Towards Lagrangian approach to quantum computations (revised)

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Abstract

In this work is discussed possibility and actuality of Lagrangian approach to quantum computations. Finite-dimensional Hilbert spaces used in this area provide some challenge for such consideration. The model discussed here can be considered as an analogue of Weyl quantization of field theory via path integral in L. D. Faddeev’s approach. Weyl quantization is possible to use also in finite-dimensional case, and some formulas may be simply rewritten with change of integrals to finite sums. On the other hand, there are specific difficulties relevant to finite case.

1 Introduction

One initial reason to consider possibility of Lagrangian formalism in quantum computations was an idea to use analogues of a minimal action principle in some quantum optimization algorithms (cf Ref. [1]).

In quantum physics the minimal action principle has standard correspondence with classical one: any possible trajectory $P$ of some particle has contribution $\exp(\frac{i}{\hbar} \int_P \mathcal{L}(t) dt)$, where $\mathcal{L}$ is Lagrange function. Such an expression has an oscillatory behavior, and only a trajectory near extremum of action $A = \int_P \mathcal{L}(t) dt$ matters, because other paths compensate each other due to interference (cf Ref. [2]).

Does it possible to use such principle in the quantum information science for finding an extremum of some function using a quantum mechanical system with appropriate Lagrangian? The idea encounters specific obstacles because Hilbert spaces used in quantum computations are finite-dimensional. On the other hand some analogue of Lagrangian theory may be really built and the present paper describes some basic properties of such models. In Section 2 are briefly revisited ideas and formulas used in continuous case, and necessary for a further revision with finite-dimensional Hilbert spaces discussed in Section 3. A relevance to the theory of quantum computations is discussed in Section 4.
2 Continuous case revisited

2.1 Weyl quantization

Let us recall briefly the idea of Weyl quantization with most attention to topics necessary for further applications to finite-dimensional Hilbert spaces.

In continuous case Weyl quantization uses a function \( f(p, q) \) with two real arguments \( p, q \) and with Fourier co-image \( \tilde{f}(\alpha, \beta) \) described by expression

\[
f(p, q) = \int \int \exp(i\alpha p + i\beta q) \tilde{f}(\alpha, \beta) \, d\alpha \, d\beta. \tag{1}
\]

Such a function is associated with an operator \( \hat{f} \) defined as

\[
\hat{f} = \int \int \exp(i\alpha \hat{p} + i\beta \hat{q}) \tilde{f}(\alpha, \beta) \, d\alpha \, d\beta. \tag{2}
\]

Here \( \hat{p} \) and \( \hat{q} \) are momentum and coordinate operators. In exponential form used in Eq. (2) it is defined a Weyl system, i.e., two families of operators:

\[
\hat{U}(\alpha) = \exp(i\alpha \hat{p}), \quad \hat{V}(\beta) = \exp(i\beta \hat{q}) \tag{3}
\]

satisfying relation (in system of units with \( \hbar = 1 \))

\[
\hat{U}(\alpha)\hat{V}(\beta) = \exp(i\alpha \beta)\hat{V}(\beta)\hat{U}(\alpha), \tag{4}
\]

equivalent to usual Heisenberg relation for coordinate and momentum

\[
[\hat{p}, \hat{q}] = \hat{p}\hat{q} - \hat{q}\hat{p} = -i. \tag{5}
\]

Formally Eq. (4) follows from Eq. (5) due to a Campbell-Hausdorff formula

\[
\exp(\hat{a} + \hat{b}) = \exp(\hat{a}) \exp(\hat{b}) \exp(-\frac{1}{2}[\hat{a}, \hat{b}]) \exp R_2,
\]

where \( R_2 \) is a term with commutators of higher order, \( R_2(\hat{p}, \hat{q}) = 0 \). Using this formula it is possible also to rewrite Eq. (2) as

\[
\hat{f} = \int \int \tilde{f}(\alpha, \beta) \exp(i\alpha\beta/2)\hat{U}(\alpha)\hat{V}(\beta) \, d\alpha \, d\beta. \tag{6}
\]

Weyl quantization via Eq. (1) and Eq. (2) produces a method of construction of some operator \( \hat{f} \) for any function \( f(p, q) \) with two variables \( \mathcal{W}: f \rightarrow \hat{f} \). It is enough to use the inverse Fourier transform in accordance with Eq. (1) to create \( \hat{f} \) and use it for construction of the operator \( \hat{f} \).

