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On the large order asymptotics of general states in semiclassical quantum mechanics

by

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ABSTRACT. — We consider the limit $\hbar \to 0$ of the solution $\Phi(t, x, \hbar)$ of Schrödinger equation:

$$i\hbar \frac{\partial \Phi(t, x, \hbar)}{\partial t} = -\frac{\hbar^2}{2m} \frac{d^2 \Phi(t, x, \hbar)}{dx^2} + V(x) \Phi(t, x, \hbar).$$

We prove that, for any integer $l \geqq 2$ and any initial condition $\Phi(0, x, \hbar)$ that belongs to Schwartz-class, a solution $\Phi^*(t, x, \hbar)$ of the semiclassical equation approximates $\Phi(t, x, \hbar)$ such as

$$\| \Phi^*(t, \cdot, \hbar) - \Phi(t, \cdot, \hbar) \|_{L^2} \leqq C \hbar^{l/2} \qquad (\hbar \to 0)$$

RÉSUMÉ. — On considère la limite $\hbar \to 0$ de la solution $\Phi(t, x, \hbar)$ de l'équation de Schrödinger:

$$i\hbar \frac{\partial \Phi(t, x, \hbar)}{\partial t} = -\frac{\hbar^2}{2m} \frac{d^2 \Phi(t, x, \hbar)}{dx^2} + V(x) \Phi(t, x, \hbar).$$

Nous prouvons que, pour tout nombre entier $l \geqq 2$ et toute condition initiale $\Phi(0, x, \hbar)$ qui appartient à Schwartz-classe, une solution $\Phi^*(t, x, \hbar)$ de l'équation semi-classique approche $\Phi(t, x, \hbar)$ tel que

$$\| \Phi^*(t, \cdot, \hbar) - \Phi(t, \cdot, \hbar) \|_{L^2} \leqq C \hbar^{l/2} \qquad (\hbar \to 0).$$

1. INTRODUCTION

It was shown in [2] that the approximate solutions to the Schrödinger equation agree with the exact solution modulo errors on the order of $\hbar^{l/2}$. However, the initial states of the equation were merely dealt with certain Gaussian states or their finite linear combinations. In this paper we shall prove that G. A. Hagedorn's results also hold for more general states which belong to Schwartz class if we somewhat modify several conditions. For simplicity, we will restrict attention to one space dimension. Our proofs rely heavily on the results of G. A. Hagedorn concerning the semiclassical behavior of certain Gaussian initial states.

We now introduce enough notations and definitions to allow us to state our main result.

ASSUMPTION 1.1. — *We assume that* $V(x) \in C^{l+2}(\mathbb{R})$, *namely* V *is* $l+2$-*th continuous differentiable function, and there exist positive constants* M, C_1 *and* C_2 *such that* $-C_2 \leqq V(x) \leqq C_1 e^{Mx^2}$ *for all* $x \in \mathbb{R}$.

ASSUMPTION 1.2. — *We assume that* $V(x) \in C^{l+2}(\mathbb{R})$ *and there exist positive constants* M, C_1 *and* C_2 *such that* $-C_2 \leqq V(x) \leqq C_1 (1+|x|)^M$ *for all* $x \in \mathbb{R}$.

Also, we assume that the quantum Hamiltonian

$$H(\hbar) = -(\hbar^2/2m)(d^2/dx^2) + V(x) = H_0(\hbar) + V$$

is essentially self-adjoint on the infinitely differentiable functions of compact support in $L^2(\mathbb{R})$. Under this Hamiltonian we shall study the evolution of states which are finite or infinite linear combinations of the Gaussian states $\varphi_j(A, B, \hbar, a, \eta, x)$, which are defined below.

DEFINITION 1. — *Let* A *and* B *be non-zero complex numbers which satisfy*

$$\operatorname{Re} BA^{-1} = |A|^{-2} (\equiv (A\bar{A})^{-1}). \tag{1.1}$$

Let $a, \eta \in \mathbb{R}$, *and* $0 < \hbar \leqq 1$. *Then for* $j = 0, 1, 2, \ldots$, *we define*

$$\varphi_j(A, B, \hbar, a, \eta, x) = (2^j j!)^{-1/2} (\pi\hbar)^{-1/4} (\bar{A})^{j/2} A^{-(j+1)/2}$$
$$\times H_j(\hbar^{-1/2} |A|^{-1} (x-a)) \exp\{-BA^{-1}(x-a)^2/2\hbar + i\eta(x-a)/\hbar\}. \tag{1.2}$$

Here H_j *denotes the* j-th *order Hermite polynomial that is defined by*

$$H_0(x) = 1 \quad \text{and} \quad H_1(x) = 2x. \tag{1.3-1}$$

$$H_{j+1}(x) = 2x H_j(x) - 2j H_{j-1}(x). \tag{1.3-2}$$

And the branch of the square root will be specified in the context in which the functions φ_j *are used. We note that, for any fixed values of* A, B, $\hbar$, a *and* η, $\{\varphi_j(A, B, \hbar, a, \eta, x)\}_{j=0}^{\infty}$ *is a complete orthonormal basis in* $L^2(\mathbb{R})$.

The following theorem was proved by G. A. Hagedorn [2] in 1981.

