Quantum Fluid Dynamics from Path Integrals

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In this work we develop analytical solutions to the general problem of computing Quantum Trajectories, within the framework of quantum fluid dynamics (QFD). The state-of-the-art technique in the field is to simultaneously solve the non-linear, coupled partial differential equations (PDEs) numerically. We, however, set off from Feynman Path Integrals, and analytically compute the propagator for a general system. This, then, is used to compute the Quantum Potential, which can generate Quantum Trajectories. For cases, where closed form solution is not possible, the problem is shown to be reducible to a single real-valued numerical integration (linear time complexity). The work formally bridges the Path Integral approach with Quantum Fluid Dynamics. As a model application to illustrate the method, we solve for the Quantum Potential of Quartic Anharmonic Oscillator, and delve in seeking insight into one of the long standing debates with regard to Quantum Tunneling.

I. INTRODUCTION

The hydrodynamic formulation of Quantum Mechanics is fulcrummed upon the Madelung Transformation$^1$. The computational methods in the field has historically played an important role owing to the analytical complexity in the attempts of developing solutions. Bohm$^2$ had suggested that the best way to analytically obtain the Quantum Potential(QP), which serves as the quantum correction term in the Hamilton-Jacobi framework of Quantum Fluid Dynamics (QFD), is to solve the time dependent Schrodinger’s equation first. This has been considered to be the most serious drawback of QFD; what point may extra computations serve when the solution of the Schrodinger Equation contains all the physically relevant information anyway. Till date this has been addressed mainly by computational remedies.$^3$ The current algorithms generally involve simultaneously solving set of non-linear coupled partial differential equations (PDEs) using either grids or basis sets. One of the difficulties in computation arises from the presence of spatial derivatives quantities, which are solved for. This often tends to make the grid unstructured after a short while.

QFD, however, has found applications in a wide spectrum of branches in Physics and chemistry. In the last half a century, it has made appearances in Quantum Foundations, theoretical Condensed Matter Physics, Nuclear Physics$^5$, Quantum Optics, Quantum transport, Computational Chemistry$^6$, in the foundations of time-dependent Density Functional Theory$^7$, study of photo-dissociation$^8$. Recently, it has been extended to the study of analogue gravity$^9$ and modelling of experimental systems of Quantum Superfluids of Light$^{10}$.

In the context of this recent upsurge in interest, we reopen the analytical quest. With the invoked question of practicality in mind, in this paper we raise the question whether there exists an analytical method of obtaining the Quantum Potential without solving the Schrodinger’s equation, and attempt a rigorous answer to it.

II. THEORY

Our derivation sets off from the Feynman theory of Path Integrals$^{12,13}$. In this paper, we present an exact analytic form for the propagator (two-point correlator) for a general applied potential. In Path Integral formalism, the correlator gives the amplitude at a point $x$, after a time of flight $t$, given it has started from an initial point $y$. This propagator serves as a Green’s function to the Schrodinger Equation$^{14}$ which renders Path Integrals its formal equivalence with the Schrodinger formulation. Equipped with this, we pose the solution to quantum trajectories, in an integral equation framework.

We exploit the Madelung transformation$^{11}$, which had opened a possibility of looking at the quantum systems as probability fluids, by decoupling the Schrodinger equation into the following two equations$^{15}$:

$$\nabla (\rho v) + \frac{\partial \rho}{\partial t} = 0$$

(1)

$$-\frac{\partial S}{\partial t} = \frac{1}{2}mv^2 + V(x,t) + Q(x,t)$$

(2)

where the quantum potential, $Q(x,t)$ is given by,

$$Q(x,t) = -\frac{\hbar^2}{2m} \nabla^2 R(x,t)$$

(3)

In the work presented through this communication we look for footing of the QP$^5$, in the Feynman Path Integrals, with the aim of developing formal analytic expression for former in terms of the applied potential and Cauchy data.

