STATEMENT OF PURPOSE

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1. Semiclassical Limit

My thesis work, under the direction of Professor Bruce Driver, is primarily devoted to the study of classical limits of quantum mechanics. Intuitively, as Planck's constant ($\hbar$) tends to zero, quantum mechanics should reduce to the laws of classical mechanics; this is the semiclassical limit which was first shown by P. Ehrenfest in [6] and Hepp in [14]. There is a large literature devoted to this topic, for a small sample see [15, 20, 18, 1, 2, 16, 7, 3, 13]. The goal of some of the literature, e.g. [9, 10, 11, 12, 8], is to approximate the solution to Schrödinger's equation by a list of parameters obtained from classical mechanics if the scale of Planck's constant $\hbar$ is insignificant within a system. Alternatively, it may be more important and interesting if experimental measurement from quantum mechanics, such as the prediction of the position of a particle, can be approximated by using only knowledge of classical mechanics. The approximation of measurements has applications in many areas, such as the computation of the $N-$ body problem, quantum dynamics, and the simulation of tunneling effect of quantum mechanics (see Figures 1.1, 1.2 and [17]).

Our work is inspired by Hepp's method in [14] and the technique of Rodnianski and Schlein's method for unbounded observables in [18]. Let $P_{\hbar}(t)$ be a time-dependent observable (possibly an unbounded linear operator) whose dynamics are governed by a Hamiltonian operator $H_{\hbar}$. For an initial state ψ which is normalized and concentrated near a point $\alpha = (q_0, p_0)$ in the position-momentum space, the quantum expectation of $P_{\hbar}(t)$ to state ψ, denoted by $\langle P_{\hbar}(t)\rangle_{\psi}$, can be considered as a function of $\hbar$ with fixed t. The main result in [4] shows that under certain conditions of $H_{\hbar}$, the quantum expectation $\langle P_{\hbar}(t)\rangle_{\psi}$ can be treated as a "Taylor series" with respect to $\hbar$ i.e.

$$\langle P_{\hbar}(t)\rangle_{\psi} = f(t) + \sqrt{\hbar} g(t) + O(\hbar). \tag{1.1}$$

where the classical limit $f(t)$ and the quantum fluctuation $g(t)$ are determined by the classical Hamiltonian equation and the linearization of the classical system respectively. From Eq. (1.1) the quantum expectation not only converges to the classical limit when $\hbar$ tends to 0, but also the first order approximation error of the quantum expectation described by the quantum fluctuation solely depends on classical mechanics, too. Another important consequence of Eq. (1.1) is the independence of any choice of quantization scheme. If two different quantizations $H_{\hbar}$ and $\widetilde{H}_{\hbar}$ both satisfy the conditions of Eq. (1.1) and their classical Hamiltonian functions are equal modulo a constant, then the quantum expectations relative to H and $\tilde{H}$ have the same classical limit and the quantum fluctuation. Interested readers may refer to Subsection 1.1 for a more detailed statement of the main result.

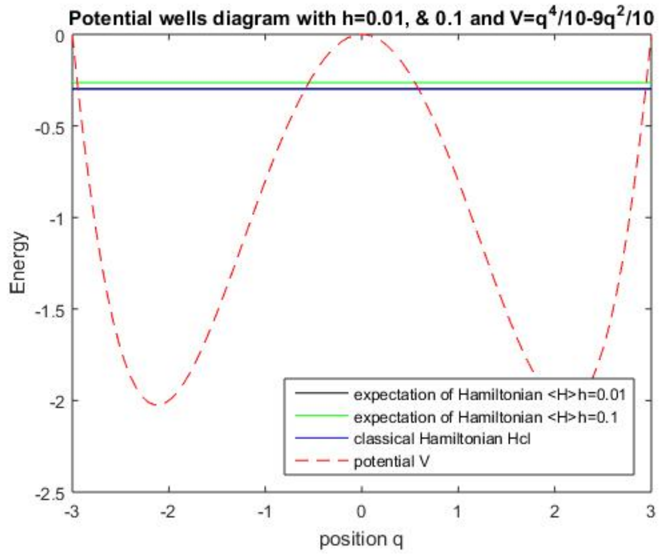

FIGURE 1.1. A simulation of a classical Hamiltonian function $H^{cl} = \frac{p^2}{2} + V(q)$ and Hamiltonian operator $H_\hbar = -\frac{\hbar}{2}\frac{d^2}{dx^2} + V(q)$. Classical energy H^{cl}, expected quantum energy $\langle H_\hbar \rangle|_{\hbar=0.1}$ and expected quantum energy $\langle H_\hbar \rangle|_{\hbar=0.01}$ cannot overcome the local peak barrier. f.3

