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JIF	= **1.500**	**SJIF** (Morocco)	= **5.667**	**OAJI** (USA)	= **0.350**

SOI: 1.1/TAS DOI: 10.15863/TAS

International Scientific Journal

Theoretical & Applied Science

p-ISSN: 2308-4944 (print) **e-ISSN:** 2409-0085 (online)

Year: 2020 **Issue:** 07 **Volume:** 87

Published: 30.07.2020 **http://T-Science.org**

QR – Issue **QR – Article**

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ONE-DIMENSIONAL SCHRODINGER OPERATOR

***Abstract**: In the article reviewed one-dimensional schrodinger operator and its self- adjointness. The use of one-dimensional schrodinger operator is one of many alternative methods to quantum mechanics, differential geometry. The mathematical theory of Schrodinger operators is used in quantum mechanics, differential geometry. It is very important for the foundations of quantum mechanics, since only self-adjoint operators describe quantum mechanical observables.*

***Key words**: schrodinger operator, one-dimensional, symmetric operator, valued function, linear function, discreteness of spectrum.*

***Language**: English*

***Citation**: Azizova, M. A. (2020). One-dimensional Schrodinger operator. *ISJ Theoretical & Applied Science, 07 (87),* 406-409.

Soi**: http://s-o-i.org/1.1/TAS-07-87-77 ***Doi: crossref https://dx.doi.org/10.15863/TAS.2020.07.87.77

***Scopus ASCC**: 2604.*

Introduction

The mathematical theory of Schrodinger operators is used in quantum mechanics, differential geometry. Allows for numerous generalizations. It is very important for the foundations of quantum mechanics, since only self-adjoint operators describe quantum mechanical observables. In quantum mechanics, the Schrödinger operator is the energy operator of a system of n charged particles in a coordinate representation. The concept of a wave function is a fundamental postulate of quantum mechanics; the wave function defines the state of the system at each spatial position, and time. Using these postulates, Schrödinger's equation can be derived from the fact that the time-evolution operator must be unitary, and must therefore be generated by the exponential of a self-adjoint operator, which is the quantum Hamiltonian. This derivation is explained below.

1. Self- adjointness

Consider an operator H_0 defined on $D(H_0) = C_0^{\infty}$ (R) by the formula

(1) $H_0 u = -u'' + V(x)u,$

where $V(x) \in L^{\infty}_{loc}(\mathrm{R})$ is a real valued function. Clearly, H_0 is a symmetric operator in $L^2(\mathrm{R})$. Recall that H_0 is said to be essentially self-adjoint if its closure H_0^{**} is a self-adjoint operator. In this case H_0 has one and only one self-adjoint extension.

1. *Assume that*

(2) $V(x) \geq -Q(x),$

where $Q(x)$ is a nonnegative continuous even function which is nondecreasing for $x \geq 0$ and satisfies

(3) $\int_{-\infty}^{\infty} \frac{dx}{\sqrt{Q(2x)}} = \infty$

Then H_0 is essentially self-adjoint.

Proof. As we have already seen in previous lectures, to prove self-adjointness of H_0^{**} it is enough to show that H_0^{**} is a symmetric operator. Hence, first we have to study the domain $D(H_0^{*})$

(i) *If* $f \epsilon D(H)_0^*$, then $f'(x)$ is absolutely continuous and $f'' \epsilon L^2_{loc}$(R).

Indeed, let $g = (H)_0^* f$. For every $\varphi \epsilon C_0^\infty$ (R) we have

$$\int_{-\infty}^{\infty} \overleftrightarrow{f(x)}\, \varphi''(x) = \int_{-\infty}^{\infty} (V(x)\, \overleftrightarrow{f(x)} - \overleftrightarrow{g(x)})\varphi(x)dx$$

Denote by $F(x)$ the second primitive function of $V(x).\, f(x)\text{-}g(x)$

Then the previous identity and integration by parts imply

$$\int_{-\infty}^{\infty} \overleftrightarrow{f}\, .\varphi'' dx = \int_{-\infty}^{\infty} \overleftrightarrow{F}.\ \varphi'' dx$$

Hence, $(F - f)'' = 0$ in the sense of distributions, i. e. $F\text{-}f$ is a linear function of x. This implies immediately the required claim.

