\frac{1}{2}}\cos(\zeta\sqrt{\lambda})\sin(x\sqrt{\lambda}) - \frac{1}{2}\lambda^{-1}[D(x)\cos(\zeta\sqrt{\lambda})\cos(x\sqrt{\lambda})\\ &\quad -D(\zeta)\sin(\zeta\sqrt{\lambda})\sin(x\sqrt{\lambda})] + \frac{1}{4}\lambda^{-\frac{3}{2}}\{[q(\zeta) + q(x) - \frac{1}{2}(D^2(\zeta)\\ &\quad +D^2(x))]\cos(\zeta\sqrt{\lambda})\sin(x\sqrt{\lambda}) - D(\zeta)D(x)\sin(\zeta\sqrt{\lambda})\cos(x\sqrt{\lambda})\}\\ &\quad +o(\lambda^{-\frac{3}{2}}), \qquad 0 \leq \zeta \leq x \leq a \end{split}$$

where

$$D(x) := xq(x) + \frac{a}{2} \left[q\left(\frac{a}{2}\right) - q\left(\frac{a}{4}\right) \right] - \int_{a/4}^{a/2} tq'(t)dt - \int_{a/4}^{x} tq'(t)dt.$$
(20)

Similar result holds for $0 \le x \le \zeta \le a$ changing the role of ζ and x.

Proof. We begin to the proof by evaluating the Wronskian function $w(\lambda)$. For this reason, we substitute (7), (8), (9) and (10) into (19). Hence,

$$w(\lambda) = 1 - \frac{1}{4}\lambda^{-1} \left[q(x) - q(0) + \frac{1}{2}D^2(x) \right] \cos^2(x\sqrt{\lambda}) + \frac{1}{4}\lambda^{-1}$$

$$\times \left[q(x) + q(0) - \frac{1}{2}D^{2}(x) \right] \sin^{2}(x\sqrt{\lambda})$$

$$+ \frac{1}{4}\lambda^{-1}D^{2}(x) + \frac{1}{4}\lambda^{-1} \left[q(x) - q(0) - \frac{1}{2}D^{2}(x) \right] \cos^{2}(x\sqrt{\lambda})$$

$$- \frac{1}{4}\lambda^{-1} \left[q(x) + q(0) + \frac{1}{2}D^{2}(x) \right] \sin^{2}(x\sqrt{\lambda}) + o(\lambda^{-1})$$

$$= 1 - \frac{1}{4}\lambda^{-1}D^{2}(x) + \frac{1}{4}\lambda^{-1}D^{2}(x) + o(\lambda^{-1})$$

$$= 1 + o(\lambda^{-1}).$$

From that, we can write

$$\frac{1}{w(\lambda)} = \frac{1}{1 + o(\lambda^{-1})} = 1 + o(\lambda^{-1}).$$
(21)

