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Semiclassical quantum mechanics, IV: large order asymptotics and more general states in more than one dimension

by

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ABSTRACT. — We solve the n-dimensional time dependent Schrödinger equation $i\hbar \dfrac{\partial\Psi}{\partial t} = -\dfrac{\hbar^2}{2m} \Delta\Psi + V\Psi$ modulo errors which have L^2 norms on the order of $\hbar^{l/2}$ for arbitrary large l. The initial conditions are fairly general states whose position and momentum uncertainties are proportional to $\hbar^{1/2}$.

RÉSUMÉ. — On résout l'équation de Schrödinger dépendant du temps $i\hbar \dfrac{d\Psi}{dt} = -\dfrac{h^2}{2m} \Delta\Psi + V\Psi$ en dimension n modulo des erreurs dont la norme dans L^2 est d'ordre $\hbar^{l/2}$ pour l'arbitrairement grand. Les conditions initiales sont des états relativement généraux dont les incertitudes de position et d'impulsion sont proportionnelles à $\hbar^{1/2}$.

§ 1. INTRODUCTION

In this paper we study the high order semiclassical asymptotics of solutions to the n-dimensional time dependent Schrödinger equation

$ih \dfrac{\partial \Psi}{\partial t} = - \dfrac{\hbar^2}{2m} \Delta \Psi + V\Psi$. We show that there exist solutions $\Psi(x, t)$ which are concentrated near the trajectory of a classical particle up to errors which are on the order of $\hbar^{l/2}$ for arbitrarily large l.

These results are generalizations of some of our earlier work [3] [4] on the semiclassical limit of quantum mechanics. In [3] we showed that there are approximate solutions to the n-dimensional Schrödinger equation which are accurate up to errors on the order of $\hbar^{1/2}$. In [4] we showed that in one dimension, there are approximate solutions which are accurate up to errors on the order of $\hbar^{l/2}$ for arbitrary l. Thus, the present paper generalizes [3] to higher dimension and [4] to higher order. The generalizations are not straightforward because it is far from clear just what the n-dimensional analogs of the functions $\phi_k(A, B, \hbar, a, \eta, x)$ of [4] are. They are not simply « products of Hermite polynomials of various arguments multiplied by a Gaussian », as stated in [4]. The complication comes from the fact that the complex unitary group $U(n, \mathbb{C})$ enters in the problem where one might expect to see the real orthogonal group $O(n, \mathbb{R})$. This forces one to study some generalizations of the usual Hermite polynomials. Once one knows that these functions are, the generalization of [4] is immediate.

The approximate solutions which we study have momentum and position uncertainties on the order of $\hbar^{1/2}$. This particular semiclassical limit was first studied by Hepp [9], who computed the first term in the small $\hbar$ asymptotics of certain expectation values. In the chemistry literature, Heller [7] used the approximation of the same type, without studying the question of whether or not the approximate solutions were asymptotic to exact solutions. He and Lee have also proposed [8] an approximation similar to the one in [4] and the one we describe here, but he has not found the natural orthonormal basis in which to do the expansion. Ralston [10] has studied approximate solutions to strictly hyperbolic systems of partial differential equations. His results are similar to the ones which we present below, but he expands the approximate solution in terms of a non-orthogonal basis for $L^2(\mathbb{R}^n)$, which leads to more complicated evolution equations for the coefficients in the expansion.

Other semiclassical limits are studied in the literature. In this regard, we recommend the reader consult the work of Yajima [14] [15]. The time independent problem for limits similar to ours has also been studied. The reader should consult the works of Combes, Duclos and Seiler [1] [2], and Simon [11] [12].

For the potentials which we consider, the quantum Hamiltonian $H(\hbar) = - \dfrac{\hbar^2}{2m} \Delta + V(x) = H_0(\hbar) + V$ on $L^2(\mathbb{R}^n)$ is essentially self-adjoint on the

$C^\infty(\mathbb{R}^n)$ functions of compact support. Under this Hamiltonian we will study the evolution of states which are linear combinations of the wave functions $\phi_k(A, B, \hbar, a, \eta, x)$, which are defined below. The state $\phi_k(A, B, \hbar, a, \eta, x)$ is concentrated near the position a and near the momentum η. Its position uncertainty is proportional to $\hbar^{1/2}$, and is determined by the matrix $|A| = [AA^*]^{1/2}$ and the multi-index k. Its momentum uncertainty is proportional to $\hbar^{1/2}$, and is determined by the matrix $|B| = [BB^*]^{1/2}$ and the multi-index k.