Now we have to examine the behavior of $f \epsilon D(H_0^*)$ as $x \to \infty$.

(ii) If $f \epsilon D(H_0^*)$, *then*

(4) $\int_{-\infty}^{\infty} \frac{|f'(x)|^2}{Q(2x)} dx < \infty$

To prove the last claim, consider the integral

$$J = \int_{-\omega}^{\omega} (1 - \frac{|x|}{\omega}) \left(f''(x)\overleftrightarrow{f(x)} + f(x)\overleftrightarrow{f''(x)}\right)$$

$$= \int_{-\omega}^{\omega} (1 - \frac{|x|}{\omega}) \left(f' \cdot \overleftrightarrow{f} + f \cdot \overleftrightarrow{f'}\right)' dx - 2\int_{-\omega}^{\omega} (1 - \frac{|x|}{\omega})|f'|^2 dx.$$

Thus, we get the following identity

$$\int_{-\omega}^{\omega} (1 - \frac{|x|}{\omega})|f'(x)|^2 dx = -\frac{1}{2}\int_{-\omega}^{\omega} \left(f'' \cdot \overleftrightarrow{f} + f \cdot \overleftrightarrow{f''}\right).\left(1 - \frac{|x|}{\omega}\right) dx + \frac{1}{2\omega}[|f(\omega)|^2 + |f(-\omega)|^2 - 2|f(0)|].$$

Multiplying the last identity by ω, integrating over $\omega \ \epsilon\ [0,\ t]$, and taking into account the identity

$$\int_0^T (\int_{-\omega}^{\omega} (\omega - |x|)h(x)dx)d\omega = \frac{1}{2}\int_{-T}^{T} (T - |x|)^2\, h(x)dx$$

we get

$$\int_{-T}^{T} (T - |x|)^2 |f|^2\, dx = \frac{1}{2}\int_{-T}^{T} (T - |x|)^2 \left(f'' \cdot \overleftrightarrow{f} + f \cdot \overleftrightarrow{f''}\right) dx + \int_0^T |f(\omega)|^2 + |f(-\omega)|^2) d\omega - 2|f(0)|^2 T,$$

or, dividing by T^2,

$$\int_{-T}^{T} (1 - \frac{|x|}{T})^2 |f'|^2 dx = -\frac{1}{2}\int_{-T}^{T} (1 - \frac{|x|}{T})^2 \left(f'' \cdot \overleftrightarrow{f} + f \cdot \overleftrightarrow{f''}\right) dx + \frac{1}{T^2}(\int_{-T}^{T} |f(x)|^2\, dx - 2|f(0)|^2 \cdot T).$$

Letting $g = -f'' + V(x)\, f$, we obtain

$$\int_{-T}^{T} (1 - \frac{|x|}{T})^2 \left|f'\right|^2 dx =$$

$$= \frac{1}{2}\int_{-T}^{T} (1 - \frac{|x|}{T})^2 (g \cdot \overleftrightarrow{f} + \overleftrightarrow{g} \cdot f)\, dx - \int_{-T}^{T} (1 - \frac{|x|}{T})^2 V(x)|f(x)|^2 dx + \frac{1}{T^2}(\int_{-T}^{T} |f(x)|^2\, dx - 2|f(0)|^2 T)$$

Now remark that $f, g\ \epsilon\ L^2$(R) and $0 \le 1 - |x|/T \le 1$ for $x\, \epsilon\, (T, -T)$.