There is also direct formula for \( \hat{f} \). Using an expression for kernel of Eq. (2) in coordinate representation

\[
(q'|e^{i\alpha \hat{p} + i\beta \hat{q}}|q'') = \exp(i\frac{q' + q''}{2} - \beta(q'' - q' + \alpha)), \tag{7}
\]
it is possible to write elements of the operator $\hat{f}$

$$\langle q' | \hat{f} | q'' \rangle = \frac{1}{2\pi} \int f \left( p, \frac{q' + q''}{2} \right) e^{ip(q'' - q')} dp.$$  \hfill (8)

It is simple to invert Fourier transformation on $p$ used in Eq. (8) and using notation $q = (q'' + q')/2$, $x = q'' - q'$ to write

$$f(p, q) = \int \langle q - x/2 | \hat{f} | q + x/2 \rangle \exp(-ipx) dx.$$  \hfill (9)

The formula Eq. (9) show, how to calculate $W^{-1}$.

It should be mentioned, that for a particular case, then $\hat{f}$ is the statistical operator ("density matrix") $\hat{\rho}$, Eq. (9) coincides with an expression for Wigner function. The property is known also as Wigner-Weyl isomorphism. Despite of such coincidence in mathematical expressions, Weyl quantization has rather different area of applications. Wigner function was suggested for presentation of mixed states, but Weyl quantization often used for description of evolution of arbitrary operator in Heisenberg picture without actual necessity to work with states and density matrices.

The Hamiltonian function here $H(p, q) = W^{-1}\hat{H}$ displays a proper correspondence principle with the classical physics, i.e., the evolution law for operators in the Heisenberg picture applied to coordinate and momentum

$$d\hat{q}/dt = i[\hat{H}, \hat{q}], \quad d\hat{p}/dt = i[\hat{H}, \hat{p}],$$  \hfill (10)

produces canonical Hamiltonian equations for classical coordinate, momentum and function $H(p, q)$

$$dq/dt = \partial H(p, q)/\partial p, \quad dp/dt = -\partial H(p, q)/\partial q.$$  \hfill (11)

In continuous case such property ensures correspondence principle, because any operator may be presented formally via series with $\hat{p}$ and $\hat{q}$. In the discrete case there are no good analogues of such operators and so other ideas should be used instead.

### 2.2 Lagrangian approach and path integral

The functional (path) integral in Weyl approach may be introduced by quite straightforward procedure. In Schrödinger picture $|\psi'\rangle = S|\psi\rangle$ and it is possible to write elements of evolution operator $S$ ("quantum gate") for small period of time $\Delta t$ as

$$\langle q'' | \hat{S}(\Delta t) | q' \rangle = \langle q'' | e^{-i\hat{H}\Delta t} | q' \rangle \cong \langle q'' | 1 - i\hat{H}\Delta t | q' \rangle.$$  \hfill (12)
Applying Eq. 8 to Eq. 12:

\[ \langle q''|\hat{S}|q'\rangle \equiv \frac{1}{2\pi} \int e^{ip(q''-q')} \left( 1 - iH(p, \frac{q''+q'}{2}) \Delta t \right) dp \]

\[ \approx \frac{1}{2\pi} \int e^{ip(q''-q')-iH(p, \frac{q''+q'}{2})\Delta t} dp \] (13)