The precise definition of the states $\phi_k(A, B, \hbar, a, \eta, x)$ is quite complicated, and requires the following notation:

Throughout the paper we will let n denote the space dimension. A multi-index $k = (k_1, k_2, \ldots, k_n)$ is an ordered n-tuple of non-negative integers. The order of k is defined to be $|k| = \sum_{i=1}^{n} k_i$, and the factorial of k is defined to be $k! = (k_1!)(k_2!) \ldots (k_n!)$. The symbol D^k denotes the differential operator $D^k = \dfrac{\partial^{|k|}}{(\partial x_1)^{k_1}(\partial x_2)^{k_2} \ldots (\partial x_n)^{k_n}}$, and the symbol x^k denotes the monomial $x^k = x_1^{k_1} x_2^{k_2} \ldots x_n^{k_n}$. We denote the gradient of a function f by $f^{(1)}$, and we denote the matrix of second partial derivatives of f by $f^{(2)}$. With a slight abuse of notation, we view $\mathbb{R}^n$ as a subset of $\mathbb{C}^n$, and let e_i denote the ith standard basis vector in $\mathbb{R}^n$ or $\mathbb{C}^n$. The inner product on $\mathbb{R}^n$ or $\mathbb{C}^n$ is $\langle v, w \rangle = \sum_{i=1}^{n} \bar{v}_i w_i$.

Our generalizations of the zeroth and first order Hermite polynomials are

$$\widetilde{\mathscr{H}}_0(x) = 1$$

and

$$\widetilde{\mathscr{H}}_1(v; x) = 2 \langle v, x \rangle,$$

where v is an arbitrary non-zero vector in $\mathbb{C}^n$. Our generalizations of the higher order Hermite polynomials are defined recursively as follows: Let $v_1, v_2, \ldots, v_m$ be m arbitrary non-zero vectors in $\mathbb{C}^n$. Then,

$$\widetilde{\mathscr{H}}_m(v_1, v_2, \ldots, v_m; x) = 2 \langle v_m, x \rangle \widetilde{\mathscr{H}}_{m-1}(v_1, v_2, \ldots, v_{m-1}; x)$$
$$- 2 \sum_{i=1}^{m-1} \langle v_m, \bar{v}_i \rangle \widetilde{\mathscr{H}}_{n-2}(v_1, \ldots, v_{i-1}, v_{i+1}, \ldots, v_{m-1}; x).$$

One can prove inductively that these functions do not depend on the ordering of the vectors $v_1, v_2, \ldots, v_m$. Furthermore, if the space dimension is $n = 1$ and the vectors $v_1, v_2, \ldots, v_m$ are all equal to $1 \in \mathbb{C}^1$, then

$\tilde{\mathscr{H}}_m(v_1, v_2, \ldots, v_m; x)$ is equal to the usual Hermite polynomial of order m, $H_m(x)$.

Now suppose A is a complex invertible $n \times n$ matrix. We define $|A| = [AA^*]^{1/2}$, where A^* denotes the adjoint of A. By the polar decomposition theorem, there exists a unique unitary matrix U_A so that $A = |A| U_A$. Given a multi-index k, we define the polynomial

$$\mathscr{H}_k(A; x) = \tilde{\mathscr{H}}_{|k|}(\underbrace{U_A e_1, \ldots, U_A e_1}_{k_1 \text{ entries}}, \underbrace{U_A e_2, \ldots, U_A e_2}_{k_2 \text{ entries}}, \ldots, \underbrace{U_A e_n, \ldots, U_A e_n}_{k_n \text{ entries}}; x).$$

We are now in a position to define the functions $\phi_k(A, B, \hbar, a, \eta, x)$.

