Lagrangian form of Schrödinger equation

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Abstract Lagrangian formulation of quantum mechanical Schrödinger equation is developed in general and illustrated in the eigenbasis of the Hamiltonian and in the coordinate representation. The Lagrangian formulation of physically plausible quantum system results in a well defined second order equation on a real vector space. The Klein–Gordon equation for a real field is shown to be the Lagrangian form of the corresponding Schrödinger equation.

1 Introduction

Schrödinger evolution equation of quantum mechanics [1] is of the first order in time and is formulated on the complex Hilbert space of the system. In these respects, it is similar to the evolution equation of a Hamiltonian dynamical system[2,3]. The latter have an equivalent Lagrangian formulation in terms of equations of the second order in time. On the other hand, something like a Lagrangian formulation of the abstract Schrödinger equation is usually not considered. The question of a second order evolution equation equivalent to the Schrödinger equation in coordinate representation was considered for the first time by Schrödinger himself [4]. However, he did not consider the problem as the one of relation between Hamiltonian (Schrödinger) and Lagrange frameworks. An interesting analysis of this problem, again formulated in the coordinate representation, appeared in [5]. Construction of an appropriate Lagrangian formulation of the quantum Schrödinger evolution in the general case is the task of

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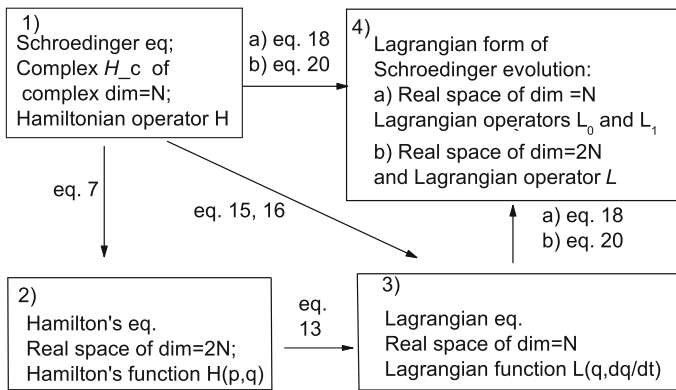Vinca Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

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Fig. 1 Illustrates relations between various formulations of quantum Schrödinger evolution.

this paper. This is quite different from the standard application of the action functional in the Lagrangian (or Hamiltonian) form of the functional integral representation of the quantum propagator [6,7].

Our strategy and the main result could be schematically summarized as in Fig. 1. We shall start from the quantum Schrödinger equation on an abstract complex Hilbert space, which we consider as given. This is the box 1 in Fig.1. It is well known that the Schrödinger equation is equivalent to the appropriate Hamiltonian dynamical system on the corresponding phase space [8–11]. This is the box 2 in Fig.1. In fact, the geometric Hamiltonian form of the Schrödinger evolution could be extended to an equivalent formulation of the quantum mechanics [10], and is quite suitable for treatment of problems like nonlinear constraints[12,13], imbedding of classical into quantum mechanics [14,15] and hybrid theories [16–18]. We shall apply the standard transition procedure from Hamiltonian to Lagrangian formulation in order to obtain the Lagrangian form of the Hamiltonian formulation of the Schrödinger equation. The result is the box 3 in Fig. 1. The final step is the transition from the Lagrangian dynamical system in box 3 to the Lagrangian form of the Schrödinger equation, which turns out to be a second order equation on a real Hilbert space. This is the box 4 in Fig. 1. The transitions between boxes, represented by the arrows in Fig. 1, are explained in detail, and in the general case, in the next section.

Of course, the Lagrangian form, when it exists, is equivalent to the Hamiltonian Schrödinger equation. Therefore, our main motivation for the derivation of the Lagrangian form of the general (linear) Schrödinger equation is purely formal. One further motivation is that the Lagrangian form of the Schrödinger equation is more suitable for Lorentz invariant models. In fact, we shall see that the Klein-Gordon equation [19] for the relativistic state vector is noting else but the Lagrangian formulation of the Schrödinger equation with the corresponding Hamiltonian. Also, symmetries are more naturally considered as morphisms of the Lagrangian form and not as time evolution, while the Hamiltonian formulation, i.e. the Schrödinger equation, on the other hand, offers the framework in which the time evolution is an automorphism of the relevant symplectic structure. However, one should bare on mind that the canonical

coordinates and momenta in the Hamiltonian and velocities in the Lagrangian formulations of the Schrödinger equation are in fact the coefficients in a basis expansion of the quantum state vector.

