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APPROXIMATION OF THE SCHRÖDINGER DIFFERENTIAL EQUATION BY (0,2)-INTERPOLATIONAL SPLINE FUNCTIONS

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1. Introduction

In this paper we give the approximate solution of the Schrödinger differential equation

$$\psi''(x) = (x^2 - \lambda)\psi(x) \tag{1.1}$$

for the two atom molecule by $(0,2)$-interpolational spline functions, if the initial conditions

$$\psi_0 = \psi(0) \quad \text{and} \quad \psi_0' = \psi'(0)$$

are given.

The given method approximates not only the solution function $\psi(x)$ but also the derivatives $\psi'(x)$ and $\psi''(x)$. The order of the approximation coincides with that of the best possible polynomial approximation. We give error estimates and show the cases where the method is stable.

We let in (1.1) $\lambda = AB^{-1}$, where $A = 2\mu E/\hbar^2$, $B = \sqrt{\mu k}/\hbar$; where E denotes the energy, k is the Hook-constant, $\hbar$ is the Planck constant divided by 2π, and

$$\mu = \frac{M_a M_b}{M_a + M_b},$$

where M_a, M_b denote the mass of the atoms (see e.g. [1]).

2. The definition of the (0,2)-interpolational spline functions; first approximational method

In the interval $[0,b]$ let the system of nodal points

$$\Delta : \quad x_i = i\frac{b}{n}; \qquad i = \overline{0,n}, \qquad n = 2,3,\ldots \tag{2.1}$$

be given and let ψ_i, ψ_i'' denote the exact values of the solution of (1.1) and its second derivative at the nodal points.

We define the (0, 2)-interpolational spline-function $S_\Delta(x;\psi)$ corresponding to the function ψ as it follows:

$$
\begin{aligned}
(2.2)\qquad & S_\Delta(x;\psi) \equiv S_\Delta(x) \equiv S_i(x) = \\
& = \psi_i + a_i(x-x_i) + \frac{\psi_i''}{2}(x-x_i)^2 + b_i(x-x_i)^3
\end{aligned}
$$

($i=\overline{0,n-1}$, $n=2,3,\ldots$; $x\in[x_i,x_{i+1}]\subset[0,b]$). In the spline functions defined in (2.2) the coefficients a_i, b_i are chosen in order to satisfy the following equalities:

$$
(2.3)\qquad
\begin{aligned}
&a)\quad S_\Delta(x_i;\psi) = S_\Delta(x_i) = S_i(x_i) = \psi_i; \quad i=\overline{0,n-1};\\
&b)\quad S_{n-1}(x_n) = \psi_n;\\
&c)\quad S_i(x_{i+1}) = S_{i+1}(x_{i+1}) = \psi_{i+1}; \quad i=\overline{0,n-1};\\
&d)\quad S_i''(x_i) = \psi_i''; \quad i=\overline{0,n-1};\\
&e)\quad S_{n-1}''(x_n) = \psi_n''.
\end{aligned}
$$

The equations (2.3) a) and d) are obviously satisfied by (2.2). Further, the equations b), c) and e) are satisfied if

$$
(2.4)\qquad
\begin{aligned}
&\alpha)\quad a_i + b_i h^2 = \frac{1}{h}(\psi_{i+1}-\psi_i) - \frac{h}{2}\psi_i'' \quad i=\overline{0,n-1},\\
&\beta)\quad b_i = \frac{1}{6h}(\psi_{i+1}''-\psi_i''); \quad i=\overline{0,n-1},
\end{aligned}
$$

where $h = x_{i+1}-x_i$, $i=\overline{0,n-1}$.

From the equations (2.3) c), (2.4) α) it follows obviously that the spline functions $S_\Delta(x;\psi)$ are continuous in the interval $[0,b]$, that is $S_\Delta(x;\psi)\in C([0,b])$.