Hence, estimating $-V(x)$ by $Q(x)$, we get

$$\int_{-T}^{T} (1 - \frac{|x|}{T})^2 |f'|^2 dx \le \int_{-T}^{T} (1 - \frac{|x|}{T})^2 Q(x)|f|^2 dx + c,$$

where c is independent of T. The last inequality implies clearly

(5) $\frac{1}{4}\left(\int_{-T}^{T}|f'(x)|\right)^2 dx \le \int_{-T}^{T} Q(x)|f|^2\,dx + c$

Let

$$\omega(T) = \frac{1}{4}\int_{-T/2}^{T/2}|f'|^2\,dx$$

$$\chi(T) = \int_{-T}^{T} Q(x)|f|^2\,dx + c$$

Consider the integral

$$\int_0^T \frac{\omega'(x) - \chi'(x)}{Q(x)}\,dx$$

and apply the following on mean value: *if $f(x)$ is a continuous function and $K(x) \ge 0$ is a nondecreasing continuous function, then there exists $\xi \in [a, b]$ such that*

$$\int_a^b f(x)K(x)\,dx = K(a)\int_a^{\xi} f(x)dx$$

Then, due to (5) we obtain

$$\int_0^T \frac{\omega'\chi'}{Q}dx = \frac{1}{Q(0)}\int_0^{\xi}(\omega' - \chi')dx = \frac{1}{Q(0)}[\omega(\xi) - \chi(\xi) - \omega(0) - \chi(0)] \le \frac{1}{Q(0)}[\chi(0) - \omega(0)] = C.$$

Since

$$\omega'(x) = \frac{1}{2}\left[|f'\left(\frac{x}{2}\right)|^2 + \left|f'\left(-\frac{x}{2}\right)|^2\right],\right.$$

$$\chi'(x) = Q(x)[|f(x)|^2 + |f(-x)|^2],$$

we get immediately

$$\frac{1}{8}\int_0^T \frac{|f'\left(\frac{x}{2}\right)|^2 + |f'\left(-\frac{x}{2}\right)|^2}{Q(x)}dx \le \int_0^T (|f(x)|^2 + |f(-x)|^2)dx + C.$$

Since $f \in L^2(\mathrm{R})$, the last inequality implies the required claim.

End of proof of 1. Let $f_1, f_2 \in D(H_0^*)$ and

$$g_i = -f_i'' + V(x)f_i, \quad i = 1,2.$$

We have to show that

$$\int_{-\infty}^{\infty} f_i\overleftrightarrow{g_2}dx = \int_{-\infty}^{\infty} g_i\overleftrightarrow{f_2}dx$$

First we observe that

(6) $\int_{-t}^{t}(f_i\overleftrightarrow{g_2} - g_i\overleftrightarrow{f_2})dx = \int_{-t}^{t}(f_1\overleftrightarrow{f_2''} - f_1''\overleftrightarrow{f_2})dx = |f_1\overleftrightarrow{f_2'} - f_1'\overleftrightarrow{f_2}||_{-t}^{t}$

Let

$$p(t)\frac{1}{\sqrt{Q(2t)}}, \quad P(x) = \int_0^x p(t)dt$$

Multiplying (6) by $\rho(t)$ and integrating over $[0, T]$, we obtain

(7) $\int_0^T p(t)[\int_{-t}^{t}(f_1\overleftrightarrow{g_2} - g_1\overleftrightarrow{f_2})dx]dt =$

$$= \int_0^T p(t)[f_1 - \overleftrightarrow{f_2'} - f_1'\overleftrightarrow{f_2}]|_{-t}^{t}dt$$

For the left-hand part we have (changing the order of integration)

$$\int_0^T p(t)\left[\int_{-t}^{t}(f_1\overleftrightarrow{g_2} - g_1\overleftrightarrow{f_2})dx\right]dt = \int_{-T}^{T}\left[(f_1\overleftrightarrow{g_2} - g_1\overleftrightarrow{f_2})\int_{|x|}^{T}p(t)\,dt\right]dx = \int_{-T}^{T}(f_1\overleftrightarrow{g_2} - g_1\overleftrightarrow{f_2})(P(T) - P(|x|))dx$$