The presentation in Sect. 2 is general and formal. The conditions for existence of the expression of the canonical momenta in terms of velocities will be briefly discussed in the general case near the end of Sect. 2. The possible problems will be further illustrated and discussed in Sect. 3, together with the presentation of particular examples obtained by rewriting the general formalism in particular bases. In this section we also treat the Klein-Gordon equation as an example of the Lagrangian formulation of the appropriate Schrödinger equation. Summary is given in Sect. 4.

2 Derivation of the Lagrangian Equations

The Schrödinger equation

$$i\hbar\frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle \tag{1}$$

on a complex Hilbert space $\mathcal{H}_c$ of finite or infinite complex dimension N, is equivalent to a Hamiltonian dynamical system on an appropriate real, symplectic manifold of dimension $2N$. This Hamiltonian formulation of the Schrödinger evolution equation is well known (excellent comprehensive reviews are [10,11]). Nevertheless, we need to recapitulate the notation and write down the basic definitions and formulas in their most elementary form. Derivation of the Hamiltonian form of the Eq. (1) ends with the Eqs. (10) and the rest of this section is devoted to the derivation of the Lagrangian form of the Schrödinger evolution.

A vector $|\psi\rangle \in \mathcal{H}_c$ in an abstract (arbitrary) basis $\{|n\rangle\}$ is written as

$$|\psi\rangle = \sum_n z_n|n\rangle = \sum_n (q_n + ip_n)|n\rangle \tag{2}$$

The matrix elements

$$H_{mn} = \langle m|\hat{H}|n\rangle \equiv H_{mn}^R + iH_{mn}^I \tag{3}$$

satisfy $H_{mn}^R = H_{nm}^R$, $H_{mn}^I = -H_{nm}^I$ since $\hat{H}$ is a Hermitian operator. It is not necessary for our main line of reasoning, but it is nevertheless instructive, to write down explicitly the abstract matrix form of the Schroödinger equation (1) in terms of real $2N$ dimensional vector

$$|\phi\rangle = (q_1, \ldots q_n, p_1 \ldots p_n)^T \equiv (q, p)^T \tag{4}$$

The Schrödinger equation (1) in terms of the $2N$ real vector $|\phi\rangle$ in the abstract basis reads

$$\frac{d|\phi\rangle}{dt} = \frac{1}{\hbar}\begin{pmatrix} \hat{H}^I & \hat{H}^R \\ -\hat{H}^R & \hat{H}^I \end{pmatrix}|\phi\rangle, \tag{5}$$

where $\hat{H}^I$, $\hat{H}^R$ denote $N \times N$ matrices introduced in (3). The Schrödinfer equation (1) and the representations in the abstract basis of $\mathcal{H}_c$ are the content of the box 1, and are considered as given.

The function

$$H(q, p) = \frac{1}{2\hbar} \langle \psi | \hat{H} | \psi \rangle \tag{6}$$

where q_n, p_n, $|\psi\rangle$ are as in (2) is a quadratic form given explicitly by

$$H(q, p) = \frac{1}{2\hbar} \sum_{nm} \left(q_n q_m H_{nm}^R + p_n p_m H_{nm}^R - 2q_n p_m H_{nm}^I \right). \tag{7}$$

Let us remark that the function $H(q, p)$ can also be written as $\langle \phi | \hat{H}^C | \phi \rangle$ where $|\phi\rangle$ is given by (4) but the representation is not unique, i.e. the expression (7) is given by $\langle \phi | \hat{H}^C | \phi \rangle$ where

$$\hat{H}^c = \frac{1}{2\hbar} \begin{pmatrix} \hat{H}^R & -\hat{H}^I \\ \hat{H}^I & \hat{H}^R \end{pmatrix} \tag{8}$$

or

$$\hat{H}^c = \frac{1}{2\hbar} \begin{pmatrix} \hat{H}^R & -2\hat{H}^I \\ 0 & \hat{H}^R \end{pmatrix}. \tag{9}$$

or other similar matrces.

It is easily checked that the Hamilton equations with the Hamilton's function $H(q, p)$ (7):

$$\dot{q}_n = \frac{\partial H(q, p)}{\partial p_n}, \quad \dot{p}_n = -\frac{\partial H(q, p)}{\partial q_n} \tag{10}$$

reproduce the real form of the Schrödinger equation (5). The Hamiltonian function (6) and (7) and the corresponding Hamilton's equations are the content of the box 2, and the arrow from box 1 to box 2 is given explicitly by the formula (7).