We call the spline functions $S_\Delta(x;\psi)$ interpolational functions of (0, 2)-type (see [2], [3]) by the equations (2.3) a), b) d) and e), that is, they interpolate the functions $\psi(x)$, $\psi''(x)$ at the nodal points, but they do not interpolate the function $\psi'(x)$. We remark that the function $S_\Delta(x;\psi)$ is identical with a polynomial of degree 3 by (2.2) on each subinterval $[x_i,x_{i+1}]$, $i=\overline{0,n-1}$ and by (2.4) its degree is minimal.

From the previous results we have the following

Theorem 1. *The* (0, 2)*-interpolational spline functions* $S_\Delta(x;\psi)\in C([0,b])$ *corresponding to the function* $\psi(x)$*, satisfying the equations* (2.3) *for the system of nodal points* (2.1)*, exist and are unique.*

We note that we do not need an equidistant subdivision, the theorem remains valid for any division, where $x_{i+1} - x_i = h_i$, $i = \overline{0, n-1}$, and the h_i's are different.

We prove the convergence theorem. For any interval $x_i \leq x \leq x_{i+1}$, $i = \overline{0, n-1}$ by (2.2) and (2.4) β) the substitution $x = x_i + th$, $0 \leq t \leq 1$ gives

$$\begin{aligned} &|\psi''(x) - S''_\Delta(x)| = |\psi''(x) - S''_i(x)| = \\ (2.5)\qquad &= |\psi''(x) - \psi''_i - 6b_i(x - x_i)| = \left|\psi''(x) - \frac{1}{h}(\psi''_{i+1} - \psi''_i)(x - x_i)\right| = \\ &= \left|\psi''(x) - \left[\psi''_{i+1}t + (1-t)\psi''_i\right]\right| = |\psi''(x) - \psi''(\xi_i)| \leq \omega(h; \psi''), \end{aligned}$$

where $x_i \leq \xi_i \leq x_{i+1}$ and $\omega(x; \psi'')$ denotes the modulus of continuity of the function $\psi''(x)$, that is

$$\omega(h; \psi'') = \omega(h) = \max_{|x' - x''| \leq h} |\psi''(x') - \psi''(x'')|; \quad x', x'' \in [0, b].$$

We consider the function $g(x) = \psi(x) - S_i(x)$, $x \in [x_i, x_{i+1}]$, then by (2.3) a), b) we have $g(x_{i+1}) = 0$, $g(x_i) = 0$ and the theorem of Rolle gives

$$g'(\eta_i) = \psi'(\eta_i) - S'_i(\eta_i) = 0, \quad x_i < \eta_i < x_{i+1}. \tag{2.6}$$

If we integrate (2.5), then for $x_{i+1} > \eta_i \geq x$ we have by (2.6)

$$\begin{aligned} &|\psi'(x) - S'_i(x)| = \left|\int_x^{\eta_i} \left[\psi''(t) - S''_i(t)\right] dt\right| \leq \\ (2.7)\qquad &\leq \int_x^{\eta_i} \left|\psi''(t) - S''_i(t)\right| dt \leq \omega(h)(\eta_i - x) \leq \omega(h)(x_{i+1} - x) \leq \omega(h)h. \end{aligned}$$

Further for $x_i < \eta_i \leq x$ by integrating (2.5), (2.6) implies

$$\begin{aligned} &|\psi'(x) - S'_i(x)| = \left|\int_{\eta_i}^{x} \left[\psi''(t) - S''_i(t)\right] dt\right| \leq \\ (2.8)\qquad &\leq \int_{\eta_i}^{x} \left|\psi''(t) - S''_i(t)\right| dt \leq \omega(h)(x - \eta_i) \leq \omega(h)(x - x_i) \leq \omega(h)h. \end{aligned}$$