DEFINITION. — Let A and B be complex $n \times n$ matrices with the following properties:

$$A \text{ and } B \text{ are invertible}; \tag{1.1}$$

$$BA^{-1} \text{ is symmetric ([real symmetric]} + i \text{[real symmetric]}); \tag{1.2}$$

$$\text{Re } BA^{-1} = \frac{1}{2}[(BA^{-1}) + (BA^{-1})^*] \text{ is strictly positive definite}; \tag{1.3}$$

$$(\text{Re } BA^{-1})^{-1} = AA^*. \tag{1.4}$$

Let $a \in \mathbb{R}^n$, $\eta \in \mathbb{R}^n$, $\hbar > 0$. Then for each multi-index k, we define

$$\begin{aligned}
\phi_k(A, B, \hbar, a, \eta, x) = {} & 2^{-|k|/2}(k!)^{-1/2}\pi^{-n/4}\hbar^{-n/4}[\det A]^{-1/2} \\
& \times \mathscr{H}_k(A; \hbar^{-1/2}|A|^{-1}(x - a)) \\
& \times \exp\{-\langle(x-a), BA^{-1}(x-a)\rangle/2\hbar + i\langle\eta, (x-a)\rangle/\hbar\}.
\end{aligned}$$

The choice of the branch of the square root of $[\det A]^{-1}$ in this definition will depend on the context, and will always be specified.

Remarks.

1. Whenever we write $\phi_k(A, B, \hbar, a, \eta, x)$, we tacitly assume that the conditions (1.1)-(1.4) are fulfilled.

2. Condition (1.4) can be rewriten in a more symmetrical way. It is equivalent to the condition

$$A^*B + B^*A = 2I,$$

where I is the $n \times n$ identity matrix.

3. We prove in § 2 that for fixed A, B, $\hbar$, a, and η, the functions $\phi_k(A, B, \hbar, a, \eta, x)$ form an orthonormal basis of $L^2(\mathbb{R}^n)$.

4. Generically, U_A and U_B are complex unitary matrices, and $|A|$ and $|B|$ are Hermitian. In the special cases in which they all happen to be real, the functions $\phi_k(A, B, \hbar, 0, 0, x)$ are simply rotated, scaled versions of the eigenfunctions of the n-dimensional harmonic oscillator.

5. The scaled Fourier transform which is appropriate for the semi-classical limit is

$$[\mathscr{F}_\hbar \Psi](\xi) = (2\pi\hbar)^{-n/2} \int_{\mathbb{R}^n} \Psi(x)e^{-i\langle \xi, x\rangle/\hbar}dx\,.$$

In § 2 we prove that

$$[\mathscr{F}_\hbar \phi_k(A, B, \hbar, a, \eta, .)](\xi) = (-i)^{|k|}e^{-i\langle \eta, a\rangle/\hbar}\phi_k(B, A, \hbar, \eta, -a, \xi)\,.$$

6. In the definition of the functions $\phi_k(A, B, \hbar, a, \eta, x)$, the only place in which the matrix B appears is in the exponent. Similarly, $\phi_k(B, A, \hbar, \eta, -a, \xi)$ depends on the matrix A only through the exponential factor. This property is crucial to our proofs. It also makes the result of Remark 5 rather amazing.

The main result of this paper is the following:

THEOREM 1.1. — Suppose $V \in C^{l+2}(\mathbb{R}^n), |V(x)| \leqslant C_1 e^{M|x|^2}$, and $V(x) \geqslant -C_2$, for some constants C_1, C_2, and M. Let $a_0 \in \mathbb{R}^n$, $\eta_0 \in \mathbb{R}^n$, and let A_0 and B_0 be $n \times n$ matrices satisfying (1.1)-(1.4). Given a positive integer J, a positive real number T, and complex numbers c_k for $|k| \leqslant J$, there exists a constant C_3 such that

$$\left\| e^{-itH(\hbar)/\hbar} \sum_{|k|\leqslant J} c_k\phi_k(A_0, B_0, \hbar, a_0, \eta_0, .)\right.$$

$$\left. - e^{iS(t)/\hbar} \sum_{|k|\leqslant J+3l-3} c_k(t, \hbar)\phi_k(A(t), B(t), \hbar, a(t), \eta(t), .)\right\| \leqslant C_3\hbar^{l/2} \quad (1.5)$$

whenever $|t| \leqslant T$ (det $A(t)$) is never zero, and the branch of the square root of (det $A(t))^{1/2}$ in the definition of $\phi_k(A(t), B(t), \hbar, a(t), \eta(t), x)$ is determined by continuity in t). Here $[A(t), B(t), a(t), \eta(t), S(t)]$ is the unique solution of the system of ordinary differential equations:

$$\frac{\partial \eta}{\partial t}(t) = -V^{(1)}(a(t))\,, \tag{1.6}$$

$$\frac{\partial a}{\partial t}(t) = \eta(t)/m\,, \tag{1.7}$$

$$\frac{\partial A}{\partial t}(t) = iB(t)/m\,, \tag{1.8}$$

$$\frac{\partial B}{\partial t}(t) = iV^{(2)}(a(t))A(t)\,, \tag{1.9}$$

$$\frac{\partial S}{\partial t}(t) = [\eta(t)]^2/2m - V(a(t))\,, \tag{1.10}$$

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 $c_k(t, \hbar)$ are the unique solution to the system of coupled ordinary differential equations

$$\frac{dc_k}{dt}(t, \hbar) = \sum_{0 \leqslant |j| \leqslant J + 3l - 3} \sum_{3 \leqslant |m| \leqslant l+1} -i\hbar^{(|m|-2)/2}(m!)^{-1}[D^m V](a(t)) \times b_{k,m,j}(A(t))c_j(t, \hbar), \quad (1.11)$$

subject to the initial conditions $c_k(0, \hbar) = c_k$ for $|k| \leqslant J$ and $c_k(0, \hbar) = 0$ for $J + 1 \leqslant |k|$. In this equation, the quantity $b_{k,m,j}(A)$ is a numerical quantity which is computed in the remarks below.

Remarks.

1. The quantity $b_{k,m,j}(A)$ is a product of some quantities which are related to the symmetric tensor representations of the matrices $|A|$, U_A, and $\overline{U_A}$. To explicitly compute these quantities, we need some notation. Given a sequence of integers $i_1, i_2, \ldots, i_N$ which satisfy $1 \leqslant i_j \leqslant n$, we define ind $(i_1, i_2, \ldots, i_N)$ to be the multi-index k with the property that the number j occurs in the sequence $i_1, i_2, \ldots, i_N$, exactly k_j times. Let A be a non-singular complex $n \times n$ matrix, and let k and m be multi-indices with $|k| = |m|$. We fix $j_1, j_2, \ldots, j_{|m|}$ so that ind $(j_1, j_2, \ldots, j_{|m|}) = m$, and define

$$d_{m,k}(A) = \left(\frac{k!}{m!}\right)^{1/2} \sum_{\substack{i_1, i_2, \ldots, i_{|k|} \\ \text{ind}(i_1,\ldots,i_{|k|})=k}} \overline{[U_A]_{i_1,j_1}[U_A]_{i_2,j_2}\cdots[U_A]_{i_{|k|},j_{|k|}}}.$$

In addition, let k, l, and m be any three multi-indices, and choose $i_1, i_2, \ldots, i_N$ with ind $(i_1, i_2, \ldots, i_N) = k$. Then we define

$$e_{l,k,m}(A) = \sum_{p=1}^{|k|} \sum_{j_p=1}^{n} \langle l, x^{j_1}x^{j_2}\cdots x^{j_{|k|}}m \rangle \prod_{q=1}^{|k|} |A|_{i_q,j_q},$$

where $\langle l, x^{j_1}x^{j_2}\cdots x^{j_{|k|}}m \rangle$ denotes the matrix element of $x^{j_1}x^{j_2}\cdots x^{j_{|k|}}$ in the usual harmonic oscillator basis (i. e., the basis $\{\phi_k(I, I, 1, 0, 0, x)\}$). With these definitions, the numerical quantity $b_{k,m,j}$ which appears in the theorem is:

$$b_{k,m,j}(A) = \sum_{\substack{|l|=|j| \\ |i|=|k|}} d_{j,l}(A)e_{l,m,i}(A)\overline{d_{i,k}(A)}.$$

2. The quantities in the above remark arise from the computation of the matrix elements

$$\langle \phi_k(A, B, \hbar, a, \eta, x), \quad (x-a)^m \phi_j(A, B, \hbar, a, \eta, x) \rangle.$$

These matrix elements do not depend on a or η, and the $\hbar$ dependence

scales out to give a factor of $\hbar^{|m|/2}$. The U_A dependence is in the quantity $d_{m,k}(A)$. It enters the computation through the formula:

$$\phi_m(A, B, 1, 0, 0, x)/\phi_0(A, B, 1, 0, 0, x)$$

$$= \sum_{|k| = |m|} d_{m,k}(A)\phi_k(I, I, 1, 0, 0, |A|^{-1}x)/\phi_0(I, I, 1, 0, 0, |A|^{-1}x).$$

The $|A|$ dependence is in the quantity

$$e_{l,k,m}(A) = \langle \phi_l(I, I, 1, 0, 0, |A|^{-1}x), \quad x^k\phi_m(I, I, 1, 0, 0, |A|^{-1}x) \rangle.$$

All of these formulas may be proved by using the definition of $\phi_k(A, B, \hbar, a, \eta, x)$, induction, and explicit computation.