In order to derive the Lagrangian form of the Hamilton's equations (10) we need to express the canonical momenta p_n in terms of the velocities $\dot{q}_n$. This is done in the standard way, and using the explicit form of the Eqs. (10). In fact, from (10a)

$$\sum_m H_{nm}^R p_m = \hbar \dot{q}_n - \sum_m H_{nm}^I q_m \tag{11}$$

Therefore

$$p_k = \sum_n \left((H^R)^{-1} \right)_{kn} \left(\hbar \dot{q}_n - \sum_m H_{nm}^I q_m \right), \tag{12}$$

or in a more compact form $p = (\hat{H}^R)^{-1}(\hbar\dot{q} - \hat{H}^I q)$. At this point we do not care about the existence of the inverse operator $(\hat{H}_R)^{-1}$. The relation (12) is substituted into the definition of the Lagrange function $L = \sum_l p_l \dot{q}_l - H(q, p)$ to obtain, after

some manipulation

$$L(q, \dot{q}) = \frac{\hbar}{2} \sum_{n,m} \dot{q}_n \left((H^R)^{-1} \right)_{nm} \dot{q}_m + \sum_{n,m,k} q_n H^I_{nk} \left((H^R)^{-1} \right)_{km} \dot{q}_m$$

$$- \frac{1}{2\hbar} \sum_{n,m} q_n \left[\sum_{k,j} H^I_{n,k}((H^R)^{-1})_{k,j} H^I_{j,m} + H^R_{n,m} \right] q_m \qquad (13)$$

The previous formula for the Lagrangian function $L(q, \dot{q})$ in terms of the Hamiltonian $\hat{H}$ could be rewritten in a perhaps more systematic form

$$L(q, \dot{q}) = \sum_{nm} \dot{q}_n L^{\dot{q}\dot{q}}_{nm} \dot{q}_m + \sum_{nm} q_n L^{q\dot{q}}_{nm} \dot{q}_m + \sum_{nm} q_n L^{qq}_{nm} q_m \qquad (14)$$

where $L^{\dot{q}\dot{q}}$, $L^{q\dot{q}}$, L^{qq} are given in terms of $\hat{H}^R$, $(\hat{H}^R)^{-1}$, $\hat{H}^I$ in the following compact form

$$L^{\dot{q}\dot{q}} = \frac{\hbar}{2}(\hat{H}^R)^{-1}, \ L^{q\dot{q}} = \hat{H}^I(\hat{H}^R)^{-1}, \ L^{qq} = \frac{-1}{2\hbar}[H^I(\hat{H}^R)^{-1}\hat{H}^I + \hat{H}^R]. \quad (15)$$

The Lagrange function (14) is uniquely related to the original Hamiltonian operator in (1). The corresponding Lagrangian equations are

$$\ddot{q}_m = \frac{-1}{2} \sum_{n,i} (L^{\dot{q}\dot{q}}_{m,i})^{-1} L^{q\dot{q}}_{n,i} \dot{q}_n + \frac{1}{2} \sum_{n,i} (L^{\dot{q}\dot{q}}_{m,i})^{-1} L^{q\dot{q}}_{i,n} \dot{q}_n$$

$$+ \sum_{n,i} (L^{\dot{q}\dot{q}}_{m,i})^{-1} L^{qq}_{i,n} q_n, \qquad (16)$$

where $L^{\dot{q}\dot{q}}$, $L^{q\dot{q}}$, L^{qq} are given by (15).

The Lagrangian (14) with transition formulas (15) is the content of the box 3 and the arrow from the box 1 to the box 3.

Let us remark that the Lagrangian (14) can be written in the form resembling the Eq. (6) by introducing 2N-dimensional vector $|\kappa\rangle = (q, \dot{q})^T$. Then

$$L(q, \dot{q}) = \langle \kappa | \begin{pmatrix} \frac{-1}{2\hbar}[H^I(\hat{H}^R)^{-1}\hat{H}^I + \hat{H}^R] & \frac{1}{2}\hat{H}^I(\hat{H}^R)^{-1} \\ \frac{-1}{2}(\hat{H}^R)^{-1}\hat{H}^I & \frac{\hbar}{2}(\hat{H}^R)^{-1} \end{pmatrix} | \kappa \rangle \qquad (17)$$