It is possible to divide finite interval of time on \( N \) small periods and use expression \( \hat{S} = \prod \exp(i\hat{H}(t)\Delta t) \). For \( N \to \infty \) and \( \Delta t \to 0 \) such products of Eq. 13 corresponds to expression for functional (continual, path) integral along all paths in coordinate and momentum space

\[ \langle q''|\hat{S}|q'\rangle = \int_P \exp\left( i \int (p\dot{q} - H(p, q)) dt \right) DpDq. \] (14)

The function \( \mathcal{A} = \int (p\dot{q} - H(p, q)) dt \) here is limit \( \Delta t \to 0 \) of finite sums in Eq. 13 and coincides with classical action. More details about finite sums used in the passage to the continuous limit may be found also in description of Eq. 24 below.

### 3 Finite-dimensional case

#### 3.1 Weyl pair

An advantage of Weyl relations Eq. 4 for purposes of present paper is possibility to write an analogue of such operators in finite, \( n \)-dimensional case. It is enough to use Weyl pair of \( n \times n \) matrices \( \hat{U}, \hat{V} \):

\[ \hat{U}_{jk} = \delta_{j,k+1 \mod n}, \quad \hat{V}_{jk} = \exp\left( \frac{2\pi i}{n} j \right) \delta_{jk} \] (15)

with property

\[ \hat{U}\hat{V} = \exp(2\pi i/n)\hat{V}\hat{U}. \] (16)

Let us consider finite analogues of other expressions. Let \( \hat{M}(a, b) \) is function of two integer arguments \( a, b = 0, \ldots, n-1 \). It is possible to use discrete Fourier transform for both arguments and write analogue of Eq. 1

\[ M(p, q) = \frac{1}{n} \sum_{a,b=0}^{n-1} \exp\left( \frac{2\pi i}{n} (ap + bq) \right) \hat{M}(a, b). \] (17)

The function \( M(p, q) \) is defined for any real \( p, q \), but integer values are enough to find \( \hat{M}(a, b) \) via inverse Fourier transform, and so value of \( M(p, q) \) for any real values.

Analogue of operator \( \hat{f} \) defined by Eq. 6 is \( n \times n \) matrix \( \hat{M} \) could be written as

\[ \hat{M} = \frac{1}{n} \sum_{a,b=0}^{n-1} \exp\left( \frac{\pi i}{n} ab \right) \hat{U}^a\hat{V}^b\hat{M}(a, b), \] (18)
but it produces some problems due to using of modular arithmetics, e.g. unlike with continuous case the operator Eq. (18) $\hat{M}$ is not Hermitian for real function $M(p, q)$ Eq. (17). Anyway, for simpler illustration of suggested approach, it is enough to consider asymmetric construction, i.e.,

$$\hat{M} = \frac{1}{n} \sum_{a,b=0}^{n-1} \hat{U} a \hat{V} b \tilde{M}(a, b),$$  \hspace{1cm} (19)$$

For such operator true discrete asymmetric analogue of expression Eq. (8)

$$\hat{M}_{kj} = \langle j|\hat{M}^l|k \rangle = \frac{1}{n} \sum_{p=0}^{n-1} e^{\frac{2\pi i}{n} p(j-k)} M(p, k).$$  \hspace{1cm} (20)$$

It can be checked directly using Eq. (17) and Eq. (19):

$$\frac{1}{n} \sum_{p=0}^{n-1} e^{\frac{2\pi i}{n} p(k-j)} M(p, k) = \frac{1}{n} \sum_{p,a,b=0}^{n-1} e^{\frac{2\pi i}{n} (p(k-j) + ap + bk)} \hat{M}(a, b)$$

$$= \frac{1}{n} \sum_{a,b=0}^{n-1} \hat{M}(a, b) \sum_{p=0}^{n-1} e^{\frac{2\pi i}{n} p(k-j+a)} = \sum_{a,b=0}^{n-1} \delta_{j-k,a} e^{\frac{2\pi i}{n} bk} \hat{M}(a, b) = \hat{M}_{kj}.$$  \hspace{1cm} (22)$$

Inverse transformation for Eq. (20) also may be simply found

$$M(p, q) = \sum_{j=0}^{n-1} e^{-\frac{2\pi i}{n} pj} \hat{M}^l_{q+j}, \hspace{1cm} p, q \in \mathbb{Z}.$$  \hspace{1cm} (21)$$

It should be mentioned also, that in equations above notation for modular arithmetic is often omitted for simplicity, e.g., $q + j$ used instead of $q + j \mod n$.