According to Path Integral approach, the dynamics of a particle from one point to another, is contributed by all the possible paths that connects them; their contributions being weighted by exp $\frac{iS[x]}{\hbar}$, where $S(x(t))$ is the action or Hamilton’s principal function associated with the corresponding path. The net propagator $K(x_b,t;x_a,0)$ is obtained by summing the
contributions of all paths. The integral
\[ \Psi(x_b,t) = \int_{x_a}^{x_b} K(x_b,t;x_a,0)\Psi_0(x_a)dx_a \]  \hspace{1cm} (4)
gives the time evolution of the wave-function.

To elaborate the scheme of unification, we consider a particle with mass \( m \), moving in one dimension under the action of a conservative force generated by potential \( V(x) \). The Path-Integral formulation postulates that the particle can opt for any possible path from its initial position \( x_i \), to a final position \( x_f \) after a time of flight, \( t \). Let \( x(t) \) be such a general path. Any such general path can be broken down as
\[ x(t) = x^c(t) + y(t). \]  \hspace{1cm} (5)
where \( x^c(t) \) is the corresponding action-minimized classically legal path. Varying \( y(t) \) to span the space of continuous functions on \([t_0, t]\) subjected to the boundary conditions,
\[ y(t_0) = y(t_f) = 0 \]
is tantamount to spanning the space of allowed paths of Path Integral formulation, over which we need to integrate in order to obtain the propagator.

One way to compute the path integral is to first discretise time into \( n \) moments.
\[ t_0 = 0; t_i = i\epsilon; t_n = t \]
Equation (5) then becomes,
\[ x(t_i) = x(t) = x^c_i + y_i. \]  \hspace{1cm} (6)
at each of these moments. The potential over the general path can be Taylor expanded around the classical position at each of these moments:\[ V(x_i) = V(x^c_i + y_i) = V(x^c_i) + \sum_{r=2}^n \frac{y^r}{r!} \frac{\partial^r V(x)}{\partial x^r} \Big|_{x=x^c_i} \]  \hspace{1cm} (7)
The kinetic energy is quadratic in velocity and can be split into,
\[ \frac{m}{2} v_i^2 = \frac{m}{2} (x_i^{c,2} + 2x_i^{c,2}y_i + y_i^2) \]  \hspace{1cm} (8)
The net contribution of all the terms which are independent of \( y_i \), in the propagator is simply \( e^{iS(x;x_0,0)/\hbar} \). All the terms linear in \( y \) does not contribute to the integral as the first variation of the action around the classical path is by definition zero\[ \lim_{n \to \infty} \left( \frac{1}{n} \right)^n \int \exp \left\{ \frac{i\epsilon}{\hbar} \sum_{r=1}^n \frac{m(y_r-y_{r-1})^2}{2\epsilon^2} + \right. \]
\[ \left. \sum_{r=2}^n \frac{y^r}{r!2^r} \frac{\partial^r V(x)}{\partial x^r} \Big|_{x=x^c_i} \right\} Dy \]
which can be rewritten as,
\[ \lim_{n \to \infty} \left( \frac{1}{n} \right)^n \int \exp \left\{ \frac{i\epsilon}{\hbar} \sum_{r=1}^n \frac{m(y_r-y_{r-1})^2}{2\epsilon^2} + \right. \]
\[ \left. \left( y_r + y_{r-1} \frac{\partial^r V(x)}{\partial x^r} \Big|_{x=x^c_i} \right) \right\} Dy \]
where,
\[ \kappa = \frac{i\epsilon}{\hbar} \sum_{r=3}^n \frac{(y_r + y_{r-1})^2}{2r!2^r} \frac{\partial^r V(x)}{\partial x^r} \Big|_{x=x^c_i} \]
The algebra for obtaining the first term (zeroth-order of \( \kappa \)) is the same as that of the simple harmonic oscillator. If the potential is exactly quadratic, then this is the only surviving term. For this class of systems the propagator can always be written as
\[ K(x,t;x_0,0) = F(t)e^{\frac{i\epsilon^2}{4\hbar}} \]  \hspace{1cm} (9)
where \( F(t) \) is an undetermined normalization constant dependent only on the time elapsed. The contribution from higher orders in potential makes the pre-factor position dependent as well. The complete propagator is sum of all such contributions. Smaller the higher order derivatives of the potential are, that is the smoother it is, better can the propagator be approximated just by exponentiating the classical action. This is precisely the WKB approximation of quantum mechanics\[ \text{[12]} \]
The rest of the integrals, unfortunately is not so straightforward to carry out analytically and forms the thesis of the present paper. Consider the terms constituting the linear order in \( \kappa \). The \( i^{th} \) moment integral is of the form,
\[ \int_{-\infty}^{\infty} \exp \left\{ \frac{i\epsilon}{\hbar} \left[ \frac{m(y^2_i)}{2\epsilon^2} + \frac{(y_i + y_{i-1})^2}{2} \right] \right\} \frac{dy_i}{2!} \]
where,
\[ K = \frac{1}{2!} \frac{\partial^2 V(x)}{\partial x^2} \Big|_{x=x^c_i} \]
For simplicity of calculations, \( \frac{(y_{i+1} + y_{i-1})}{2} \) can be replaced by \( y_i \), as in the limit, \( y_i \) and \( y_{i-1} \) comes infinitesimally close.
The general integral can then be reduced to sum of simpler Gaussian integrals of the form,
\[ \int_{-\infty}^{\infty} \exp \left\{ \frac{i\epsilon}{\hbar} \left[ \frac{m}{\epsilon^2} - K \right] y^2_i - \frac{m}{\epsilon^2} \left( (y_i + y_{i-1}) \right) \right\} dy_i \]
All these integrals can be carried out in a closed form for all powers of \( y_i \) and the expression is as follows.
\[ \int_{-\infty}^{\infty} e^{k(y_i^2 + ay_i^2)} dy_i = \sqrt{\frac{\pi}{k1+i\tau}} e^{-\frac{a^2k}{4}} \left( \mathcal{Y} \left( \frac{-\pi^2 k}{4}, r \right) \right) \]  \hspace{1cm} (10)
where \( \mathcal{Y}(x,m) \)s represent a class of hypergeometric polynomials, which are of the order of \( m/2 \) in \( x \), and are closely related
to the Kummer confluent hypergeometric function. First few of the $\Upsilon$ s are,