In order to go from the box 3 to the box 4 we introduce operators $\hat{L}_0$ and $\hat{L}_1$, acting on a real N-dimensional space, which are defined in terms of $\hat{H}^R$, $\hat{H}^I$, $(\hat{H}^R)^{-1}$ (Eq. (3)) as follows

$$\hat{L}_0 = \frac{-1}{\hbar^2} \left[\hat{H}^R \hat{H}^I (\hat{H}^R)^{-1} \hat{H}^I + (\hat{H}^R)^2 \right], \quad \hat{L}_1 = \frac{1}{\hbar} \left[\hat{H}^I + \hat{H}^R \hat{H}^I (\hat{H}^R)^{-1} \right]. \qquad (18)$$

The Lagrangian equations (16) are written as

$$\frac{d^2|q\rangle}{dt^2} = \hat{L}_1 \frac{d|q\rangle}{dt} + \hat{L}_0 |q\rangle \tag{19}$$

where $|q\rangle \in \mathcal{H}_R$. This is the content of the box 4. and represents the Lagrangian form of the quantum Schroedinger equation on the complex space $\mathcal{H}_c$.

Suppose that the operators $\hat{L}_0$ and $\hat{L}_1$ satisfying (18) exist for a given operator $\hat{H}$ in (1). Then any orbit $|q(t)\rangle$ of (19) in $\mathcal{H}_R^N$ can be used to construct the corresponding orbit of the Schrödinger equation on $\mathcal{H}_c^N$, and the Schrödinger orbit is given by $|\psi(t)\rangle = |q(t)\rangle + i|p(t)\rangle$, where $|p(t)\rangle$ is given in terms of $|q(t)\rangle$ and $|\dot{q}(t)\rangle$ by the formula (12). Also, the initial conditions for the Lagrangian formulation $q(t_0)$, $\dot{q}(t_0)$ are related to the initial state of the Hamiltonian equations or of the Schrödinger equation essentially by the equation (12). Thus, the crucial question for the construction of the Lagrangian formulation is the existence of the operators $\hat{L}_0$, $\hat{L}_1$, which is essentially the question of the existence of the inverse operator $(\hat{H}^R)^{-1}$. The Hamiltonian operator $\hat{H}$ in (1) uniquely determines the operators $\hat{H}^R$ and $\hat{H}^I$. However, a singular choice of basis in $\mathcal{H}_c$ might imply that the operator $\hat{H}^R$ (or $\hat{H}^I$) is represented by zero and $(H_{nm}^R)^{-1}$ does not exist (see example in 3.1). However, in a typical basis $\hat{H}^R$ is represented by a nonzero operator. The existence of $(\hat{H}^R)^{-1}$ then depends on the physical problem. If $(\hat{H}^R)^{-1}$, for the system with the Hilbert space $\mathcal{H}_c$ does not exist, then redefinition of the system by restriction on an appropriate subspace of $\mathcal{H}_c$ would lead to a well defined $(\hat{H}^R)^{-1}$. Alternatively, in terms of the Hamiltonian and the corresponding Lagrangian formulations nonexistence of $(\hat{H}^R)^{-1}$ corresponds to constrained Hamiltonian and singular Lagrangian systems, and the relation between the two formalisms is treated by the appropriate methods [3].

The Lagrangian system (18) on N dimensional $\mathcal{H}_R$ can be trivially written in the form of an evolution equations on real 2N dimensional real space:

$$\frac{d|\kappa\rangle}{dt} = \mathcal{L}|\kappa\rangle \tag{20}$$

where

$$\mathcal{L} = \begin{pmatrix} 0 & 1 \\ \hat{L}_0 & \hat{L}_1 \end{pmatrix}, \tag{21}$$

and $|\kappa\rangle \in \mathcal{H}_R^{2N}$ was defined just before the Eq. (17).

3 Examples and Discussion

In this section we present a series of examples, in the order of increasing complexity, which are aimed to illustrate the problems that might occur in the construction of the Lagrangian formulation.

3.1 Discrete Finite Basis

The first example is rather trivial and artificial, but points out that problems in the construction of the Lagrangian formulation might be apparent and induced by specific choice of a singular basis. Consider the simplest possible quantum system of a single $1/2$ spin with the Hamiltonian $\hat{H} = \hat{\sigma}_y$. In the eigenbasis of the $\hat{\sigma}_z$ the Hamiltonian is represented by

$$\hat{H}_{mn} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{22}$$

The real part of the Hamiltonian is zero, there is no $(H^R_{nm})^{-1}$ and the Hamilton's function is

$$H(q, p) = \frac{1}{\hbar}(q_1 p_2 - q_2 p_1) \tag{23}$$

and there apparently is no Lagrangian formulation. However, by an arbitrary small change of basis the real part becomes nonzero. In the eigenbasis of $\hat{\sigma}_y$ the imaginary part becomes zero and the real part of the Hamiltonian becomes

$$\hat{H}_{mn} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{24}$$

The Lagrangian formulation is now constructed as in the next example.