THEOREM 1. — *Suppose* $V(x)$ *satisfies Assumption* 1.1 *for some integer* $l \geqq 2$. *Let* $a_0, \eta_0 \in \mathbb{R}$, *and let* $A_0, B_0 \in \mathbb{C}$ *which satisfy* (1.1). *Then, for any* $T > 0$, *any* $J \in \mathbb{N}$ *and any* $c_0, c_1, \ldots, c_J \in \mathbb{C}$, *there exists* C_3 *such that*

$$\Bigg\| e^{-itH(\hbar)/\hbar} \sum_{j=0}^{J} c_j \varphi_j(A_0, B_0, \hbar, a_0, \eta_0, \cdot) - e^{iS(t)/\hbar} \sum_{j=0}^{J+3(l-1)} c_j(t, \hbar)\, \varphi_j(A(t), B(t), \hbar, a(t), \eta(t), \cdot) \Bigg\|_{L^2(\mathbb{R})} \leqq C_3 \hbar^{l/2} \quad (1.4)$$

whenever $t \in [0, T]$ *and* $0 < \hbar \leqq 1$. *Here* $[A(t), B(t), a(t), \eta(t), S(t)]$ *is the unique bounded solution to the system of ordinary differential equations*:

$$\text{(i)} \qquad \frac{da}{dt}(t) = \eta(t)/m,$$

$$\text{(ii)} \qquad \frac{d\eta}{dt}(t) = -V'(a(t)),$$

$$\text{(iii)} \qquad \frac{dA}{dt}(t) = i B(t)/m,$$

$$\text{(iv)} \qquad \frac{dB}{dt}(t) = i V''(a(t))\, A(t),$$

$$\text{(v)} \qquad \frac{dS}{dt}(t) = \eta(t)^2/2m - V(a(t)),$$

subject to the initial conditions $A(0) = A_0$, $B(0) = B_0$, $a(0) = a_0$, $\eta(0) = \eta_0$ *and* $S(0) = 0$. *The* $\{c_j(t, \hbar)\}_{j=0}^{J+3(l-1)}$ *is the unique solution to the system of coupled ordinary differential equations*

$$\frac{dc_j}{dt}(t, \hbar) = \sum_{n=0}^{J+3(l-1)} \sum_{k=3}^{l+1} -i\hbar^{(k-2)/2} |A(t)|^k (\overline{A(t)}/A(t))^{(n-j)/2} \times V^{(k)}(a(t)) \langle j, x^k n \rangle c_n(t, \hbar)/k! \quad (1.5)$$

subject to the initial conditions $c_j(0, \hbar) = c_j$ *for* $0 \leqq j \leqq J$ *and* $c_j(0, \hbar) = 0$ *for* $J + 1 \leqq j \leqq J + 3(l-1)$. *In this equations,* $V^{(k)}$ *denotes* $d^k V/dx^k$, *and* $\langle j, x^k n \rangle$ *are defined by*

$$\langle j, x^k n \rangle = \int_{\mathbb{R}} x^k \varphi_n(1, 1, 1, 0, 0, x)\, \varphi_j(1, 1, 1, 0, 0, x)\, dx.$$

We define $\langle j, x^k n \rangle = 0$, *if* $j < 0$ *or* $n < 0$.

In Theorem 1, only finite linear combinations of $\{\varphi_j\}_{j=0}^{\infty}$ was treated, so that we shall improve this theorem to infinite linear combinations. For this purpose, we must modify the definition of $c_j(t, \hbar)$, because the system of ordinary differential equation (1.5) is depended on J. Then we propose to replace $\{c_j(t, \hbar)\}_{j=0}^{J+3(l-1)}$ with $\{d_j(t, \hbar)\}_{j=0}^{\infty}$ that each $d_j(t, \hbar)$

is independent of J. We define each $d_j(t, \hbar)$ as follows: for each $j\in\{0, 1, 2, 3, \dots\}$,

$$d_j(t, \hbar)=c_j+\sum_{n=0}^{\infty} c_n\Bigg[\sum_{q=1}^{l-1}(-i)^q \sum_{3q\leqq a_1+\dots+a_q\leqq (l-1)+2q}$$

$$\sum_{n+n_1\dots+n_q=j}\int_0^t\int_0^{s_{q-1}}\dots\int_0^{s_2}\int_0^{s_1} ds_{q-1}\,ds_{q-2}\dots ds_1\,ds_0$$

$$\prod_{p=1}^{q}\{\hbar^{(a_p-2)/2}\langle(n+n_1+\dots+n_p), x^{a_p}(n+n_1+\dots+n_{p-1})\rangle$$

$$\times|\mathrm{A}(s_{p-1})|^{a_p}(\mathrm{A}(s_{p-1})/\overline{\mathrm{A}(s_{p-1})})^{n_p/2}\cdot \mathrm{V}^{(a_p)}(a(s_{p-1}))/a_p!\}\Bigg] \quad (1.6)$$

where, for each $p=1, 2, \dots, l-1$, $a_p\in\{3, 4, \dots, l+1\}$, and n_p is integer except $n_0=0$ which satisfies $-a_p\leqq n_p\leqq a_p$.

We have the following main theorem.

THEOREM 2. — *Suppose* $\mathrm{V}(x)$ *satisfies Assumption* 1.2 *for some integer* $l\geqq 2$. *Let* a_0, $\eta_0\in\mathbb{R}$, *and let* A_0, $\mathrm{B}_0\in\mathbb{C}$ *which satisfy* (1.1). *Let* $\{c_j\}_{j=0}^{\infty}(\subset\mathbb{C})$ *be a complex sequence such that* $\sum_{j=0}^{\infty}|c_j|\cdot j^p<\infty$ *for all* $p>0$. *Then, for* $\mathrm{T}>0$, *there exists* $\mathrm{C}_3>0$ *such that*

$$\Bigg\|e^{-it\,\mathrm{H}(\hbar)/\hbar}\sum_{j=0}^{\infty}c_j\varphi_j(\mathrm{A}_0, \mathrm{B}_0, \hbar, a_0, \eta_0, \cdot)$$

$$-e^{i\,\mathrm{S}(t)/\hbar}\sum_{j=0}^{\infty}d_j(t, \hbar)\varphi_j(\mathrm{A}(t), \mathrm{B}(t), \hbar, a(t), \eta(t), \cdot)\Bigg\|_{\mathrm{L}^2(\mathbb{R})}\leqq \mathrm{C}_3\hbar^{l/2} \quad (1.7)$$

whenever $t\in[0, \mathrm{T}]$ and $0<\hbar\leqq 1$. *Here* $[\mathrm{A}(t), \mathrm{B}(t), a(t), \eta(t), \mathrm{S}(t)]$ *is the unique solution to the system of equation* (i)$\sim$(v). *Justly each* $d_j(t, \hbar)$ *is defined in* (1.6).