Assume the Hamiltonian operator $H_\hbar$ is non-negative and self-adjoint and let $\mathcal{N}_\hbar = \hbar\mathcal{N}$, where $\mathcal{N}$ is the closure of $-\frac{1}{2}\frac{d^2}{dx^2} + \frac{x^2}{2} - \frac{1}{2}$. The key assumption for the main result in [4] is that for all $\beta \geq 0$, there exists $C_\beta < \infty$ such that

$$\left\langle \mathcal{N}_\hbar^\beta \psi, \psi \right\rangle \leq C_\beta \left\langle H_\hbar^\beta \psi, \psi \right\rangle \text{ for all } \psi \in D\left(H_\hbar^\beta\right), \tag{1.2}$$

equ.1.2

where $\langle \cdot, \cdot \rangle$ is the standard L^2 inner product with respect to Lebesgue measure. One natural example of $H_\hbar$ satisfying Eq. (1.2) is a polynomial of $N_\hbar$ with a positive leading coefficient and degree at least 1 (see Proposition 1.11 in [4]). This $H_\hbar$ is a finite dimensional analogue of the type of Hamiltonian found in multiple papers which study Bose-Einstein condensation, see for example, [1, 18]. In general, it is difficult to check the condition in Eq. (1.2) for other classes of Hamiltonian operators. However, two main results in [5] show that the operator inequality of Eq. (1.2) does indeed hold for a large class of Hamiltonian operators which is contained in the collection of differential operators with polynomial coefficients. [This class of operators contains differential operators of arbitrary even order.] For this class of operators, the first result (see Theorem 1.9 in [5]) is that the Schwartz space is a core for $H_\hbar^\beta$ for $\beta \geq 0$; the second result (see Corollary 1.20 in [5]) finds sufficient conditions on the polynomial coefficients of two operators, $H_\hbar$ and $\tilde{H}_\hbar$, in this class so that the operator inequality of Eq. (1.2) holds with $\mathcal{N}_\hbar$ is replaced by $\tilde{H}_\hbar$. Thus, Eq. (1.2) is a special case of the second result (see Corollary 1.23 in [5]). Moreover, this second result can be thought of as an "extension" of the Löwner-Heinz inequality. Indeed, if $H_\hbar \geq \tilde{H}_\hbar$ (in the sense described in Eq. (1.2) with $\beta = 1$), then the Löwner-Heinz inequality shows $H_\hbar^\beta \geq \tilde{H}_\hbar^\beta$ for $0 \leq \beta \leq 1$. The second

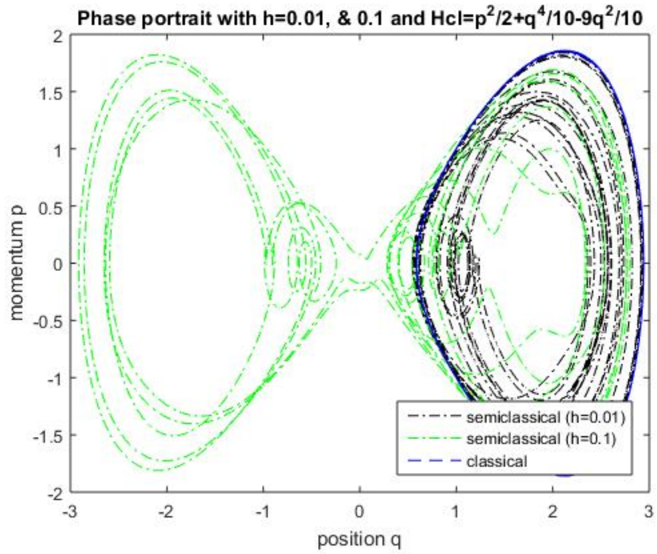

FIGURE 1.2. A figure eight shaped phase orbit corresponding to semiclassical mechanics with $\hbar = 0.1$ indicates that a particle can jump from one well to another in Figure f.3 1.1 even though the energy of the particle is lower than the local peak barrier. This is the tunneling effect in quantum mechanics. Moreover, by comparing between the two phase orbits with $\hbar = 0.1$ and $\hbar = 0.01$, a phase orbit corresponding to semiclassical mechanics converges to the phase orbits corresponding to classical mechanics as $\hbar \to 0$. f.4

result mentioned above shows a similar inequality holds (under our assumptions) for $\beta > 1$ even though the function $x \to x^{\beta}$ is non "operator monotone."