As $\psi(x_i) - S_i(x_i) = 0$, by integrating (2.7), (2.8) we have

$$|\psi(x) - S_i(x)| \leq \omega(h)\frac{h^2}{2}. \tag{2.9}$$

By (2.5), (2.7), (2.8) and (2.9) we have

Theorem 2. *In the interval* $0 \leq x \leq b$ *we have the following inequalities for* $x \in [x_{i+1}, x_i]$, $i = \overline{0, n-1}$ *and for the nodal points* (2.1)*:*

$$\begin{aligned} |\psi^{(r)}(x) - S_\Delta^{(r)}(x)| &\equiv |\psi^{(r)}(x) - S_i^{(r)}(x)| \leq \omega(h)h^{2-r}; \quad r = 1, 2; \\ |\psi(x) - S_\Delta(x)| &\equiv |\psi(x) - S_i(x)| \leq \omega(h)\frac{h^2}{2}. \end{aligned} \tag{2.10}$$

The equations (2.10) imply that the $(0, 2)$-interpolational spline function defined by (2.2) and its first and second derivatives converge to the functions $\psi(x)$, $\psi'(x)$ and $\psi''(x)$. We note that the order of the approximation coincides with the order of the best polynomial approximation (see e.g. [4]).

Now we prove that with the help of the $(0, 2)$-interpolational spline function defined in (2.2) we can approximate the Schrödinger differential equation (1.1) with the initial conditions ψ_0, ψ_0'.

By (2.2) and (2.1) we obviously have the initial conditions

$$\begin{aligned} S_\Delta(0; \psi) &= S_0(0) = \psi_0, \\ S_\Delta'(0; \psi) &= S_0'(0) = a_0. \end{aligned} \tag{2.11}$$

Here we show that $a_0 \to \psi_0'$, whenever $h \to 0$, that is $n \to \infty$. Indeed, by (2.4) we obtain

$$a_0 = \frac{1}{h}(\psi_1 - \psi_0) - \frac{h}{2}\psi_0'' - \frac{h}{6}(\psi_1'' - \psi_0''),$$

but the finite Taylor-formula gives

$$\frac{\psi_1 - \psi_0}{h} = \psi_0' + \frac{\psi''(\xi_0)}{2}h, \quad 0 < \xi_0 < x_1;$$

and the triangle inequality shows that

$$|a_0 - \psi_0'| \leq \frac{h}{2}|\psi''(\xi_0) - \psi_0''| + \frac{h}{6}|\psi_1'' - \psi_0''| \leq \frac{2}{3}\omega(h)h, \tag{2.12}$$

where $\omega(h)$ denotes the modulus of continuity of the function $\psi''(x)$. Hence by (2.11) and (2.12) the $(0, 2)$-interpolational spline functions satisfy, resp., approximate the ψ_0, resp., ψ_0' initial conditions.

We prove the following

Theorem 3. *For the system of nodal points* (2.1) *in the subintervals* $x \in$ $\in [x_i, x_{i+1}]$, $i = \overline{0, n-1}$ *we have*

$$\begin{aligned} &|S''_{\Delta}(x;\psi) - (x^2-\lambda)S_{\Delta}(x;\psi)| = \\ &= |S''_i(x) - (x^2-\lambda)S_i(x)| \leq \omega(x;\psi'')(1+(x^2+|\lambda|)h^2). \end{aligned} \tag{2.13}$$

Proof. By (1.1) and (2.10) the triangle inequality implies for $x \in [x_i, x_{i+1}]$, $i = \overline{0, n-1}$

$$|S''_{\Delta}(x;\psi) - (x^2-\lambda)S_{\Delta}(x;\psi)| = |S''_i(x) - \psi''(x) + (x^2-\lambda)[\psi(x) - S_i(x)]| \leq$$

$$\leq |S''_i(x) - \psi''(x)| + |x^2-\lambda||\psi(x) - S_i(x)| \leq \omega(h;\psi'')\left(1 + |x^2-\lambda|\frac{h^2}{2}\right).$$

We note that the $(0,2)$-interpolational spline functions defined in (2.2) really approximate by (2.13) the solution of (1.1) with the initial conditions ψ_0, ψ'_0 in the interval $[0, b]$. By (2.1) we have $h = x_{i+1} - x_i = \frac{b}{n}$; $i = \overline{0, n-1}$, $n = 2, 3, \ldots$; further $\omega(h;\psi'') \to 0$ for $n \to 0$; and $|x^2 - \lambda| \leq b^2 + |\lambda|$, where $|\lambda|$ is a fixed value for any two atom molecule. Further, by (2.2) we have $S_{\Delta}(0;\psi) = S_0(0) = \psi_0$ and (2.12) implies that $a_0 \to \psi'_0$ for $n \to \infty$, that is, the functions $S_{\Delta}(x;\psi)$ satisfy the initial condition ψ_0 and approximate the initial condition ψ'_0.