3.2 Discrete Energy Eigenbasis

Derivation and the formulas of the Lagrangian formalism acquire specially simple form in the eigenbasis of the Hamiltonian $\hat{H}$ with a discrete, say non-degenerate, spectrum. The Hamilton's function is of the form corresponding to a system of linear oscillators

$$H(q, p) = \sum_m \frac{e_m}{2\hbar}(q_m^2 + p_m^2), \tag{25}$$

Thus, $H_{nm} = H^R_{nm} = \delta_{nm} e_m$, where e_m are real and $H^I = 0$. The momenta p_m are related to the velocities $\dot{q}_m$ by $p_m = \hbar \dot{q}_m / e_m$, which is well defined if $\hat{H}$ has no zero eigenvalue. Lagrangian function (13) is given by

$$L(q, \dot{q}) = \sum_m \left(\hbar \frac{\dot{q}_m^2}{e_m} - \frac{e_m q_m^2}{2\hbar} - \hbar \frac{\dot{q}_m^2}{2e_m} \right) \tag{26}$$

and the Lagrangian equations are

$$\ddot{q}_m = -\frac{e_m^2}{\hbar^2} q_m, \tag{27}$$

or

$$\ddot{\phi} = \hat{L}_0 \phi, \tag{28}$$

where $\hat{L}_0 = -\hat{H}^2/\hbar^2$ operates on the real space $\mathbf{R}^N$. The only possible obstacle to the existence of the Lagrangian formulation is possible zero eigenvalue of the Hamiltonian. If there is a zero eigenvalue then the restriction of the Schrödinger equation onto the orthogonal complement of the zero eigenspace generates the Hamiltonian system with the canonical pair q_0, p_0 that does not appear in the Hamilton's function (25), and for which there is the corresponding Lagrangian formulation on $\mathbf{R}^{N-1}$.

From these two examples we see that the construction of the Lagrangian formulation might fail if one makes a choice of the singular basis and/or includes nonphysical states.

3.3 Coordinate Representation

Construction of the Lagrangian formulation for the Schrödinger equation in the coordinate representation follows the same steps as in the general case, or can be obtained by applying the general formulas (18) and (19) written in the coordinate basis. The only potential problem is, like in the general case, non-existence of the inverse of the real part of the Hamiltonian operator $(\hat{H}^R)^{-1}$, appearing in (12). This operator typically has non-diagonal elements in almost all bases and, of course, this fact is irrelevant for the question of its existence. In the coordinate representation, the non-diagonal character of $(\hat{H}^R)^{-1}$ appears as non-locality of the relevant differential operator, and this fact, like its analog in the general case, is irrelevant for the existence of the Lagrangian formulation.

Consider a Hamiltonian of the form

$$\hat{H} = \frac{\hat{P}_x^2}{2m} + V(\hat{X}). \tag{29}$$

In the representation of the coordinate $\hat{X}$, the evolution equation (1) becomes the Schrödinger linear partial differential equation of mathematical physics

$$i\hbar \frac{\partial \psi(t, x)}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi(t, x) + V(x)\psi(t, x), \tag{30}$$

where $\Delta = \frac{\partial^2}{\partial x^2}$. This equation is equivalent to the Hamiltonian functional equations for the canonical fields $\phi(x)$, $\pi(x)$ introduced by $\psi(t, x) = \phi(t, x) + i\pi(t, x)$. The Hamilton's functional is obtained by applying the general rule

$$H(\phi, \pi) = \langle \psi | \hat{H} | \psi \rangle = \int dx \frac{1}{2\hbar} (\phi - i\pi)(-\frac{\hbar^2}{2m} \Delta + V)(\phi + i\pi)$$

$$= \int dx \frac{1}{2\hbar} \left[-\frac{\hbar^2}{2m} (\phi \Delta \phi + \pi \Delta \pi) + V(\phi^2 + \pi^2) \right] \tag{31}$$