$$
\begin{align*}
\Upsilon(x, 0) &= 1 \\
\Upsilon(x, 1) &= -\sqrt{x} \\
\Upsilon(x, 2) &= (x + 1/2) \\
\Upsilon(x, 3) &= -\sqrt{x}(x + 3/2) \\
\Upsilon(x, 4) &= ((x + 3)x + 3/4)
\end{align*}
$$

These polynomials are the main source of difficulty, which makes the evaluation of successive integrals increasingly difficult. What rescues us, is the fact that the physically relevant quantity, the propagator, is defined only at a limit $n \to \infty$, $\epsilon \to 0$, $m \epsilon = t$. At this Riemannian limit, only the terms independent in $\epsilon$ in the denominator have finite contribution, and after integrating out the $n$-th integral for $r$-th order has the form,

$$
i\epsilon \left( \sum_{l=1}^{n} l^r (x'_l + x'_f) + \sum_{l=1}^{n} (n - 2l)! \left( (x_l + x_f) - (x'_l + x'_f) \right) \right)
\left( \sqrt{\frac{2\pi \hbar}{m}} \right)^{n-1} \hbar^{r+1/2}
$$

The normalization constant is given by,

$$A = \sqrt{\frac{2\pi i\hbar}{m}} \tag{11}$$

In the limit the final contribution to the propagator from each moment thus can be expressed analytically as,

$$v_r(x,t) \exp \left( \frac{im(x_f - x_i)^2}{2\hbar t} \right) \tag{12}$$

where,

$$v_r(x,t) = \frac{x'_r + x'_f + \frac{(x_i + x_f)' - (x'_i + x'_f)}{2}}{\sqrt{\frac{2\pi \hbar}{m}} } \tag{13}$$