### 3.2 Lagrangian approach to discrete models

Using Eq. (20) it is possible to write analogue of Lagrangian function Eq. (8)

$$\langle j|\hat{S}^l|k \rangle \approx 1 \sum_{p=0}^{n-1} e^{\frac{2\pi i}{n} p(j-k)} (1 - iH(p,j)\Delta t)$$

$$\approx 1 \sum_{p=0}^{n-1} e^{\frac{2\pi i}{n} p(j-k) - iH(p,j)\Delta t}.$$  \hspace{1cm} (22)$$

Here $\langle j|\hat{S}|k \rangle = \hat{S}_{kj}$ are simply indexes of matrix. For interval of time divided on $N$ segments we have

$$\langle q_0|\hat{S}|q_N \rangle = \sum_{q_1,\cdots,q_{N-1}=0}^{n-1} \langle q_0|\hat{S}_1|q_1 \rangle \cdots \langle q_{N-1}|\hat{S}_N|q_N \rangle.$$  \hspace{1cm} (23)$$

5
Using Eq. (22) it is possible to write

$$
\langle q_0 | \hat{S}_l | q_N \rangle \cong \frac{1}{n^N} \sum_{q_1, \ldots, q_{N-1}=0}^{n-1} \exp(i \mathfrak{A}^l_{q,p})
$$

where discrete analogue of action

$$
\mathfrak{A}^l_{q,p} = \sum_{k=0}^{N-1} \left( 2 \pi \frac{n}{n} p_k (q_{k+1} - q_k) - H(p_k, q_k) \Delta t \right)
$$

is calculated along all $n^{N-1}$ possible paths $q_k$ between two fixed points and with $n^N$ different momentum $p_k$ for each separate segment of such broken line. Approximate expression Eq. (24) converges to value $\hat{S}_l q_0 q_N$ in limit $N \to \infty$, $\Delta t \to 0$. For continuous limit $n \to \infty$ the Eq. (25) for asymmetric ordering may look even more traditional.

### 3.3 Precise expression with “effective Lagrangian”

For further analysis of discrete models it is possible to introduce some “effective Lagrangian” to have precise value of $\hat{S}_l j k$ for any division of time interval, including $N = 1$. Really, errors in expressions above was related with two consequent approximations like $\exp(i \epsilon) \approx 1 + i \epsilon$. Let us instead of application of (discrete) Weyl quantisation to Hamiltonian apply it directly to operator $\hat{S}_l$ in Eq. (22).

$$
\langle j | \hat{S}_l | k \rangle = \frac{1}{n} \sum_{p=0}^{n-1} e^{\frac{2\pi i}{n} p (j-k)} S(p, j)
$$

with straightforward generalization to sum like Eq. (24), precise for any $N \geq 1$. It is only necessary to change $H$ to $H'_\Delta t \equiv i \ln S(\Delta t)/\Delta t$, it is an “effective Hamiltonian,” $H'_\Delta t \to H$, $\Delta t \to 0$. Here all paths with terms $S(p, q) = 0$ should be simply omitted.