Remark 1. — It should be noted that the resulting approximate dynamics is not unitary under these $d_j(t, \hbar)$ which are defineded by (1.6). For this fact, *see* G. A. Hagedorn [2]. However we think that this disadvantage can be enough to recover by the fact that J can be taken ∞.

Remark 2. — It is easily show that, by (1.6), that we can put

$$\sum_{j=0}^{\infty}d_j(t, \hbar)\varphi_j(\mathrm{A}(t), \mathrm{B}(t), \hbar, a(t), \eta(t), x)$$

$$=\sum_{j=0}^{\infty}c_j\{\varphi_j(\mathrm{A}(t), \mathrm{B}(t), \hbar, a(t), \eta(t), x)+\mathrm{F}_j(t, x)\} \quad (1.8)$$

where each $F_j(t.x)$ is defined by

$$F_j(t, x)=\sum_{q=1}^{l-1}(-i)^q \sum_{3q\leqq a_1+\ldots+a_q\leqq(l-1)+2q} \sum_{n_1=-a_1}^{a_1}\ldots\sum_{n_q=-a_q}^{a_q}$$
$$\times\int_0^t\int_0^{s_{q-1}}\ldots\int_0^{s_2}\int_0^{s_1} ds_{q-1}\,ds_{q-2}\ldots ds_1\,ds_0$$
$$\times\prod_{p=1}^{q}\{\hbar^{(a_q-2)/2}\langle (j+n_1+\ldots+n_p), x^{a_p}(j+n_1+\ldots+n_{p-1})\rangle$$
$$\times|A(s_{p-1})|^{a_p}(A(s_{p-1})/\overline{A(s_{p-1})})^{n_p/2}V^{(a_p)}(a(s_{p-1}))/a_p!\}$$
$$\times\varphi_{j+n_1+\ldots+n_q}(A(t), B(t), \hbar, a(t), \eta(t), x). \quad (1.9)$$

Remark 3. — For Schwartz class function $f\in\mathscr{S}(\mathbb{R})$, let c_j be chosen so that $f(x)=\sum_{j=0}^{\infty}c_j\varphi(1, 1, 1, 0, 0, x)$, then, we note that $\sum_{j=0}^{\infty}|c_j|\cdot j^p<\infty$ for all $p>0$. Therefore we notice that Theorem 1 is extended to the state $f\in\mathscr{S}(\mathbb{R})$ because of replacing $c_j(t, \hbar)$ with $d_j(t, \hbar)$.

2. SOME PRELIMINARY LEMMAS

Throughout this section we mention three preliminary lemmas for the proof of Theorem 2. The first lemma gives the basic formula in semiclassical quantum mechanics. This important fact was obtained by G. A. Hagedorn in [1]. The second one means that

$$\sum_{j=0}^{\infty}d_j(t, \hbar)\varphi_j(a(t), \eta(t), \hbar, A(t), B(t), \cdot)$$

belongs to L^2-class. The last lemma is the estimate in the polynomial approximation of the potential $V(x)$.

LEMMA 2.1 (See *G. A. Hagedorn* [1]). — *Let* a_0, $\eta_0\in\mathbb{R}$, *and let* A_0, $B_0\in\mathbb{C}$ *which satisfy* (1.1). *If* $V(x)$ *is a polynomial of degree* 2 *and* $V(x)\geqq -C$, *then, the following equality holds*:

$$e^{-itH(\hbar)/\hbar}\varphi_j(A_0, B_0, \hbar, a_0, \eta_0, x) = e^{iS(t)/\hbar}\varphi_j(A(t), B(t), \hbar, a(t), \eta(t), x) \quad (2.1)$$

for all $t\in\mathbb{R}$ *and all* $j\in\{0, 1, 2, \ldots\}$.

LEMMA 2.2. — *Suppose the potential* $V(x)$ *satisfies Assumption* 1.1 *for some integer* $l\geqq 2$. *Then, there exists* $C(T, l)>0$ *such that*

$$\|F_j(t, \cdot)\|_{L^2(\mathbb{R})}\leqq C(T, l).[j+(l+1)^2]^{3(l-1)/2} \quad (2.2)$$

for all $j\in\{0, 1, 2, \ldots\}$ *and all* $t\in[0, T]$.

Proof. — The hypothesis imply the existences of Γ and R, such that $|A(t)|\leqq\Gamma$ and $|a(t)|\leqq R$ for all $t\in[0, T]$. Then, for any $t\in[0, T]$, we see that

$$\|F_j(t,\cdot)\|_{L^2(\mathbb{R})}\leqq\sum_{q=1}^{l-1}\sum_{3q\leqq a_1+\ldots+a_q\leqq(l-1)+2q}|T|^q\sum_{n_1=-a_1}^{a_1}\ldots\sum_{n_q=-a_q}^{a_q}$$
$$\times\prod_{p=1}^{q}\left\{\hbar^{(a_p-2)/2}|\langle(j+n_1+\ldots+n_p), x^{a_p}(j+n_1+\ldots+n_{p-1})\rangle|\right.$$
$$\left.\times\Gamma^{a_p}\cdot\max_{t\in[0,T]}\frac{|V^{(a_p)}(a(t))|}{a_p!}\right\}$$
$$\leqq C'(T, l)\sum_{q=1}^{l-1}\sum_{3q\leqq a_1+\ldots+a_q\leqq(l-1)+2q}\sum_{n_1=-a_1}^{a_1}\ldots\sum_{n_q=-a_q}^{a_q}$$
$$\times\prod_{p=1}^{q}\|x^{a_p}\varphi_{j+n_1+\ldots+n_p}(1, 1, 1, 0, 0,\cdot)\|_{L^2(\mathbb{R})}.$$