Finally, using (7), (8), (21) in (18) we find

$$\begin{split} \frac{\phi_1(\zeta,\lambda)\phi_2(x,\lambda)}{w(\lambda)} &= \{\cos(\zeta\sqrt{\lambda}) + \frac{1}{2}\lambda^{-\frac{1}{2}}D(\zeta)\sin(\zeta\sqrt{\lambda}) + \frac{1}{4}\lambda^{-1}[q(\zeta) - q(0) \\ &- \frac{1}{2}D^2(\zeta)]\cos(\zeta\sqrt{\lambda}) + o(\lambda^{-1})\} \\ &\times \{\lambda^{-\frac{1}{2}}\sin(x\sqrt{\lambda}) - \frac{1}{2}\lambda^{-1}D(x)\cos(x\sqrt{\lambda}) + \frac{1}{4}\lambda^{-\frac{3}{2}} \\ &\times \left[q(x) + q(0) - \frac{1}{2}D^2(x)\right]\sin(x\sqrt{\lambda}) + o(\lambda^{-\frac{3}{2}})\}\{1 + o(\lambda^{-1})\} \\ &= \{\lambda^{-\frac{1}{2}}\cos(\zeta\sqrt{\lambda})\sin(x\sqrt{\lambda}) - \frac{1}{2}\lambda^{-1}D(x)\cos(\zeta\sqrt{\lambda})\cos(x\sqrt{\lambda}) \\ &+ \frac{1}{4}\lambda^{-\frac{3}{2}}\left[q(x) + q(0) - \frac{1}{2}D^2(x)\right]\cos(\zeta\sqrt{\lambda})\sin(x\sqrt{\lambda}) \\ &+ \frac{1}{2}\lambda^{-1}D(\zeta)\sin(\zeta\sqrt{\lambda})\sin(x\sqrt{\lambda}) - \frac{1}{4}\lambda^{-\frac{3}{2}}D(\zeta)D(x) \\ &\times \sin(\zeta\sqrt{\lambda})\cos(x\sqrt{\lambda}) + \frac{1}{4}\lambda^{-\frac{3}{2}}\left[q(\zeta) - q(0) - \frac{1}{2}D^2(\zeta)\right] \\ &\times \cos(\zeta\sqrt{\lambda})\sin(x\sqrt{\lambda}) + o(\lambda^{-\frac{3}{2}})\} \times \{1 + o(\lambda^{-1})\} \\ &= \lambda^{-\frac{1}{2}}\cos(\zeta\sqrt{\lambda})\sin(x\sqrt{\lambda}) - \frac{1}{2}\lambda^{-1}[D(x)\cos(\zeta\sqrt{\lambda})\cos(x\sqrt{\lambda}) \\ &- D(\zeta)\sin(\zeta\sqrt{\lambda})\sin(x\sqrt{\lambda})] + \frac{1}{4}\lambda^{-\frac{3}{2}} \\ &\times \{\left[q(\zeta) + q(x) - \frac{1}{2}\left(D^2(\zeta) + D^2(x)\right)\right]\cos(\zeta\sqrt{\lambda})\sin(x\sqrt{\lambda}) \\ &- D(\zeta)D(x)\sin(\zeta\sqrt{\lambda})\cos(x\sqrt{\lambda})\} + o(\lambda^{-\frac{3}{2}}). \end{split}$$

Thus, the proof is completed.

Theorem 6. Green's function of the periodic problem with symmetric double well potential satisfies, as $n \to \infty$

$$\begin{aligned} G(x,\zeta,n) &= \frac{a}{2(n+1)\pi} \cos \frac{2(n+1)\pi\zeta}{a} \sin \frac{2(n+1)\pi x}{a} - \frac{a^2}{8(n+1)^2\pi^2} \\ &\times [D(x) \cos \frac{2(n+1)\pi\zeta}{a} \cos \frac{2(n+1)\pi x}{a} \\ &- D(\zeta) \sin \frac{2(n+1)\pi\zeta}{a} \sin \frac{2(n+1)\pi x}{a}] \\ &+ \frac{a^3}{32(n+1)^3\pi^3} \left\{ \left[q(\zeta) + q(x) - \frac{1}{2} \left(D^2(\zeta) + D^2(x) \right) \right] \right\} \\ &\times \cos \frac{2(n+1)\pi\zeta}{a} \sin \frac{2(n+1)\pi x}{a} - D(\zeta)D(x) \sin \frac{2(n+1)\pi\zeta}{a} \\ &\times \cos \frac{2(n+1)\pi\chi}{a} \right\} + o(n^{-3}) \end{aligned}$$

for $0 \leq \zeta \leq x \leq a$. Similar result holds for $0 \leq x \leq \zeta \leq a$ changing the role of ζ and x.

Theorem 7. Green's function of the semi-periodic problem with symmetric double well potential satisfies, as $n \to \infty$

$$\begin{split} G(x,\zeta,n) &= \frac{a}{(2n+1)\pi} \cos\frac{(2n+1)\pi\zeta}{a} \sin\frac{(2n+1)\pi x}{a} - \frac{a^2}{2(2n+1)^2\pi^2} \\ &\times [D(x)\cos\frac{(2n+1)\pi\zeta}{a}\cos\frac{(2n+1)\pi x}{a} \\ &- D(\zeta)\sin\frac{(2n+1)\pi\zeta}{a}\sin\frac{(2n+1)\pi x}{a}] + \frac{a^3}{4(2n+1)^3\pi^3} \\ &\times \left\{ \left[q(\zeta) + q(x) - \frac{1}{2} \left(D^2(\zeta) + D^2(x) \right) \right] \cos\frac{(2n+1)\pi\zeta}{a} \\ &\times \sin\frac{(2n+1)\pi x}{a} - D(\zeta)D(x)\sin\frac{(2n+1)\pi\zeta}{a}\cos\frac{(2n+1)\pi x}{a} \right\} \\ &+ o(n^{-3}) \end{split}$$

for $0 \leq \zeta \leq x \leq a$. Similar result holds for $0 \leq x \leq \zeta \leq a$ changing the role of ζ and x.