### 3.4 Discrete Fourier transform

For some cases the precise expression Eq. (24) may be quite simple. Let us consider for example discrete Fourier transform

$$
\tilde{F}_{jk} = \frac{1}{\sqrt{n}} \exp\left( \frac{2\pi i}{n} jk \right).
$$

1Strictly speaking, such limit for path integrals is usually not well-defined.
Using inverse transformation Eq. (21) it is possible to find

\[ F(p, q) = \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} e^{\frac{2\pi i}{n} (q(j+j^{-})-pj)} = \sqrt{n} e^{\frac{2\pi i}{n} q^2} \delta_{pq} = \sqrt{n} e^{\frac{2\pi i}{n} (p^2+q^2)} \delta_{pq}. \]  

Here “effective Hamiltonian” \( q^2 \) was rewritten in symmetric form \( (q^2 + p^2)/2 \) due to term \( \delta_{pq} \). It is convenient also, because for quantum computation with continuous variables the Hamiltonian of harmonic oscillator really may be used for realization of Fourier transform \[7\].

4 Discussion

In general, quantum computation is theory about efficient solving of computationally hard problems using quantum systems and processes. Difficulty of computational problems relevant with Lagrangian approach and calculation of sums over paths has two reasons. First one is usual exponential growth of Hilbert space dimension with respect to number of quantum systems, i.e., calculations with \( n \) qubits requires operations with \( 2^n \times 2^n \) matrices (multiplications, exponents, etc.). The second one is well-known difficulty with definition and calculation of functional (path) integrals, it may be described as unspecified growth of number of terms in sums like Eq. (24) due to using expressions with limits \( \Delta t \rightarrow 0, \ N \rightarrow \infty \).

It was already mentioned some mathematical resemblance with theory of Wigner functions in continuous case. For discrete models some methods from theory of Wigner function like doubling of lattice, using reflection operator and Galois fields \[8, 9\] do not have simple extensions for theory considered here, but maybe it provides promising challenge. Anyway, it is quite likely, that due to some analogy between theory of Weyl quantization and Wigner function, it is possible to combine such techniques for particular tasks related with statistical description of ensembles in theory of quantum computations and communications.

In considered theory Fourier transform is related with simplest quadratic Hamiltonian similar with harmonic oscillator. In usual, continuous theory only quadratic Hamiltonians produce possibility of more or less rigor calculation of path integral. In discrete theory used here all expressions may be calculated for any functional dependence, but simple representation of Fourier transformation may be convenient, because it is a fundamental tool for many quantum algorithms \[10\] including Shor’s factoring one \[11\].

It is also possible to compare such approach with yet another propositions for quantum algorithms, despite they may look different from traditional one. For example it was suggested \[12\] to use many-slits interference with different paths for resolution of NP-complete problems on quantum computer.

It should be mentioned also idea of quantum optimization algorithms discussed in introduction. It works, if due to oscillatory behaviour and appropriate Lagrangian, all paths except optimal are vanishing. It is usual for classical limit.
On the other hand, the method may be useful for calculation of sum itself, even if it is not related directly with any optimization task. For example, application of sum over paths for computing of polynomial equation over finite fields was discussed recently in [13]. It was also noted there, that many basic papers about quantum computing complexity use some variants of sum over path approach (see [13] and references therein).

Some difference between the just mentioned models and the method considered in this paper similar with distinction between earlier version with sum other spatial paths and more recent version with paths in the phase \((p,q)\) space [4, 6].

The models discussed in [13] exploit straightforward representation of matrix multiplication via path summation Eq. (23) with only one kind of indexes \((q_k)\), but in present paper is also used more general expressions with sum other paths in whole discrete phase space \((p_k, q_k)\) Eq. (24). Only for some particular cases, like quadratic Hamiltonians or “effective Hamiltonian” with \(\delta\) symbol Eq. (28), the summation on \(p_k\) may be cancelled.

The detailed representation in phase space is essential, because one purpose of this paper was to find relations between physical models and abstract quantum computations, e.g., it becomes clearer from equations considered above, how Lagrangian term \(p\Delta q − H\Delta t\) appears in expressions for sum over paths, how classical limit may be obtained for quantum system due to growth of Hilbert space dimension, etc.

There are also other tasks relevant to given approach. For example, Lagrangian formalism is standard method for description of interacting quantum fields and it may be useful for more adequate models of quantum gates and computation.

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