Now we can easily show the following estimate from the induction with respect to $n\in\mathbb{N}$: for all $j=0, 1, 2, \ldots$ and all $n\in\mathbb{N}$,

$$\|x^n\varphi_j(1, 1, 1, 0, 0,\cdot)\|_{L^2(\mathbb{R})}\leqq 3^n\cdot(j+n)^{n/2}. \tag{2.3}$$

Therefore, we see that

$$\|F_j(t,.)\|_{L^2(\mathbb{R})}\leqq C'(T, l)\cdot\sum_{q=1}^{l-1}\sum_{3q\leqq a_1+\ldots+a_q\leqq(l-1)+2q}\sum_{n_1=-a_1}^{a_1}\ldots\sum_{n_q=-a_q}^{a_q}$$
$$\times\prod_{p=1}^{q}3^{a_p}\cdot(j+n_1+\ldots+n_p+a_p)^{a_p/2}$$
$$\leqq C'(T, l)\cdot 3^{3(l-1)}\cdot[j+(l+1)^2]^{3(l-1)/2}\sum_{q=1}^{l-1}\sum_{3q\leqq a_1+\ldots+a_q\leqq(l-1)+2q}$$
$$\times\sum_{n_1=-a_1}^{a_1}\ldots\sum_{n_q=-a_q}^{a_q}1=C(T, l)\cdot[j+(l+1)^2]^{3(l-1)/2}.$$

Hence, the inequality (2.2) was proved. □

LEMMA 2.3. — *Suppose* $V(x)$ *satisfies Assumption* 1.2 *for some integer* $l\geqq 2$. *Let* $\Gamma>0$, $R>0$, *and let* $Y_a(x)=\sum_{k=0}^{l+1}V^{(k)}(a)\cdot(x-a)^k/k!$ Then, $|A|\leqq\Gamma$ *and* $|a|\leqq R$ *implies*

$$\|(e^{-itV(.)/\hbar}-e^{-itY_a(.)/\hbar})\varphi_j(A, B, \hbar, a, \eta,\cdot)\|_{L^2(\mathbb{R})}$$
$$\leqq C(C_1, l, R, M)\cdot\max[\Gamma^{l+2}, \Gamma^{2p}]\cdot|t|\cdot(j+2p)^p\cdot\hbar^{l/2} \tag{2.4}$$

for all $j\in\{0, 1, 2, \ldots\}$ *and* $t\in\mathbb{R}$, *where*

$p=\max[(l+2)/2, M]$, $\quad C(C_1, l, R, M)=\max[D_1(l, R), D_2(C_1, l, R, M)]$

which each $D_1 = D_1(l, R)$ *and* $D_2 = D_2(C_1, l, R, M)$ *is defined by*

$$D_1 = \max_{|y| \leqq R+1} \frac{|V^{(l+2)}(y)|}{(l+2)!}, \qquad D_2 = C_1 \cdot (R+2)^{2p} + \max_{|y| \leqq R} \sum_{k=0}^{l+1} \frac{|V^{(k)}(y)|}{k!}.$$

Proof. – From the assumption of $V(x) \in C^{l+2}(\mathbb{R})$, we can use Taylor's formula. Hence, we obtain that $|a| \leqq R$ and $|x-a| \leqq 1$ imply

$$|V(x) - Y_a(x)| \leqq D_1(l, R) \cdot |x-a|^{l+2}.$$

And the growth of $|V(x)| \leqq C_1 \cdot (1+|x|)^M$ means that there exist $p = \max[(l+2)/2, M]$ and $D_2(C_1, l, R, M) > 0$ such that $|a| \leqq R$ and $|x-a| \geqq 1$ imply

$$|V(x) - Y_a(x)| \leqq D_2(C_1, l, R, M) \cdot |x-a|^{2p}.$$

Therefore, we show that, for $|A| \leqq \Gamma$ and $|a| \leqq R$,

$$\begin{aligned}
&\| (e^{-it V(\cdot)/\hbar} - e^{-it Y_a(\cdot)/\hbar}) \varphi_j(A, B, \hbar, a, \eta, \cdot) \|_{L^2(\mathbb{R})} \\
&\qquad \leqq \hbar^{-1} \cdot |t| \cdot \| \, |V(\cdot) - Y_a(\cdot)| \cdot \varphi_j(A, B, \hbar, a, \eta, \cdot) \|_{L^2(\mathbb{R})} \\
&\qquad \leqq D_1(l, R) \cdot \hbar^{-1} \cdot |t| \cdot \| (x-a)^{l+2} \varphi_j(A, B, \hbar, a, \eta, \cdot) \|_{L^2(\mathbb{R})} \\
&\qquad\qquad + D_2 \cdot \hbar^{-1} \cdot |t| \cdot \| (x-a)^{2p} \varphi_j(A, B, \hbar, a, \eta, \cdot) \|_{L^2(\mathbb{R})} = I + II.
\end{aligned}$$

Here, from the estimate (2.3), we see that,

$$\begin{aligned}
I &= D_1(l, R) \cdot \hbar^{-1} \cdot |t| \cdot |A|^{l+2} \cdot \hbar^{(l+2)/2} \cdot \| x^{l+2} \varphi_j(1, 1, 1, 0, 0, \cdot) \|_{L^2(\mathbb{R})} \\
&\leqq D_1(l, R) \cdot \Gamma^{l+2} \cdot |t| \cdot \hbar^{l/2} \cdot 3^{l+2} \cdot (j+l+2)^{(l+2)/2}, \qquad (\forall j \in \{0, 1, 2, \dots\}) \\
II &= D_2 \cdot \hbar^{-1} \cdot |t| \cdot |A|^{2p} \cdot \hbar^p \cdot \| x^{2p} \varphi_j(1, 1, 1, 0, 0, \cdot) \|_{L^2(\mathbb{R})} \\
&\leqq D_2 \cdot \Gamma^{2p} \cdot |t| \cdot \hbar^{p-1} \cdot 3^{2p} \cdot (j+2p)^p, \qquad (\forall j \in \{0, 1, 2, \dots\}).
\end{aligned}$$