3. As in [3] [4] [5] [6] [13], $A(t)$ and $B(t)$ are determined by the relations

$$A(t) = \frac{\partial a(t)}{\partial a(0)} A(0) + i\frac{\partial a(t)}{\partial \eta(0)} B(0)$$

$$B(t) = \frac{\partial \eta(t)}{\partial \eta(0)} B(0) - i\frac{\partial \eta(t)}{\partial a(0)} A(0)$$

4. One can prove another theorem which allows some infinite linear combinations of the functions $\phi_k(A, B, \hbar, a, \eta, x)$ if one is willing to do computations modulo errors on the order of $\hbar^{1/2}$. We have not stated this theorem here, since it is the obvious analog of Theorem 1.2 of [4]. Given the results of §2 of the present paper, it is easy to generalize the proof of Theorem 1.2 of [4] to the n-dimensional case.

5. One can generalize Theorem 1.1 to include more general Hamiltonians. Hamiltonians which are arbitrary smooth functions of $x, p = -i\nabla$, and t can be accommodated. In particular, one can include magnetic fields, or one can study problems with time dependent potentials which are quadratic in x and p (jointly). See e. g., [5] [13] and [6] for applications of these ideas.

In the rest of the paper we give the technical details necessary for the proof of Theorem 1.1. We do not actually give a proof of the theorem, since many of the steps are virtually identical to the analogous steps in the 1-dimensional case.

§ 2. THE TECHNICALITIES

In this section we give proofs of the crucial lemmas involving the properties of the functions $\phi_k(A, B, \hbar, a, \eta, x)$. We also present a very rough outline of the proof of Theorem 1.1. We do not give the full proof because

(once the lemmas are proved) it is essentially identical to the proof of Theorem 1.1 of [4].

LEMMA 2.1. — The functions $\phi_k(A, B, \hbar, a, \eta, x)$ form an orthonormal basis of $L^2(\mathbb{R}^n)$.

Proof. — By scaling out the $|A|$ dependence of the functions $\phi_k(A, B, \hbar, a, \eta, x)$, we need only prove this lemma for the case in which $|A| = I$. Furthermore, because of relation (1.4), the value of B is irrelevant in the computation of inner products of the ϕ_k's with one another. So, we can assume $B = I$, also. Similarly, it is sufficient to consider only the case of $\eta = 0$ and $\hbar = 1$. Let $\omega_j = U_A e_j$ for $1 \leqslant j \leqslant n$. Define $a(\omega_j)$ to be the differential operator $a(w_j) = \langle \overline{w_j}, x \rangle + \langle \overline{w_j}, \nabla \rangle$ defined on the Schwartz space $\mathscr{S}(\mathbb{R}^n)$, and let $a(w_j)^*$ be its adjoint. On Schwartz space, $a(w_j)^*$ acts as the differential operator $a(w_j)^* = \langle w_j, x \rangle - \langle w_j, \nabla \rangle$. The self-adjoint operators $N(w_j) = a(w_j)^* a(w_j)$ for $1 \leqslant j \leqslant n$ are easily seen to commute with one another. Suppose $v_1, v_2, \ldots, v_m$ are chosen from the set (w_j). Then, by explicit computation.

$$a(w_j)\widetilde{\mathscr{H}}_m(v_1, v_2, \ldots, v_m; x)e^{-x^2/2}$$

$$= 2 \sum_{i=1}^m \langle \overline{w_j}, \overline{v_i} \rangle \widetilde{\mathscr{H}}_{m-1}(v_1, \ldots, v_{i-1}, v_{i+1}, \ldots, v_m; x)e^{-x^2/2},$$

and

$$a(w_j)^* \widetilde{\mathscr{H}}_m(v_1, v_2, \ldots, v_m; x)e^{-x^2/2} = \widetilde{\mathscr{H}}_{m+1}(v_1, \ldots, v_m, w_j; x)e^{-x^2/2}.$$