The computation of $v_r(x,t)$s for terms constituting higher orders of $x$, follows the same algorithm, and the computation of the propagator reduces to a multinomial combinatorics problem of calculating the corresponding coefficients, $B_r$s. In principle, the whole Kernel can be obtained so, analytically, as long as the sum converges, and the general formula looks like,

$$K(x,t;\chi_0) = F(t) \sum_r B_r v_r(x,t) \tag{14}$$

where $S_{\text{free}}$ is the classical action of the free particle. Equation (14) gives the general propagator for any general potential. The derivation was carried out for single particle and one dimension. But it can be generalized to any dimensions and any number of particles in the obvious way. We assume a general initial complex wave-function, expressed in polar form as

$$\Psi_0(x_0) = R_0 e^{i\frac{S_{\text{free}}}{\hbar}} \tag{15}$$

The general wave function depicting the system at time $t$ according to path integral formulation can be written as,

$$\Psi(x,t) = F(t) \int_{-\infty}^{\infty} R_{0e} \frac{(S_{\text{cl}} + S_{\text{free}} + S_0)}{\hbar} \sum_r B_r v_r(x,t) dx_0 \tag{16}$$

using equation (4). The wave-function is undetermined up to a time dependent normalization. However the QP can be obtained precisely by decoupling this wave-function into real and complex parts and carrying out the integrals. Expressing the resultant wave function in polar form as,

$$F(t) R(x,t) \exp \left( \frac{(S_{\text{cl}} + S_{\text{free}} + S_0)}{\hbar} \right) \tag{17}$$

the QP is obtained using equation (3). The function $F(t)$, being independent of $x$, gets canceled. This can be used to generate the fluid trajectories, equivalently by using (18).

$$\frac{d^2x}{dt^2} = -\nabla (V + Q) \tag{18}$$

The formula (14) provides a general formal expression for the path integral propagator in closed form, subject to the availability of the classical action in closed form. This bridges the Path Integral formulation with QFD. In cases where the trajectories cannot be obtained in closed form, we have argued that the problem can be reduced to numerically computing a single real valued integral (16). The algorithm we propose hence has linear time complexity, which supersedes speeds of all its predecessor.

III. TOY SYSTEM: ANHARMONIC OSCILLATOR

As a simple model application of the method, we illustrate here the case the Quartic Anharmonic Oscillator potential, primarily to showcase the ease of computation. Study of this well known system can be found in many standard textbook of Quantum Mechanics or Path Integral. Despite its simplicity, it is applied widely in condensed matter theory, in modelling double well potentials, like in isomerization, reactions with symmetric potential barriers and study of inversion of ammonia and Nitrogen-Vacancy Defect Center. Our interest in this model stems from the aim of probing tunneling using a simple enough system.

As stated earlier, exact computation of the propagator in closed form depends on the availability of classical action in closed form. Unfortunately, that is not the case with Anharmonic Oscillator, and the classical action can only be studied using perturbation. That restricts our venture to the perturbative regime, even though the path integral computation as we have presented does not demand it. It might be noteworthy, unlike the Schulman treatment, we do not do an asymptotic analysis, we do not neglect any contribution from paths,
be substituted by $x_i, x_f$ to convert it into the boundary value problem. The obtained action is denoted by $S_{cl}$ for the rest of the discussion.