Therefore, we can easily obtain the inequality (2.4), because of $p \geqq l/2 + 1$. □

3. PROOF OF THEOREM 2

We shall divide the interval [0, T] into N-pieces. Then, we will be led to the following discrete time analogs of the equation (i)∼(v) and $F_j(t, x)$: Let

$$a_N(0) = a_0, \qquad \eta_N(0) = \eta_0, \qquad A_N(0) = A_0, \qquad B_N(0) = B_0, \qquad S_N(0) = 0$$

and

$$F_{N,j}(0, x) = 0,$$

$$\text{(i')} \qquad \tilde{a}(nT/N) \equiv a_N(n) = a_N(0) + \left(\frac{T}{N}\right) \cdot \frac{i}{m} \sum_{k=1}^{n} \eta_N(k)$$

(ii') $$\tilde{\eta}(n\mathrm{T}/\mathrm{N}) \equiv \eta_{\mathrm{N}}(n) = \eta_{\mathrm{N}}(0) - \left(\frac{\mathrm{T}}{\mathrm{N}}\right) \sum_{k=1}^{n} \mathrm{V}'(a_{\mathrm{N}}(k-1))$$

(iii') $$\tilde{\mathrm{A}}(n\mathrm{T}/\mathrm{N}) \equiv \mathrm{A}_{\mathrm{N}}(n) = \mathrm{A}_{\mathrm{N}}(0) + \left(\frac{\mathrm{T}}{\mathrm{N}}\right) \cdot \frac{i}{m} \sum_{k=1}^{n} \mathrm{B}_{\mathrm{N}}(k)$$

(iv') $$\tilde{\mathrm{B}}(n\mathrm{T}/\mathrm{N}) \equiv \mathrm{B}_{\mathrm{N}}(n) = \mathrm{B}_{\mathrm{N}}(0) + \left(\frac{\mathrm{T}}{\mathrm{N}}\right) \cdot i \sum_{k=1}^{n} \mathrm{V}''(a_{\mathrm{N}}(k-1))\, \mathrm{A}_{\mathrm{N}}(k-1)$$

(v') $$\tilde{\mathrm{S}}(n\mathrm{T}/\mathrm{N}) \equiv \mathrm{S}_{\mathrm{N}}(n) = \left(\frac{\mathrm{T}}{\mathrm{N}}\right) \sum_{k=1}^{n} \left[\frac{\eta_{\mathrm{N}}^{2}(k)}{2m} - \mathrm{V}(a_{\mathrm{N}}(k-1))\right].$$

And the discrete version of $\mathrm{F}_j(t, x)$ is that

$$\begin{aligned}\tilde{\mathrm{F}}_j(n\mathrm{T}/\mathrm{N}, x) \equiv \mathrm{F}_{\mathrm{N},j}(n, x) = \sum_{q=1}^{l-1} (-i)^q \sum_{3q \leqq a_1 + \ldots + a_q \leqq (l-1) + 2q} \\ \sum_{n_1=-a_1}^{a_1} \cdots \sum_{n_q=-a_q}^{a_q} \left(\frac{\mathrm{T}}{\mathrm{N}}\right)^q \sum_{k_{q-1}=q-1}^{n-1} \sum_{k_{q-2}=q-2}^{k_{q-1}-1} \cdots \sum_{k_1=1}^{k_2-1} \sum_{k_0=0}^{k_1-1} \\ \times \prod_{p=1}^{q} \{ \hbar^{(a_p-2)/2} \langle (j+n_1+\ldots+n_p),\, x^{a_p}(j+n_1+\ldots+n_{p-1}) \rangle \\ \times |\mathrm{A}_{\mathrm{N}}(k_{p-1})|^{a_p} \cdot (\mathrm{A}_{\mathrm{N}}(k_{p-1})/\overline{\mathrm{A}_{\mathrm{N}}(k_{p-1})})^{n_p/2} \cdot \mathrm{V}^{(a_p)}(a_{\mathrm{N}}(k_{p-1}))/a_p! \} \\ \times \varphi_{j+n_1+\ldots+n_q}(\mathrm{A}_{\mathrm{N}}(n), \mathrm{B}_{\mathrm{N}}(n), \hbar, a_{\mathrm{N}}(n), \eta_{\mathrm{N}}(n), x). \quad (3.1)\end{aligned}$$

By taking N sufficiently large we can make these $a_{\mathrm{N}}(n)$, $\eta_{\mathrm{N}}(n)$, $\mathrm{A}_{\mathrm{N}}(n)$, $\mathrm{B}_{\mathrm{N}}(n)$, $\mathrm{S}_{\mathrm{N}}(n)$ and $\mathrm{F}_{\mathrm{N},j}(n, x)$ approximate $a(t)$, $\eta(t)$, $\mathrm{A}(t)$, $\mathrm{B}(t)$, $\mathrm{S}(t)$ and $\mathrm{F}_j(t, x)$ if $t = n\mathrm{T}/\mathrm{N}$. From Lemma 2.2 and $\sum_{j=0}^{\infty} |c_j| . j^p < \infty$ for $\forall p > 0$, we immediately note that

$$\sum_{j=0}^{\infty} c_j \{ \varphi_j(\mathrm{A}(t), \mathrm{B}(t), \hbar, a(t), \eta(t), \cdot) + \mathrm{F}_j(t, \cdot) \} \in \mathrm{L}^2(\mathbb{R}).$$

Therefore, we can combine the results of G. A. Hagedron [2] and the previous preliminary lemmas. Then, we can know the following results [I] ~ [V].