From these relations it is easy to see that

$$N(w_j)\widetilde{\mathscr{H}}_m(v_1, v_2, \ldots, v_m; x)e^{-x^2/2} = 2 \sum_{i=1}^n \langle \overline{w_j}, \overline{v_i} \rangle \widetilde{\mathscr{H}}_m(v_1, v_2, \ldots, v_m; x)e^{-x^2/2}.$$

Thus, $\widetilde{\mathscr{H}}_m(v_1, v_2, \ldots, v_m; x)e^{-x^2/2}$ is an eigenfunction of $N(w_j)$ with eigenvalue equal to twice the number of occurrances of w_j in the sequence $v_1, v_2, \ldots, v_m$. Since this is true for each j, and the $N(w_j)$'s are commuting self-adjoint operators, the functions $\phi_k(A, B, \hbar, a, \eta, x)$ are orthogonal.

The function $\widetilde{\mathscr{H}}_m(v_1, v_2, \ldots, v_m; x)e^{-x^2/2}$ is equal to

$$a(v_1)^* a(v_2)^* \ldots a(v_m)^* e^{-x^2/2},$$

so using the relations given above, one can easily see that the functions $\phi_k(A, B, \hbar, a, \eta, x)$ are properly normalized.

To prove the completeness of the functions $\phi_k(A, B, \hbar, a, \eta, x)$, one should note that the operator $\sum_{j=1}^n N(w_j) = -\Delta + x^2$ is simply twice the usual

Harmonic oscillator Hamiltonian. The states $\phi_k(A, B, 1, 0, 0, x)$ are eigenfunctions if $|A| = I$, and for each eigenvalue, one easily sees that there are as many $\phi_k(A, B, 1, 0, 0, x)$'s as the dimension of the corresponding eigenspace. ■

LEMMA 2.2. — Let $[\mathscr{F}_\hbar \Psi](\xi) = (2\pi\hbar)^{-n/2} \int_{\mathbb{R}^n} \Psi(x) e^{-i\langle \xi, x\rangle/\hbar} dx.$

Then $[\mathscr{F}_\hbar \phi_k(A, B, \hbar, a, \eta, \cdot)](\xi) = (-i)^{|k|} e^{-i\langle \eta, a\rangle/\hbar} \phi_k(B, A, \hbar, \eta, -a, \xi).$

Proof. — By elementary manipulations, it is sufficient to consider the case $\hbar = 1$, $a = \eta = 0$. For the cases $|k| = 0, 1$, we prove the lemma by explicit calculation. For the larger values of $|k|$, we use induction and the following two formulas:

$$\widetilde{\mathscr{H}}_{m+1}(v_1, v_2, \ldots, v_{m+1}; x) = 2\langle v_{m+1}, x\rangle \widetilde{\mathscr{H}}_m(v_1, v_2, \ldots, v_m; x)$$

$$-2\sum_{i=1}^{m} \langle v_{m+1}, \bar{v}_i\rangle \widetilde{\mathscr{H}}_{m-1}(v_1, \ldots, v_{i-1}, v_{i+1}, \ldots, v_m; x),$$

and

$$\langle w, \nabla\rangle \widetilde{\mathscr{H}}_m(v_1, v, \ldots, v_m; x) = 2\sum_{i=1}^{m} \langle w, \bar{v}_i\rangle \widetilde{\mathscr{H}}_{m-1}(v_1, \ldots, v_{i-1}, v_{i+1}, \ldots, v_m; x).$$

The only difficult step in the induction is the following: Assume the lemma is correct for all multi-indices m with $|m| \leqslant M$, and let k be a multi-index with $|k| = M + 1$. Choose vectors $v_j = e_{i_j}$ for $1 \leqslant j \leqslant M + 1$, so that ind $(i_1, i_2, \ldots, i_{M+1}) = k$. Let $u_j = U_A v_j$, $w_j = U_B v_j$, and $C_k = 2^{-|k|/2}(k!)^{-1/2}\pi^{-n/4}$. Then,