3. Second approximational method

In §.2 as we constructed the $(0,2)$-interpolational spline functions we assumed that the values $\psi_i = \psi(x_i)$ are given at the nodal points of the system (2.1), and $\psi''_i = (x_i^2 - \lambda)\psi_i$. However, these values are practically unknown, only ψ_0 and ψ'_0 are given. In this paragraph we construct approximate values $\bar{\psi}_i \approx \psi_i$ by an iterational method at the nodal points, for which the respective sequence of $(0,2)$-interpolational spline functions satisfy similar approximation theorems as in §.2.

We assume at the iterational method that $\psi_0 \neq 0$ is given and $\psi'_0 = 0$. These assumptions are often satisfied in the applications.

If $\psi_0 \neq 0$ is given and $\psi'_0 = 0$ are the initial values then the exact value ψ_i at the point x_i of the system (2.1) can be given – by the differential equation (1.1) – as follows:

$$\psi_i = \psi_0 + \int_0^{x_i}\int_0^{t_1} \psi''(t_2)dt_2dt_1 = \psi_0 + \int_0^{x_i}\int_0^{t_1} (t_2^2 - \lambda)\psi(t_2)dt_2dt_1 =$$

$$= \psi_0\left[1+\int_0^{x_i}\int_0^{t_1}(t_2^2-\lambda)dt_2dt_1\right]+\int_0^{x_i}\int_0^{t_1}\left[(t_2^2-\lambda)\int_0^{t_2}\int_0^{t_3}\psi''(t_4)dt_4dt_3\right]dt_2dt_1 =$$

$$= \psi_0\left[1+\int_0^{x_i}\int_0^{t_1}(t_2^2-\lambda)dt_2dt_1\right]+$$

$$+\int_0^{x_i}\int_0^{t_1}\left[(t_2^2-\lambda)\int_0^{t_2}\int_0^{t_3}(t_4^2-\lambda)dt_4dt_3\right]dt_2dt_1+\ldots+$$

$$(3.1)\qquad +\int_0^{x_i}\int_0^{t_1}\left[(t_2^2-\lambda)\int_0^{t_2}\int_0^{t_3}(t_4^2-\lambda)\left[\times\ldots\right.\right.$$

$$\left.\left.\ldots\times(t_{2n-2}^2-\lambda)\int_0^{t_{2n-2}}\int_0^{t_{2n-1}}(t_{2n}^2-\lambda)dt_{2n}dt_{2n-1}\right]\ldots\right]dt_2dt_1+$$

$$+\int_{x_i}^{0}\int_0^{t_1}\left[(t_2^2-\lambda)\int_0^{t_2}\int_0^{t_3}(t_4^2-\lambda)\left[\times\ldots\times\right.\right.$$

$$\left.\left.\times(t_{2n}^2-\lambda)\int_0^{t_{2n}}\int_0^{t_{2n+1}}\psi''(t_{2n+2})dt_{2n+2}dt_{2n+1}\right]\ldots\right]dt_2dt_1=$$

$$= \psi_0[r_n(x)]+I_n,$$

that is, we choose the value on the right hand side of (3.1) in the square bracket – depending only on ψ_0 and λ – for $\bar{\psi}_i$, $i=\overline{1,n}$. In (3.1) $\times$ denotes a double integral.