For all $\varepsilon > 0$, there exists $\mathrm{N}_1 > 0$ such that $\mathrm{N} \geqq \mathrm{N}_1$ implies that, for all $0 \leqq n \leqq \mathrm{N}$,

[I] $\mathrm{A}_{\mathrm{N}}(n)$ is invertible,

$$|\mathrm{A}_{\mathrm{N}}(n)| \leqq \Gamma \text{ and } |a_{\mathrm{N}}(n)| \leqq \mathrm{R} \text{ for some } \Gamma > 0,\ \mathrm{R} > 0,$$

[II] $$\Bigg\| e^{i\mathrm{S}(n\mathrm{T}/\mathrm{N})/\hbar} \sum_{j=0}^{\infty} c_j \{ \varphi_j(\mathrm{A}_{\mathrm{N}}(n), \mathrm{B}_{\mathrm{N}}(n), \hbar, a_{\mathrm{N}}(n), \eta_{\mathrm{N}}(n), \cdot) + \mathrm{F}_{\mathrm{N},j}(n, \cdot) \} - e^{i\mathrm{S}(t)/\hbar} \sum_{j=0}^{\infty} c_j \{ \varphi_j(\mathrm{A}(t), \mathrm{B}(t), \hbar, a(t), \eta(t), \cdot) + \mathrm{F}_j(t, \cdot) \} \Bigg\|_{\mathrm{L}^2(\mathbb{R})} \leqq \frac{\varepsilon}{3},$$

[III] $$\left\| \left(e^{-itH(\hbar)/\hbar} - [e^{-i(T/N)H_0(\hbar)/\hbar} \cdot e^{-i(T/N)V(\cdot)/\hbar}]^n\right) \times \sum_{j=0}^{\infty} c_j \varphi_j(A_0, B_0, \hbar, a_0, \eta_0, \cdot) \right\|_{L^2(\mathbb{R})} \leqq \frac{\varepsilon}{3},$$

[IV] $$\| (e^{-i(T/N)V(\cdot)/\hbar} - e^{-i(T/N)Y_{a_N(n)}(\cdot)/\hbar}) \times \{ \varphi_j(A_N(n), B_N(n), \hbar, a_N(n), \eta_N(n), \cdot) + F_{N,j}(n, \cdot) \} \|_{L^2(\mathbb{R})}$$
$$\leqq \frac{C_1(l, T)}{N} \cdot [j+4p^2]^{4p} \cdot \hbar^{l/2}, \qquad (\forall j \in \{0, 1, 2, \ldots\}),$$

[V] $$\left\| \left[e^{-i(T/N)Z_{a_N(n)}(\cdot)/\hbar} - 1 + \left(\frac{T}{N}\right) \cdot \frac{i}{\hbar} \cdot Z_{a_N(n)}(\cdot) \right] \times \{ \varphi_j(A_N(n), B_N(n), \hbar, a_N(n), \eta_N(n), \cdot) + F_{N,j}(n, \cdot) \} \right\|_{L^2(\mathbb{R})}$$
$$\leqq \frac{\varepsilon}{3KN} \cdot [j+(l+1)^2]^{3l}, \qquad (\forall j \in \{0, 1, 2, \ldots\}),$$

where

$$Z_{a_N(n)}(x) = \sum_{k=3}^{l+1} V^{(k)}(a_N(n)) \cdot (x - a_N(n))^k / k!$$

and

$$K = \sum_{j=0}^{\infty} |c_j| \cdot [j+4p^2]^{4p} < \infty.$$

From [II] and [III], we notice that the proof will be complete if we show the following inequality: namely, for all $0 \leqq n \leqq N$,

$$\left\| [e^{-i(T/N)H(\hbar)/\hbar} \cdot e^{-i(T/N)V(\cdot)/\hbar}]^n \times \sum_{j=0}^{\infty} c_j \varphi_j(A_0, B_0, \hbar, a_0, \eta_0, \cdot) - e^{iS_N(n)/\hbar} \times \sum_{j=0}^{\infty} c_j \{ \varphi_j(A_N(n), B_N(n), \hbar, a_N(n), \eta_N(n), \cdot) + F_{N,j}(n, \cdot) \} \right\|_{L^2(\mathbb{R})}$$
$$\leqq C_3 \hbar^{l/2} + \frac{\varepsilon}{3}$$

where C_3 is a positive constant which is independent of ε, N and $\hbar$.

At first we put $W_{a_N(n)}(x)=\sum_{k=0}^{2} V^{(k)}(a_N(n))\cdot(x-a_N(n))^k/k!$ Then, from Lemma 2.1 and (2.1), we can calculate that, for $0\leqq n\leqq N-1$,

$$
\begin{aligned}
&e^{-i(T/N)H_0(\hbar)/\hbar}\cdot e^{-i(T/N)W_{a_N(n)}(x)/\hbar}\cdot\left[1-\left(\frac{T}{N}\right)\cdot\frac{i}{\hbar}\cdot Z_{a_N(n)}(x)\right]\\
&\quad\times e^{iS_N(n)/\hbar}\cdot\{\varphi_j(A_N(n), B_N(n), \hbar, a_N(n), \eta_N(n), x)+F_{N,j}(n,x)\}\\
&\quad=e^{iS_N(n+1)/\hbar}\cdot\{\varphi_j(A_N(n+1), B_N(n+1), \hbar, a_N(n+1), \eta_N(n+1), x)\\
&\qquad\qquad+F_{N,j}(n+1,x)\}+\mathscr{F}_{N,j}(n,x), \qquad (3.2)
\end{aligned}
$$

where $\mathscr{F}_{N,j}(n,x)$ is that

$$
\begin{aligned}
\mathscr{F}_{N,j}(n,x)=&-\left(\frac{T}{N}\right)\cdot\frac{i}{\hbar}\cdot e^{iS_N(n)/\hbar}\cdot e^{-i(T/N)H_0(\hbar)/\hbar}\cdot e^{-i(T/N)W_{a_N(n)}(x)/\hbar}\\
&\times\sum_{q=1}^{l-1}\sum_{r=q}^{l-1}\left[\sum_{k=l+2-r}^{l+1}\frac{V^{(k)}(a_N(n))\cdot(x-a_N(n))^k}{k!}\right]\cdot(-i)^q\\
&\times\sum_{a_1+\ldots+a_q=r+2q}\ \sum_{n_1=-a_1}^{a_1}\cdots\sum_{n_q=-a_q}^{a_q}\left(\frac{T}{N}\right)^q\\
&\times\sum_{k_{q-1}=q-1}^{n-1}\ \sum_{k_{q-2}=q-2}^{k_{q-1}-1}\cdots\sum_{k_1=1}^{k_2-1}\sum_{k_0=0}^{k_1-1}
\end{aligned}
$$