$C_k^{-1}(2\pi)^{n/2}[\mathscr{F}_1 \phi_k(A, B, 1, 0, 0, \cdot)](\xi)$

$$= [\det A]^{-1/2} \int \widetilde{\mathscr{H}}_{M+1}(u_1, u_2, \ldots, u_{M+1}; |A|^{-1}x)$$
$$\times \exp\{-\langle x, BA^{-1}x\rangle/2 - i\langle \xi, x\rangle\} dx$$

$$= [\det A]^{-1/2} \int [2\langle u_{M+1}, |A|^{-1}x\rangle \mathscr{H}_M(u_1, u_2, \ldots, u_M; |A|^{-1}x)$$

$$-2\sum_{j=1}^{M} \langle u_{M+1}, \overline{u}_j\rangle \mathscr{H}_{M-1}(u_1, \ldots, u_{j-1}, u_{j+1}, \ldots, u_M; x)]$$
$$\times \exp\{-\langle x, BA^{-1}x\rangle/2 - i\langle \xi, x\rangle\} dx$$

$$= [\det A]^{-1/2} \int 2\langle |A|^{-1}u_{M+1}, x\rangle \mathscr{H}_M(u_1, u_2, \ldots, u_M; |A|^{-1}x)$$
$$\times \exp\{-\langle x, BA^{-1}x\rangle/2 - i\langle \xi, x\rangle\} dx$$

$$-2\sum_{j=1}^{M} \langle u_{M+1}, \overline{u}_j\rangle [\det A]^{-1/2} \int \widetilde{\mathscr{H}}_{M-1}(u_1, \ldots, u_{j-1}, u_{j+1}, \ldots, u_M; x)$$
$$\times \exp\{-\langle x, BA^{-1}x\rangle/2 - i\langle \xi, x\rangle\} dx$$

$$= [\det A]^{-1/2} \int 2 \langle |A|^{-1}u_{M+1}, i\nabla_\xi \rangle \tilde{\mathscr{H}}_M(u_1, u_2, \ldots, u_M; |A|^{-1}x)$$
$$\times \exp\{-\langle x, BA^{-1}x\rangle/2 - i\langle \xi, x\rangle\}\, dx$$
$$- 2\sum_{j=1}^M \langle u_{M+1}, \overline{u}_j\rangle \frac{(2\pi)^{n/2}}{C_{k_{j,M+1}}} [\mathscr{F}_1 \phi_{k_{j,M+1}}(A, B, 1, 0, 0, .)](\xi)$$

$$= \frac{(2\pi)^{n/2}}{C_{k_{M+1}}} 2i \langle |A|^{-1}u_{M+1}, \nabla_\xi \rangle [\mathscr{F}_1 \phi_{k_{M+1}}(A, B, 1, 0, 0, .)](\xi)$$

$$- 2\sum_{j=1}^M \langle u_{M+1}, \overline{u}_j\rangle \frac{(2\pi)^{n/2}}{C_{k_{j,M+1}}} [\mathscr{F}_1 \phi_{k_{j,M+1}}(A, B, 1, 0, 0, .)](\xi),$$

where $\quad k_{M+1} = \text{ind}\,(i_1, \ldots, i_M)$

and $\quad k_{j,M+1} = \text{ind}\,(i_1, \ldots, i_{j-1}, i_{j+1}, \ldots, i_M).$

By the induction hypothesis, this is equal to

$$2(-i)^M i(2\pi)^{n/2} \langle |A|^{-1}u_{M+1}, \nabla_\xi \rangle [\det B]^{-1/2}$$
$$\times \tilde{\mathscr{H}}_M(w_1, w_2, \ldots, w_M; |B|^{-1}\xi) \exp\{-\langle \xi, AB^{-1}\xi\rangle/2\}$$

$$- 2(-i)^{M-1}(2\pi)^{n/2} \sum_{j=1}^M \langle u_{M+1}, \overline{u}_j\rangle [\det B]^{-1/2}$$

$$\times \tilde{\mathscr{H}}_{M-1}(w_1, \ldots, w_{j-1}, w_{j+1}, \ldots, w_M; |B|^{-1}\xi) \times \exp\{-\langle \xi, AB^{-1}\xi\rangle/2\}$$

$$= 2(-i)^{M+1}(2\pi)^{n/2} [\det B]^{-1/2} \langle |A|^{-1}u_{M+1}, AB^{-1}\xi \rangle$$
$$\times \tilde{\mathscr{H}}_M(w_1, w_2, \ldots, w_M; |B|^{-1}\xi) \exp\{-\langle \xi, AB^{-1}\xi\rangle/2\}$$