To prove Theorem 6 and Theorem 7, the related eigenvalues given by (2) and (3) are used together with Theorem 5.

4. The Whittaker-Hill Equation

Consider the Whittaker-Hill equation

$$y'' + [\lambda + 2k\cos(2x) + 2\ell\cos(4x)]y = 0, \quad x \in [0, 2\pi], \quad \lambda, k, \ell \in \mathbb{R}$$
(22)

under the periodic boundary conditions $y(0) = y(2\pi)$, $y'(0) = y'(2\pi)$, or the semiperiodic boundary conditions $y(0) = -y(2\pi)$, $y'(0) = -y'(2\pi)$. Here, our goal is to seek the eigenfunction and Green's function asymptotics of the described problem. This problem is a special case of (1) when $q(x) = 2k\cos(2x)+2\ell\cos(4x)$ and $a = 2\pi$. Also, note that q is a continuous function on $[0,2\pi]$ which is symmetric on $[0,2\pi]$ as well as on $[0,\pi]$ and non-increasing on $[0,\frac{\pi}{2}]$, i. e., $q(x) = q(2\pi - x) = q(\pi - x)$. So, we say that q is a symmetric double well potential (see Figure 1). Last of all, we can apply the obtained results in Sections 2 and 3 to this problem.

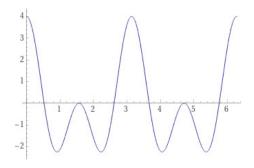


FIGURE 1. Graph of q when $k = \ell = 1$

Following two theorems give the results about the eigenfunctions.

Theorem 8. The eigenfunctions of the Whittaker-Hill equation satisfying the periodic boundary conditions are, as $n \to \infty$

$$\begin{split} \phi_1(x,n) &= \cos((n+1)x) + \frac{1}{2(n+1)} \left[k\sin(2x) + \frac{\ell}{2}\sin(4x) \right] \sin((n+1)x) \\ &+ \frac{1}{4(n+1)^2} \{ 2k\cos(2x) + 2\ell\cos(4x) - 2(k+\ell) - \frac{1}{2} [k\sin(2x) \\ &+ \frac{\ell}{2}\sin(4x)]^2 \} \cos((n+1)x) + o(n^{-2}), \end{split}$$

$$\phi_2(x,n) &= \frac{1}{n+1} \sin((n+1)x) - \frac{1}{2(n+1)^2} \left[k\sin(2x) + \frac{\ell}{2}\sin(4x) \right] \cos((n+1)x) \\ &+ \frac{1}{4(n+1)^3} \{ 2k\cos(2x) + 2\ell\cos(4x) + 2(k+\ell) - \frac{1}{2} [k\sin(2x) \\ &+ \frac{\ell}{2}\sin(4x)]^2 \} \sin((n+1)x) + o(n^{-3}). \end{split}$$

Theorem 9. The eigenfunctions of the Whittaker-Hill equation satisfying the semiperiodic boundary conditions are, as $n \to \infty$

$$\begin{split} \phi_1(x,n) &= \cos \frac{(2n+1)x}{2} + \frac{1}{2n+1} \left[k \sin(2x) + \frac{\ell}{2} \sin(4x) \right] \sin \frac{(2n+1)x}{2} \\ &+ \frac{1}{(2n+1)^2} \{ 2k \cos(2x) + 2\ell \cos(4x) - 2(k+\ell) - \frac{1}{2} [k \sin(2x) \\ &+ \frac{\ell}{2} \sin(4x)]^2 \} \cos \frac{(2n+1)x}{2} + o(n^{-2}), \end{split}$$

$$\phi_2(x,n) &= \frac{2}{2n+1} \sin \frac{(2n+1)x}{2} - \frac{2}{(2n+1)^2} \left[k \sin(2x) + \frac{\ell}{2} \sin(4x) \right] \cos \frac{(2n+1)x}{2} \\ &+ \frac{2}{(2n+1)^3} \{ 2k \cos(2x) + 2\ell \cos(4x) + 2(k+\ell) - \frac{1}{2} [k \sin(2x) + \frac{\ell}{2} \sin(4x)]^2 \} \sin \frac{(2n+1)x}{2} + o(n^{-3}). \end{split}$$

To prove Theorem 8 and Theorem 9, we take $q(x) = 2k\cos(2x) + 2\ell\cos(4x)$ and $a = 2\pi$ in Theorem 3 and Theorem 4, respectively.