$$
\begin{aligned}
\prod_{p=1}^{q}&\{\hbar^{(a_p-2)/2}\langle(j+n_1+\ldots+n_p), x^{a_p}(j+n_1+\ldots+n_{p-1})\rangle\\
&\times|A_N(k_{p-1})|^{a_p}\cdot(A_N(k_{p-1})/\overline{A_N(k_{p-1})})^{n_p/2}\,V^{(a_p)}(a_N(k_{p-1}))/a_p!\}\\
&\times\varphi_{j+n_1+\ldots+n_q}(A_N(n), B_N(n), \hbar, a_N(n), \eta_N(n), x).
\end{aligned}
$$

Then, we can estimate the L^2-norm of $\mathscr{F}_{N,j}(n,x)$, that is, there exists $C_2(T,l)>0$ such that $0\leqq n\leqq N$ implies

$$
\left.\begin{aligned}
&\|\mathscr{F}_{N,j}(n,\cdot)\|_{L^2(\mathbb{R})}\leqq\frac{C_2(T,l)}{N}\cdot\hbar^{l/2}\cdot[j+(l+1)^2]^{3l/2},\\
&(\forall j\in\{0,1,2,\ldots\}).
\end{aligned}\right\}\qquad(3.3)
$$

This fact can be shown as follows:

$$
\begin{aligned}
\|\mathscr{F}_{N,j}(n,.)\|_{L^2(\mathbb{R})}\leqq&\frac{C'(T,l)}{\hbar N}\sum_{q=1}^{l-1}\sum_{r=q}^{l-1}\sum_{k=l+2-r}^{l+1}\\
&\times\sum_{a_1+\ldots+a_q=r+2q}\ \sum_{n_1=-a_1}^{a_a}\cdots\sum_{n_q=-a_q}^{a_q}\\
&\times\frac{1}{N^q}\sum_{k_{q-1}=q-1}^{n-1}\ \sum_{k_{q-2}=q-2}^{k_{q-1}-1}\cdots\sum_{k_1=1}^{k_2-1}\sum_{k_0=0}^{k_1-1}\prod_{p=1}^{q}
\end{aligned}
$$

$$\times [\hbar^{(a_p-2)/2}\cdot \| x^{a_p}\varphi_{j+n_1+\ldots+n_p}(1,1,1,0,0,\cdot)\|]$$
$$\times \| (x-a_N(n))^k \varphi_{j+n_1+,,,+n_q}(A_N(n), B_N(n), \hbar, a_N(n), \eta_N(n), \cdot)\|$$
$$\leqq \frac{C'(T,l)}{\hbar N}\sum_{q=1}^{l-1}\sum_{r=q}^{l-1}\sum_{k=l+2-r}^{l+1}$$
$$\times \sum_{a_1+\ldots+a_q=r+2q}\ \sum_{n_1=-a_1}^{a_1}\ldots\sum_{n_q=-a_q}^{a_q}\frac{N^q}{N^q}$$
$$\times \hbar^{(a_1+\ldots+a_q-2q)/2}\cdot 3^{a_1+\ldots+a_q}\cdot (j+n_1+a_1)^{a_1/2}\ldots(j+n_1+\ldots+n_q+a_q)^{a_q/2}$$
$$\times \Gamma^k\cdot\hbar^{k/2}\cdot 3^k\cdot (j+n_1+\ldots+n_q+k)^{k/2}$$
$$\leqq \frac{C'(T,l)}{\hbar N}\cdot \max[|\Gamma|^{l+1},1]\cdot 3^{3l}\sum_{q=1}^{l-1}\sum_{r=q}^{l-1}\sum_{k=l+2-r}^{l+1}\ \sum_{a_1+\ldots+a_q=r+2q}$$
$$\times \sum_{n_1=-a_1}^{a_1}\ldots\sum_{n_q=-a_q}^{a_q}\hbar^{r/2}\cdot [j+(l+1)^2]^{(a_1+\ldots+a_q)/2}\cdot \hbar^{k/2}\cdot [j+(l+1)^2]^{k/2}$$
$$\leqq \frac{C''(T,l)}{N\hbar}\cdot \hbar^{(l+2)/2}\cdot [j+(l+1)^2]^{3l/2}$$
$$\sum_{q=1}^{l-1}\sum_{r=q}^{l-1}\sum_{k=l+2-r}^{l+1}\ \sum_{a_1+\ldots+a_q=r+2q}$$
$$\times \sum_{n_1=-a_1}^{a_1}\ldots\sum_{n_q=-a_q}^{a_q} 1 = \frac{C_2(T,l)}{N}\cdot \hbar^{l/2}\cdot [j+(l+1)^2]^{3l/2}.$$

Hence, we have obtained the inequality (3.3).