$$- 4(-i)^{M+1}(2\pi)^{n/2} [\det B]^{-1/2} \sum_{j=1}^M \langle |A|u_{M+1}, |B|^{-1}\overline{w}_j \rangle$$

$$\times \tilde{\mathscr{H}}_{M-1}(w_1, \ldots, w_{j-1}, w_{j+1}, \ldots, w_M| B|^{-1}\xi) \exp\{-\langle \xi, AB^{-1}\xi\rangle/2\}$$

$$+ 2(-i)^{M+1}(2\pi)^{n/2} [\det B]^{-1/2} \sum_{j=1}^M \langle u_{M+1}, \overline{u}_j \rangle$$

$$\times \tilde{\mathscr{H}}_{M-1}(w_1, \ldots, w_{j-1}, w_{j+1}, \ldots, w_M; |B|^{-1}\xi) \times \exp\{-\langle \xi, AB^{-1}\xi\rangle/2\}$$

$$= 2(-i)^{M+1}(2\pi)^{n/2} [\det B]^{-1/2} \langle w_{M+1}, |B|^{-1}\xi \rangle$$
$$\times \tilde{\mathscr{H}}_M(w_1, w_2, \ldots, w_M; |B|^{-1}\xi) \exp\{-\langle \xi, AB^{-1}\xi\rangle/2\}$$

$$+ 2(-i)^{M+1}(2\pi)^{n/2} [\det B]^{-1/2}$$

$$\times \sum_{j=1}^M \left[\langle u_{M+1}, \overline{u}_j \rangle - 2\langle e_{i_{M+1}}, A^{-1}(B^t)^{-1}\overline{v_{i_j}} \rangle \right]$$

$$\times \ \tilde{\mathscr{H}}_{M-1}(w_1, \ldots, w_{j-1}, w_{j+1}, \ldots, w_M; |B|^{-1}\xi) \times \exp\{-\langle \xi, AB^{-1}\xi \rangle /2\}$$
$$= (-i)^{M+1}(2\pi)^{n/2} \ [\det B]^{-1/2}\tilde{\mathscr{H}}_{M+1}(w_1, \ldots, w_{M+1}; |B|^{-1}\xi)$$
$$\times \exp\{-\langle \xi, AB^{-1}\xi \rangle /2\}$$
$$= (-i)^{|k|}C_k^{-1}(2\pi)^{n/2} \phi_k(B, A, 1, 0, 0, \xi).$$

With one exception, all the steps are either straightforward applications of standard facts about the Fourier transform or applications of the identities given above. That exception occurs in the second to last step, where we have used the identity:

$$(U_A)^* \overline{U_A} - 2A^{-1}(B^t)^{-1} = -(U_B)^* \overline{U_B}.$$

By using the polar decompositions of A and B, we see that this identity is equivalent to the first equality in the identity

$$A^*(A^t)^{-1} + B^*(B^t)^{-1} = 2A^{-1}(B^t)^{-1} = 2B^{-1}(A^t)^{-1}.$$

This identity is proved as follows: By condition (1.2), we have $B^t A = A^t B$. If we take inverses on both sides of this equation, we obtain

$$A^{-1}(B^t)^{-1} = B^{-1}(A^t)^{-1} = C.$$

As in Remark 2 after the definition of the ϕ_k's, condition (1.4) is equivalent to $A^*B + B^*A = 2I$. We multiply this identity on the right by the two forms of the matrix C to obtain the desired identity. ∎

Given the two lemmas above, the proof of Theorem 1.1 is obtained by closely mimicking the proof of Theorem 1.1 of [4]. One uses the Trotter Product Formula to separate the effects of the kinetic and potential terms in the Hamiltonian. Then one expands the potential in its Taylor series of order $l + 1$ about the point $a(t)$. The errors committed are of order $\hbar^{l/2}$ due to the $\hbar$ dependence of the functions $\phi_k(A, B, \hbar, a, \eta, x)$. The terms of order less than or equal to 2 in the kinetic energy and the approximate potential give rise to the equations (1.6)-(1.10). The higher order terms from the approximate potential give rise to the system (1.11). There is an additional error of order $\hbar^{l/2}$ due to the fact that we have truncated the sums which occur in the system (1.11) in order to avoid dealing with an infinite system.

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