According to our prescription then, the perturbative propagator till the first order is given by,

$$K(x,t; x_0, 0) = F(t) e^{S_{cl}} \left( 1 - \frac{i}{\hbar} \sum_{m=3}^{4} \frac{1}{m!} \left( \frac{\partial^m}{\partial x^m} V(x^f) V_{m}(x,t) \right) \right)$$

Where the $x^f_i$ is the classical path till zeroth order, which is nothing but the path of the simple harmonic oscillator, when solved as a BVP. The figure reports the probability density and the Quantum Potential as function of space and time, computed numerically using equations (4), for the parameter values $m = 1, k = -2, \lambda = 10^{-4}, \hbar = 1$ and the initial wavefunction,

$$\Psi_0(x_0) = 0.997356 e^{-3.125(3.16228 + x_0)^2} \quad (22)$$

The parameters of the initial wave function is chosen such that the probability of finding the particle in the left well is $\sim 1$, as well as it is centered very close to the barrier wall to show some interesting dynamics, even in its initial time of flight.

A part of the probability density is clearly observed to cross the classically forbidden barrier, which is situated at $x = 0$. The QP shows to develop a deep groove in the left well along with a smaller one in the right one. It is the sum of QP and the applied potential $V(x)$, that governs the dynamics of the quantum fluid.

Bohm had interpreted the mechanism of tunneling by proposing that the Quantum Potential creates channels, by lowering the applied potential and then the whole dynamics can be seen as a blob of fluid traversing through it. On the other hand according to Wyatt it is the initial position dependent acceleration during initial period of flight that causes certain fluid elements to fly over the classical barrier. Our results indicate a reconciliation of the two seemingly contradicting views. The fact that Bohm’s interpretation is validated is obvious from the flat groove travelling towards the right well in the Quantum Potential, as well as, the fact that, initially the QP is steep, and thus its gradient is big. Depending on the initial position of the fluid element, the force directs it to either the left or the right well. However, with time the QP becomes flat and thus its gradient becomes zero. Thus, it is only the initial time of flight that decides the fate of the fluid element in crossing the barrier, and to a good approximation the QP can be neglected for further dynamics, as was conceived by Wyatt. Both the interpretations are thus found to be completely consistent with each other.

In a double well potential the Probability amplitude is expected to oscillate between two wells, which is not so evident in our plots, and probably is rendered due to higher order corrections. The higher order effects were not incorporated as
our main interest was in tunneling, which is well studied even within first order. However, as is suggested by the formulation the incorporation should be straight forward. We reserve this material for further study and discourse.

IV. DISCUSSION

QP is regarded as the origin of non-locality in QFT\cite{13}. Invoking Feynman’s idea of contribution from all possible paths in governing the dynamics, and quantifying their overall effect in \( \psi_n(x,t) \), the formulation presented in this paper, unravels a new arena of possibilities in the understanding of the processes quantum nonlocality and entanglement, which are of utmost importance in the fields of Quantum Meteorology, Quantum Optics and most importantly in developing Quantum Computers. We won’t be exploring this direction further in the limited scope of this paper.

It might be worthwhile to note, as we have not used any extra assumptions than the original quantum theories and have merely mathematically connected two preexisting seemingly disconnected nodes, all the standard results and predictions of both the theories, as well as those of the orthodox theory are simply translated unchanged. However, since the Quantum Fluids have found applications in the broader non-linear framework of Gross-Pitaevskii equation,\cite{12} which governs the dynamics of BEC, soliton-polariton semiconductor systems or that of superfluid photons to name a few, there are several straight-forward scopes of generalizing our work to these domains, to generate analytical solutions. From a mathematics perspective, this problem is interesting, as the integral formulation corresponding to a non-linear PDE is not well understood. This case opens up an opportunity to study at least a special class of it.

V. CONCLUDING REMARKS

To summarize, in this paper we have presented a general derivation of the Quantum Potential of QFD from the principles of Path Integrals, expressing it analytically as a functional of the classical path and the initial wave-function of a system. This allows us to argue that the root of the non-locality in QP arises due to the consolidation of the effects in the dynamics of all possible paths as is suggested by the principles of Path Integrals. These analytical expressions are valid for any general well-behaved potential, and can be fed into machines directly, to compute the QP and trajectories, completely bypassing the task of solving the Schrodinger’s equation. For any given initial wave-function the computation requires only one numerical integration, which has linear time complexity, thus making it faster than any preceding algorithm.

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