Moreover, from [IV], [V], (3.2) and (3.3), we shall inductively prove the following estimate, that is, there exists $C_3(T, l)>0$ such that $0\leqq n\leqq N$ implies

$$\| [e^{-i(T/N)H_0(\hbar)/\hbar}\cdot e^{-i(T/N)V(\cdot)/\hbar}]^n \varphi_j(A_0, B_0, \hbar, a_0, \eta_0, \cdot)$$
$$- e^{iS_N(n)/\hbar}\cdot \{\varphi_j(A_N(n), B_N(n), \hbar, a_N(n), \eta_N(n), \cdot)+F_{N,j}(n,\cdot)\}\|_{L^2(\mathbb{R})}$$
$$\leqq \frac{n}{N}\cdot\left[C_3(T,l)\cdot\hbar^{l/2}+\frac{\varepsilon}{3K}\right]\cdot [j+4p^2]^{4p},\qquad (\forall j\in\{0,1,2,\ldots\}).$$

The above inequality is trivial at $n=0$, because of $S_N(0)=0$, $F_{N,j}(0,x)=0$ and $\mathscr{F}_{N,j}(0,x)=0$. So we assume that this inequality holds until $n=k$. Then, at $n=k+1$, we see that

$$\| [e^{-i(T/N)H_0(\hbar)/\hbar}\cdot e^{-i(T/N)V(\cdot)/\hbar}]^{k+1} \varphi_j(A_0, B_0, \hbar, a_0, \eta_0, \cdot) - e^{iS_N(k+1)/\hbar}$$
$$\times \{\varphi_j(A_N(k+1), B_N(k+1), \hbar, a_N(k+1), \eta_N(k+1), \cdot)+F_{N,j}(k+1,\cdot)\}\|_{L^2(\mathbb{R})}$$
$$\leqq \| [e^{-i(T/N)H_0(\hbar)/\hbar}\cdot e^{-i(T/N)V(\cdot)/\hbar}]^k \varphi_j(A_0, B_0, \hbar, a_0, \eta_0, \cdot)$$
$$- e^{iS_N(k)/\hbar}\cdot \{\varphi_j(A_N(k), B_N(k), \hbar, a_N(k), \eta_N(k), \cdot)+F_{N,j}(k,\cdot)\}\|_{L^2(\mathbb{R})}$$

$$+\| [e^{-i(T/N)H_0(\hbar)/\hbar}\cdot e^{-i(T/N)V(\cdot)/\hbar}]\cdot e^{iS_N(k)/\hbar}$$
$$\times\{\varphi_j(A_N(k), B_N(k), \hbar, a_N(k), \eta_N(k), \cdot)+F_{N,j}(k,\cdot)\}-e^{iS_N(k+1)/\hbar}$$
$$\times\{\varphi_j(A_N(k+1), B_N(k+1), \hbar, a_N(k+1), \eta_N(k+1), \cdot)+F_{N,j}(k+1,\cdot)\}\|_{L^2(\mathbb{R})}$$
$$\leqq\frac{k}{N}\cdot\left[C_3(T,l)\cdot\hbar^{l/2}+\frac{\varepsilon}{3K}\right]\cdot[j+4p^2]^{4p}$$
$$+\left\|\left[e^{-i(T/N)V(\cdot)/\hbar}-e^{-i(T/N)W_{a_N(k)}(\cdot)/\hbar}\cdot\left(1-\left(\frac{T}{N}\right)\cdot\frac{i}{\hbar}\cdot Z_{a_N(k)}(\cdot)\right)\right]\right.$$
$$\left.\times\{\varphi_j(A_N(k), B_N(k), \hbar, a_N(k), \eta_N(k), \cdot)+F_{N,j}(k,\cdot)\}+\mathscr{F}_{N,j}(k,\cdot)\right\|_{L^2(\mathbb{R})}$$
$$\leqq\frac{k}{N}\cdot\left[C_3(T,l)\cdot\hbar^{l/2}+\frac{\varepsilon}{3K}\right]\cdot[j+4p^2]^{4p}$$
$$+\|(e^{-i(T/N)V(\cdot)/\hbar}-e^{-i(T/N)Y_{a_N(k)}(\cdot)/\hbar})$$
$$\times\{\varphi_j(A_N(k), B_N(k), \hbar, a_N(k), \eta_N(k), \cdot)+F_{N,j}(k,\cdot)\}\|_{L^2(\mathbb{R})}$$
$$+\left\|\left(e^{-i(T/N)Z_{a_N(k)}(\cdot)/\hbar}-1+\left(\frac{T}{N}\right)\cdot\frac{i}{\hbar}\cdot Z_{a_N(k)}(\cdot)/\hbar\right)\right.$$
$$\left.\times\{\varphi_j(A_N(k), B_N(k), \hbar, a_N(k), \eta_N(k), \cdot)+F_{N,j}(k,\cdot)\}\right\|_{L^2(\mathbb{R})}$$
$$+\|\mathscr{F}_{N,j}(k,\cdot)\|_{L^2(\mathbb{R})}\leqq\frac{k+1}{N}\cdot\left[C_3(T,l)'\cdot\hbar^{l/2}+\frac{\varepsilon}{3K}\right]\cdot[j+4p^2]^{4p}$$

where $C_3(T,l)'=\max[C_1(T,l), C_2(T,l), C_3(T,l)]$.
Therefore, we have proved that this inequality also holds for $n=k+1$.

Finally, we put the constant $C_3=K\cdot C_3(T,l)>0$ which is independent of ε, N, and $\hbar$. Then, we can easily show that, for all $0\leqq n\leqq N$,

$$\left\|[e^{-i(T/N)H(\hbar)/\hbar}\cdot e^{-i(T/N)V(\cdot)/\hbar}]^n\sum_{j=0}^{\infty}c_j\varphi_j(A_0, B_0, \hbar, a_0, \eta_0, \cdot)\right.$$
$$\left.-e^{iS_N(n)/\hbar}\sum_{j=0}^{\infty}c_j\{\varphi_j(A_N(n), B_N(n), \hbar, a_N(n), \eta_N(n), \cdot)+F_{N,j}(n,\cdot)\}\right\|_{L^2(\mathbb{R})}$$
$$\leqq\left[\sum_{j=0}^{\infty}|c_j|\cdot[j+4p^2]^{4p}\right]\cdot\left[C_3(T,l)\cdot\hbar^{l/2}+\frac{\varepsilon}{3K}\right]$$
$$=K\cdot\left[C_3(T,l)\cdot\hbar^{l/2}+\frac{\varepsilon}{3K}\right]=C_3\cdot\hbar^{l/2}+\frac{\varepsilon}{3}.\quad\square$$

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