Now we prove the following

Lemma 1. *The following inequality holds:*

$$(3.2)\qquad |\psi_i-\bar{\psi}_i|\le M_0\frac{q^{2n+2}}{\sqrt{n+1}},\quad n\ge n_0(q);\quad i=\overline{1,n},$$

where $0<q<1$.

Proof. Let $M = \max_{0\le x\le b} |\psi''(x)|$. Obviously we have $|t_{2j}^2 - \lambda| \le x_i^2 + |\lambda|$, $j = \overline{1,n}$, hence by the choice of $\bar{\psi}_i$ and by the expression on the right hand side of (3.1) outside of the square bracket, we have for $x_i \le b$

$$|\psi_i - \bar{\psi}_i| = |I_n| \le M(x_i^2 + |\lambda|)^n \frac{x_i^{2n+2}}{(2n+2)!} \le M(b^2 + |\lambda|)^n \frac{b^{2n+2}}{(2n+2)!}.$$

Using the well-known Stirling formula

$$(2n+2)! = 2\sqrt{\pi(n+1)}(2n+2)^{2n+2}e^{-(2n+2)}(1+\omega_{2n+2}),$$

where $0 < \omega_{2n+2} \le e^{\frac{1}{2(n+1)}} - 1$, we obtain

$$|\psi_i - \bar{\psi}_i| \le M\frac{1}{2\sqrt{\pi(n+1)}}\left(\frac{b^2 + |\lambda|^{\frac{n}{2n+2}}eb}{2n+2}\right)^{2n+2} \le$$

$$\le M\frac{q^{2n+2}}{2\sqrt{\pi(n+1)}} = M_0\frac{q^{2n+2}}{\sqrt{n+1}},$$

where $0 < q < 1$ is an arbitrary fixed number for $n \ge n_0(q)$, and $n_0(q)$ is also fixed.

The definition of the $(0,2)$-interpolational spline functions corresponding to the function ψ is analoguous to that of (2.2), that is

$$\text{(3.3)} \quad \bar{S}_\Delta(x;\psi) \equiv \bar{S}_\Delta(x) \equiv \bar{S}_i(x) = \bar{\psi}_i + \bar{a}_i(x-x_i) + \frac{\bar{\psi}''}{2}(x-x_i)^2 + \bar{b}_i(x-x_i)^3$$

for $x \in [x_i, x_{i+1}] \subset [0,b]$, $i = \overline{0,n-1}$, $n = 2,3,\ldots$, where $\bar{\psi}_i'' = (x_i^2 - \lambda)\bar{\psi}_i$ and the system of nodal points (2.1) is given. By (3.3) we have similar equalities as in (2.3) a)-e) with $\bar{S}_i$, $\bar{\psi}_i$ and $\bar{\psi}_i''$ for S_i, ψ_i and ψ_i'' and as in (2.4) we write

$$\text{(3.4)} \quad \begin{aligned} &\alpha) \quad \bar{a}_i + \bar{b}_i h^2 = \frac{1}{h}(\bar{\psi}_{i+1} - \bar{\psi}_i) - \frac{h}{2}\bar{\psi}_i'' \quad i = \overline{0,n-1}, \\ &\beta) \quad \bar{b}_i = \frac{1}{6h}(\bar{\psi}_{i+1}'' - \bar{\psi}_i''); \quad i = \overline{0,n-1}, \end{aligned}$$

where again we have $h = x_{i+1} - x_i$. The function $\bar{S}_\Delta(x;\psi)$ is continuous by (3.3) and (3.4) in the interval $[0,b]$, that is, $\bar{S}_\Delta(x;\psi) \in C([0,b])$.

For the convergence theorems we need two lemmas.

Lemma 2. *For the coefficients a_i, b_i and $\bar{a}_i$, $\bar{b}_i$ in (2.2), resp. (3.3) we have the following inequalities:*

$$\text{(3.5)}\qquad \begin{aligned} &(i) \qquad |a_i - \bar{a}_i| \le M_2 \frac{q^{2n+2}}{h\sqrt{n+1}};\\ &(ii) \qquad |b_i - \bar{b}_i| \le M_1 \frac{q^{2n+2}}{6h\sqrt{n+1}} \end{aligned}$$

for $i = \overline{0, n-1}$, $n \ge n_0(q)$.