Following two theorems give the results about Green's functions.

Theorem 10. Green's function of the Whittaker-Hill equation under periodic boundary conditions is, as $n \to \infty$

$$\begin{split} G(x,\zeta,n) &= \frac{1}{(n+1)}\cos((n+1)\zeta)\sin((n+1)x) - \frac{1}{2(n+1)^2} \{ [k\sin(2x) + \frac{\ell}{2}\sin(4x)] \\ &\times \cos((n+1)\zeta)\cos((n+1)x) - [k\sin(2\zeta) + \frac{\ell}{2}\sin(4\zeta)]\sin((n+1)\zeta) \\ &\times \sin((n+1)x) \} + \frac{1}{4(n+1)^3} \{ [2k[\cos(2\zeta) + \cos(2x)] + 2\ell[\cos(4\zeta) \\ &+ \cos(4x)] - \frac{1}{2}[(k\sin(2\zeta) + \frac{\ell}{2}\sin(4\zeta))^2 + (k\sin(2x) + \frac{\ell}{2}\sin(4x))^2]] \\ &\times \cos((n+1)\zeta)\sin((n+1)x) - [k\sin(2\zeta) + \frac{\ell}{2}\sin(4\zeta)][k\sin(2x) \\ &+ \frac{\ell}{2}\sin(4x)]\sin((n+1)\zeta)\cos((n+1)x) \} + o(n^{-3}) \end{split}$$

for $0 \leq \zeta \leq x \leq 2\pi$. Similar result holds for $0 \leq x \leq \zeta \leq 2\pi$ changing the role of ζ and x.

Theorem 11. Green's function of the Whittaker-Hill equation under semi-periodic boundary conditions is, as $n \to \infty$

$$G(x,\zeta,n) = \frac{2}{2n+1}\cos\frac{(2n+1)\zeta}{2}\sin\frac{(2n+1)x}{2} - \frac{2}{(2n+1)^2} \{ [k\sin(2x) - \frac{2}{(2n+1)^2} \} \}$$

$$\begin{aligned} &+ \frac{\ell}{2}\sin(4x) \cos\frac{(2n+1)\zeta}{2}\cos\frac{(2n+1)x}{2} - [k\sin(2\zeta) + \frac{\ell}{2}\sin(4\zeta)] \\ &\times \sin\frac{(2n+1)\zeta}{2}\sin\frac{(2n+1)x}{2} \} + \frac{2}{(2n+1)^3} \{ [2k(\cos(2\zeta) + \cos(2x)) \\ &+ 2\ell(\cos(4\zeta) + \cos(4x)) - \frac{1}{2} [(k\sin(2\zeta) + \frac{\ell}{2}\sin(4\zeta))^2 + (k\sin(2x) \\ &+ \frac{\ell}{2}\sin(4x))^2] \cos\frac{(2n+1)\zeta}{2}\sin\frac{(2n+1)\chi}{2} - [k\sin(2\zeta) + \frac{\ell}{2}\sin(4\zeta)] \\ &\times [k\sin(2x) + \frac{\ell}{2}\sin(4x)] \sin\frac{(2n+1)\zeta}{2}\cos\frac{(2n+1)\chi}{2} + o(n^{-3}) \end{aligned}$$

for $0 \leq \zeta \leq x \leq 2\pi$. Similar result holds for $0 \leq x \leq \zeta \leq 2\pi$ changing the role of ζ and x.

To prove Theorem 10 and Theorem 11, we first calculate (20) for $q(x) = 2k \cos(2x) + 2\ell \cos(4x)$ and $a = 2\pi$. We find

$$D(x) = 2kx\cos 2x + 2\ell x\cos 4x + 4\pi k + 4k \int_{\pi/2}^{\pi} t\sin 2t dt + 8\ell \int_{\pi/2}^{\pi} t\sin 4t dt + 4k \int_{\pi/2}^{x} t\sin 2t dt + 8\ell \int_{\pi/2}^{x} t\sin 4t dt$$
$$= k\sin 2x + \frac{\ell}{2}\sin 4x.$$

Then, we substitute the obtained result of D(x) in Theorem 6 and Theorem 7, respectively. The proof is done.

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