Now we estimate the right-hand part of (7) (more precisely, its typical term):

$$\left|\int_0^T f_1(t)\overleftrightarrow{f_2'(t)}p(t)dt\right| \le \left[\int_0^T |f_1(t)|^2\,dt\int_0^T |f_2'(t)|^2p^2(t)dt\right]^{\frac{1}{2}} \le C,$$

where, due to claim 2), the constant C is independent of T. Therefore,

$$\left|\int_{-T}^{T}(P(T) - P(|x|))[f_1.\overleftrightarrow{g_2} - g_1.\overleftrightarrow{f_2}]dx\right| \le C.$$

Dividing by $P(T)$ and letting $T \to +\infty$ (hence, $P(T) \to +\infty$), we get

(8) $\lim_{t\to+\infty}\left|\int_{-T}^{T}\left(1 - \frac{P(|x|)}{P(T)}\right)[f_1.\overleftrightarrow{g_2} - g_1.\overleftrightarrow{f_2}]dx\right| = 0$

Now we have to prove that

(9) $\lim_{T\to+\infty}\left|\int_{-T}^{T}[f_1\overleftrightarrow{g_2} - g_1\overleftrightarrow{f_2}]dx\right| = 0$

To end this we fix $\epsilon > 0$. Since $f_i, g_i \in L^2(\mathrm{R})$,

$$\int_{|x|\geq\omega}(|f_1||g_2|+|g_1||f_2|)dx \leq \epsilon$$

for all ω large enough. Then, for each $T \geq \omega$ we have

$$|\int_{-\omega}^{\omega}\left(1-\frac{P(|x|)}{P(T)}\right)[f_1\overleftrightarrow{g_2}-g_1\overleftrightarrow{f_2}]dx|$$

$$\leq |\int_{-T}^{T}\left(1-\frac{P(|x|)}{P(T)}\right)[f_1\overleftrightarrow{g_2} - g_1\overleftrightarrow{f_2}]dx| + \epsilon.$$

Letting $T \longrightarrow +\infty$ and using (8), we obtain

$$|\int_{-\omega}^{\omega}(f_1\overleftrightarrow{g_2} - g_1\overleftrightarrow{f_2})dx)| \leq \epsilon,$$

which implies (9).

2. Discreteness of spectrum

Consider the operator H_0 defined by (1). Assume that $V(x) \in L^{\infty}_{loc}(\mathrm{R})$ is a real valued function and

(10) $\lim_{x\to\infty} V(x) = +\infty$

Clearly, 1 implies that H_0 is essentially self-adjoint (take as $Q(x)$ and appropriate constant). Denote by H the closure of H_0.

Assume (10). Then the spectrum $\sigma(H)$ of H is discrete, i.e. there exists an orthonormal system $y_k(x), k = 0, 1, \ldots,$ of eigenfunctions, with eigenvalues $\lambda_k \longrightarrow +\infty$ as $k \longrightarrow \infty$.

In fact, for discreteness of $\sigma(H)$ the following condition is necessary and sufficient:

$$\int_{r}^{r+1} V(x)dx \to +\infty \ as \ r \to \infty.$$

Now we supplement 3 by some additional information about eigenvalues and corresponding eigenfunctions.

Under the assumption of 3, all the eigenvalues are simple. If $\lambda_0 < \lambda_1 < \lambda_2 < \ldots$ are the eigenvalues, then any (nontrivial) eigenfunction corresponding to λ_k has exactly k nodes, i.e. takes the value 0 exactly k times. All the eigenfunctions decay exponentially fast at infinity.

For the proof we refer to [1].

Except of exponential decay, all the statements of 6 have purely 1-dimensional character. In particular, multidimensional Schr¨odinger operators may have multiple eigenvalues.

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