Proof. First we prove inequality (3.5) (ii). The inequalities (2.4) β), (3.4) β) imply by $\psi_k'' = (x_k^2 - \lambda)\psi_k$ and $\bar{\psi}_k'' = (x_k^2 - \lambda)\bar{\psi}_k$, $k = i+1, i$ and by (3.2)

$$\text{(3.5a)}\qquad \begin{aligned} |b_i - \bar{b}_i| &\le \frac{1}{6h}\left(|\psi_{i+1}'' - \bar{\psi}_{i+1}''| + |\bar{\psi}_i'' - \psi_i''|\right) \le \\ &\le 2M_0 \frac{1}{6h}\frac{(b^2 + |\lambda|)}{\sqrt{n+1}} q^{2n+2} = M_1 \frac{q^{2n+2}}{6h\sqrt{n+1}}. \end{aligned}$$

By (2.4) a), b), (3.4) α), β) and (3.2) the triangle inequality implies

$$\text{(3.5b)}\qquad |a_i - \bar{a}_i| \le M_0 \frac{1}{h\sqrt{n+1}}\left[1 + \frac{3(b^2+\lambda)}{2}\right] q^{2n+2} = M_2 \frac{q^{2n+2}}{h\sqrt{n+1}}.$$

By (3.5*b*) and (3.5*a*) we have (3.5) (i) and (ii).

Lemma 3. *The coefficient $\bar{a}_0$ in* (3.3) *approximate the value $\psi_0' = \psi'(0)$, as we have the inequality*

$$\text{(3.6)}\qquad |\psi_0' - \bar{a}_0| \le \frac{2}{3}\omega(h)h + M_2 \frac{q^{2n+2}}{h\sqrt{n+1}}, \quad n \ge n_0(q).$$

Proof. From the triangle inequality we have by (2.12) and (3.5) (i)

$$|\psi_0' - \bar{a}_0| \le |\psi_0' - a_0| + |a_0 - \bar{a}_0| \le \frac{2}{3}\omega(h)h + M_2 \frac{q^{2n+2}}{h\sqrt{n+1}}.$$

Now we turn to the proof of the convergence theorem. For all $x \in [x_i, x_{i+1}]$ $i = \overline{0, n-1}$ we have by (3.3), (2.2), (2.10) and (3.5) (ii)

$$|\psi''(x) - \bar{S}_i''(x)| + |S_i''(x) - \bar{S}_i''| \le \omega(h) + |\psi_i'' - \bar{\psi}_i''| + 6|b_i - \bar{b}_i|(x - x_i).$$

This inequality implies by $\psi_i'' = (x_i^2 - \lambda)\psi_i$, $\bar{\psi}_i'' = (x_i^2 - \lambda)\bar{\psi}_i$, $(x_i^2 - \lambda) \le b^2 + |\lambda|$ and (3.2), (3.5) (ii)

$$(3.7a)\qquad \begin{aligned} |\psi''(x) - \bar{S}_i''(x)| &\le \omega(h) + \left[\frac{(b^2+\lambda)M}{2\sqrt{\pi}} + M_1\right] q^{2n+2} = \\ &= \omega(h) + M_3 \frac{q^{2n+2}}{h\sqrt{n+1}}. \end{aligned}$$

Similarly we can prove the inequalities

$$(3.7b)\qquad |\psi'(x) - \bar{S}_i'(x)| \le \omega(h)h + M_4 \frac{q^{2n+2}}{h\sqrt{n+1}},$$

and

$$(3.7c)\qquad |\psi(x) - \bar{S}_i(x)| \le \omega(h)\frac{h^2}{2} + M_5 \frac{q^{2n+2}}{h\sqrt{n+1}},$$

by the relations (3.3), (2.2), (2.10), (3.2), (3.5) (i), (ii), where we always have $x \in [x_i, x_{i+1}] \subset [0, b]$, $i = \overline{0, n-1}$.