sub.1.1 1.1. **Technical result.** This subsection fills in some of the mathematical details of the above description of the main result of [4]. Let $L^2(m) := L^2(\mathbb{R}, dx)$ be the Hilbert space of square integrable functions on $\mathbb{R}$ equipped with the standard L^2-inner product $\langle \cdot, \cdot \rangle$ relative to Lebesgue measure. Let $a_\hbar = \sqrt{\frac{\hbar}{2}}(M_x + \partial_x)$ with domain $D(a_\hbar) = \mathcal{S}$ (Schwartz space) and $a_\hbar^\dagger := a_\hbar^\dagger|_{\mathcal{S}}$ (the formal adjoint of $a_\hbar$) be the annihilation and creation operators on $L^2(m)$ respectively. Let $P = P\left(a_\hbar, a_\hbar^\dagger\right)$ be an (unbounded) observable where $P(\theta, \theta^*) \in \mathbb{C}\langle \theta, \theta^* \rangle$ – the space of non-commutative polynomials in θ and θ^* with complex coefficients. Further let $P_\hbar(t) := e^{iH_\hbar t/\hbar} P\left(a_\hbar, a_\hbar^\dagger\right) e^{-iH_\hbar t/\hbar}$ be the observable P in the "Heisenberg picture" where $e^{-iH_\hbar t/\hbar}$ is the Schrödinger evolution associated to the self-adjoint Hamiltonian operator, $H_\hbar$.

cor.1 **1.1.** *[A Simplified version of Corollary 1.18 in [4]] Let* $H(\theta, \theta^*) \in \mathbb{R}\langle \theta, \theta^* \rangle$ *(*$\mathbb{R}\langle \theta, \theta^* \rangle \subset \mathbb{C}\langle \theta, \theta^* \rangle$ *is the collection of non-commutative polynomials in* θ *and* θ^* *with real coefficients) be a symmetric non-commutative polynomial with* $d = \deg H > 0$. *Suppose there exists constants* $1 \geq \eta > 0$ *and* $C_\beta > 0$ *for* $\beta \geq 0$ *such that for all* $\hbar \in (0, \eta)$,

(1) $H_\hbar := \overline{H\left(a_\hbar, a_\hbar^\dagger\right)}$ *is self-adjoint and* $H_\hbar \geq I$, *and*
(2) *Eq.* (1.2) *holds.*

Let $\alpha_0 \in \mathbb{C}$, $t \in \mathbb{R}$, $P(\theta,\theta^*) \in \mathbb{C}\langle \theta, \theta^* \rangle$ *and* $\psi \in \mathcal{S}$ *be an* $L^2(m)$ *– normalized state. If*

(1) $\alpha(t) \in \mathbb{C}$ *is the solution to Hamilton's (classical) equations of motion*

$$i\dot{\alpha}(t) = \frac{\partial H^{cl}}{\partial \overline{\alpha}}(\alpha, \overline{\alpha}) \quad \text{and } \alpha(0) = \alpha_0$$

where $H^{cl}(\alpha,\overline{\alpha}) = H(\alpha,\overline{\alpha})$ *is the classical Hamiltonian function associated to* $H(\theta,\theta^*)$,
(2) $a(t) = \gamma(t)\, a_1 + \delta(t)\, a_1^\dagger$ *where* $\gamma(t)$ *and* $\delta(t)$ *are determined by the linearization of* $\alpha(t)$ *relative to initial position, and*
(3) $A_\hbar(t)$ *denotes* $a_\hbar$ *in the Heisenberg picture, i.e.*

$$A_\hbar(t) := e^{iH_\hbar t/\hbar} a_\hbar e^{-iH_\hbar t/\hbar},$$

then for $0 < \hbar < \eta$, *we have*

$$\begin{aligned} &\left\langle P\left(A_\hbar(t), A_\hbar^\dagger(t)\right)\right\rangle_{U_\hbar(\alpha_0)\psi} \\ &= \left\langle P\left(\alpha(t) + \sqrt{\hbar}a(t), \overline{\alpha}(t) + \sqrt{\hbar}a^\dagger(t)\right)\right\rangle_\psi + O(\hbar). \end{aligned} \tag{1.3}$$

equ.1.24

1.2. Corollary 1.18 in [4] can even approximate the quantum expectation of the observable P in Eq. (1.3) at multiplie times $\{t_i\}_{i=1}^n$ simultaneously.

1.2. **Future Research Plan.** There are a number of ways which we plan to generalize our work. We believe that, by using the same approach as in the one dimensional case, Corollary 1.1 can be extended to $L^2(\mathbb{R}^n)$ for any $n \in \mathbb{N}$ if the Hamiltonian $H_\hbar$ satisfies the multi-dimensional version of conditions in Corollary 1.1. Our long-term goal is to develop theorems about the semiclassical limit in an infinite dimensional space which corresponds to a quantum field setting. However, the transition from a finite dimensional space to an infinite dimensional space gives way to some new problems. In particular, one must define a correct formulation of convergence in this setting. For example, one must determine the most appropriate infinite dimensional space and the norm to study the convergence for the semiclassical limit problems. Another main issue is the construction of examples of Hamiltonian operator $H_\hbar$ satisfying an infinite dimensional version of conditions in Corollary 1.1.

Another direction of our project is to prove Corollary 1.1 for a wider class of Hamiltonian operators $H_\hbar$, and give some criteria on $H_\hbar$ so that Eq. (1.2) holds. Loosely speaking, Corollary 1.1 only is valid for a Hamiltonian operator $H_\hbar$ which is a polynomial of $a_\hbar$ and $a_\hbar^\dagger$. However, some potential functions in quantum mechanics are not polynomials or even may have singularities, e.g. the Coulomb potential. Another generalization of Corollary 1.1 is to eliminate the condition that $H_\hbar$ is a non-commutative polynomial in $a_\hbar$ and $a_\hbar^\dagger$. Other conditions of $H_\hbar$, e.g. a growth control of derivatives of the potential function in $H_\hbar$, are likely required in order to ensure Corollary 1.1 is still valid if $H_\hbar$ is no longer a polynomial. Finding the necessary conditions and examples of $H_\hbar$ other than polynomials satisfying the conditions are main goals of our project. Moreover, verification of a Hamiltonian operator satisfying Eq. (1.2) may be difficult in general. However, we conjecture that if two Hamiltonian operators arise from the same classical Hamiltonian function modulo a constant, then one Hamiltonian operator satisfying Eq. (1.2) will be sufficient to show that the other Hamiltonian operator satisfies the same Eq. (1.2). Proving conjecture may ease checking Eq. (1.2) because some quantizations may have a form well-suited to compute Eq. (1.2) relative to others.

As discussed above, studying semiclassical limit can simplify computations in some problems in quantum mechanics, e.g. a quantum expectation or the solution to the Schrödinger's equation. An additional interest of mine is to develop a numerical scheme to approximate the quantum expectation in Eq. (1.3) stably at a rate faster than $O\left(\sqrt{\hbar}\right)$. The rate of convergence depends on a state function ψ, Hamiltonian operator $H_\hbar$, observable P, time $t_i \in \mathbb{R}$ and initial condition α_0. Therefore, we would like to determine if Corollary 1.1 can be extended to have a faster convergence rate; this would identify what sets of $(\psi, H_\hbar, P, , t_i, \alpha_0)$ should be picked to achieve the faster convergence. Moreover, even if $O\left(\sqrt{\hbar}\right)$ is the optimal rate of convergence in our approach, there may be other robust ways to approximate the quantum expectation at a rate $O\left(\hbar^r\right)$ where $r > \frac{1}{2}$ (see [9, 10, 11, 12, 18]).

2. Prediction of patients ' survival rate by random forest

In addition to my primary research, I am involved in a joint project with Postdoc Samad Jahandideh and Professor Adam Godzik at the Sanford Burnham Prebys Medical Discovery Institute. Cancer cells and normal cells have different protein expression; functional proteomics is a powerful approach utilizing this idea to understand the pathophysiology and therapy of cancer. Our goal is to build a novel model to predict cancer patients' survival rate, cancer stages and remaining lifespan based on functional cancer proteomics data. Unlike traditional approaches that consider one type of functional proteomics at a time, we propose to base predictions on multiple functional proteomics and their interactions to make accurate predictions for each patient. This is a machine learning problem in a high dimensional features space where each feature may depend on each other. A random forest (RF) algorithm is a base of our model as it can be successfully applied to high-dimensional and noisy large biomedical data sets. In order to improve the performance of RF and eliminate noise in data, we develop a strategy to select an optimal set of features for our biomedical data to train the model and make predictions. The initial process entailed reducing to a set of features with a large decrease in Gini Index which optimized the AUC (area under the ROC curve). From here, we manufactured new features based on the exponential ratio among the features in this reduced set and combined the new features with features in the reduced set together. Working with this increased set, we again trimmed to an optimal set by examining the Gini Index and AUC as our metrics. By using the optimal set of features with our RF algorithm, performance measures, e.g. sensitivity, specificity, Mathews correlation coefficient (MCC) and AUC, all improved (see [19]). I am interested in continuing research in this area.

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