By (3.7a), (3.7b) and (3.7c) we have the following

Theorem 4. *For every $x \in [x_i, x_{i+1}]$, $i = \overline{0, n-1}$ we have the relations*

$$(3.7)\qquad |\psi^{(r)}(x) - \bar{S}_\Delta^{(r)}(x)| \equiv |\psi^{(r)}(x) - \bar{S}_i^{(r)}(x)| \le \omega(h)h^{2-r} + M_k \frac{q^{2n+2}}{h\sqrt{n+1}}$$

for $r = 2$, $k = 3$, and for $r = 1$, $k = 4$; further

$$(3.8)\qquad |\psi(x) - \bar{S}_\Delta(x)| \equiv |\psi(x) - \bar{S}_i(x)| \le \omega(h)\frac{h^2}{2} + M_5 \frac{q^{2n+2}}{h\sqrt{n+1}}.$$

We see that the (0, 2)-interpolational spline functions $\bar{S}_\Delta(x;\psi)$ as defined in (3.3) for the system of nodal points (2.1) approximate the functions ψ, ψ', ψ'' as the functions $S_\Delta(x;\psi)$. We note, that by (3.2a), (3.5a), (3.5b) and (3.7a) the constants M_k, $k = 0, 1, 2, 3$ and the constants M_4, M_5 in (3.7b), (3.7c) are finite and independent of n and x.

We show that the sequence $\bar{S}_\Delta(x;\psi)$ approximates the solution ψ of the differential equation (1.1) and its derivatives ψ', ψ''. It satisfies the initial condition $\bar{S}_\Delta(0;\psi) = \bar{\psi}_0 = \psi_0$. As (3.6) implies $\bar{a}_0 \to \psi_0'$ for $n \to \infty$ and $\bar{S}_\Delta'(0,\psi) = \bar{S}_0'(0) = a_0$, then it approximates also the initial condition ψ_0'. We have the following

Theorem 5. *On the subinterval $x \in [x_i, x_{i+1}] \subset [0,b]$ we have the inequality*

$$|\bar{S}''_\Delta(x;\psi) - (x^2-\lambda)\bar{S}_\Delta(x;\psi)| = |\bar{S}''_i(x;\psi) - (x^2-\lambda)\bar{S}_i(x;\psi)| \leq$$
$$\leq M_6\omega(h) + M_7\frac{q^{2n+2}}{h\sqrt{n+1}}, \qquad n \geq n_0(q), \tag{3.9}$$

where the constants M_6 and M_7 are independent of n and x.

Proof. By the triangle inequality and (1.1), (3.7), (3.8) we have

$$|\bar{S}''_i(x) - (x^2-\lambda)\bar{S}_i(x)| \leq |\bar{S}''_i(x) - \psi''(x)| + |x^2-\lambda||\psi(x) - \bar{S}_i(x)| \leq$$
$$\leq \omega(h)\left[1 + (b^2+|\lambda|)\frac{h^2}{2}\right] + \left[M_3 + (b^2+|\lambda|)M_5\right]\frac{q^{2n+2}}{h\sqrt{n+1}} \leq$$
$$\leq M_6\omega(h) + M_7\frac{q^{2n+2}}{h\sqrt{n+1}}.$$

We note that the approximational method given in §.3. is stable in the sense that if we construct functions $S^*_\Delta(x;\psi)$, similarly as in (3.3) using the values ψ^*_i, $\psi^{*\prime\prime}_i = (x_i^2-\lambda)\psi^*_i$ instead of $\bar{\psi}_i$, $\bar{\psi}''_i = (x_i^2-\lambda)\bar{\psi}_i$ then we can prove similar theorems as in §.3., if the inequality $|\bar{\psi}_i - \psi^*_i| \leq M^*\frac{q^{2n+2}}{h\sqrt{n+1}}$; $i = \overline{0, n-1}$ holds. This statement is easy to prove.

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