The Hamilton's functional (31) is traditionally (see for example [3, 10] further trans-
formed into

$$H(\phi, \pi) = \frac{1}{2\hbar} \int_X dx \left[\frac{\hbar^2}{2m} ((\partial_x \phi(x))^2 + (\partial_x \pi(x))^2) + V(x)(\phi(x)^2 + \pi(x)^2) \right],$$
(32)

but the form (31) is much more suitable for the construction of the Lagrangian formu-
lation. The Hamilton's equations corresponding to (31) (or to (32)) are

$$\dot\phi = \frac{\delta H}{\delta \pi} = \frac{1}{\hbar}(V - \frac{\hbar^2}{2m}\Delta)\pi$$

$$\dot\pi = -\frac{\delta H}{\delta \phi} = \frac{1}{\hbar}(\frac{\hbar^2}{2m}\Delta - V)\phi.$$
(33)

The generalized momentum $\pi(x)$ is expressed via $\dot\phi(x)$ using the formula (33a) and
reads

$$\pi(x) = \hbar(V - \frac{\hbar^2}{2m}\Delta)^{-1}\dot\phi$$
(34)

Observe that the differential operator $V - \frac{\hbar^2}{2m}\Delta$ maps real functions into real ones
and therefore the formula (34) is a special case of (12) $p = (\hat{H}^R)^{-1}\dot{q}$. Using the Eq.
(34) to replace π and (33a) to replace $\Delta\pi$, the Lagrangian functional corresponding
to (31) is formed by the standard rule and reads

$$L(\phi, \dot\phi) = \int dx \left[\frac{-1}{2\hbar}\phi(V - \frac{\hbar^2}{2m}\Delta)\phi + \frac{\hbar}{2}\dot\phi(V - \frac{\hbar^2}{2m}\Delta)^{-1}\dot\phi \right].$$
(35)

This is just the general formula (13) with $H^I_{nm} = 0$. Observe that the expression $\Delta\pi$
that appears in the Hamiltonian (31) is easily handled using the equation of motion
(34a). On the other hand, replacement of the generalized momenta that appear in the
term $\partial_x \pi(x)\partial_x \pi(x)$ of the equivalent Hamiltonian (32) using (34) might appear as
an additional problem in the construction of the Lagrangian. We see that the problem
is related to the particular form of the Hamiltonian (32) and does not appear in the
equivalent Hamiltonian (31).

We need the Lagrangian equations $-\frac{d}{dt}\frac{\delta L}{\delta \dot\phi} + \frac{\delta L}{\delta \phi} = 0$ with the Lagrangian (35).
Variation of the functional variation δL due to a variation of $\delta\dot\phi$ gives

$$\delta_{\delta\dot\phi}L = \int dx \frac{\hbar}{2} \left[\delta\dot\phi((V - \frac{\hbar^2}{2m}\Delta)^{-1}\dot\phi) + \dot\phi((V - \frac{\hbar^2}{2m}\Delta)^{-1}\delta\dot\phi) \right]$$
(36)

However, since the inverse of a Hermitian Hamiltonian $\hat{H}$ is also Hermitian the two
terms in the previous expression are equal and the functional derivative of L with
respect to $\dot\phi$ becomes

$$\frac{\delta L}{\delta \dot\phi} = \hbar(V - \frac{\hbar^2}{2m}\Delta)^{-1}\dot\phi.$$
(37)

The Lagrange equations become

$$\hbar^2 (V - \frac{\hbar^2}{2m}\Delta)^{-1}\ddot{\phi} = -(V - \frac{\hbar^2}{2m}\Delta)\phi \tag{38}$$

or

$$\hbar^2\ddot{\phi} = -(V - \frac{\hbar^2}{2m}\Delta)^2\phi. \tag{39}$$

Of course, the Lagrange equation (39) is the special case of the general formula (19), as was the Lagrangian (35) the special case of (13). No additional problems in the construction of the Lagrangian formulation for the Schrödinger equation (30) occur because of the special choice of the coordinate representation. Like in the general case, the only possible obstacle to the construction might be non-existence of the inverse operator $(\hat{H}_R)^{-1}$ which is in this case $(V - \frac{\hbar^2}{2m}\Delta)^{-1}$.

3.4 Klein–Gordon Equation

Consider the Schrödinger equation for a free relativistic one-dimensional scalar particle

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi = [\hbar^2 c^2\Delta + m^2 c^4]^{1/2}\psi. \tag{40}$$

Applying the general formulas from Sect. 2, or replacing everywhere in the previous example $-\frac{\hbar^2}{2m}\Delta + V(x)$ with $[\hbar^2 c^2\Delta + m^2 c^4]^{1/2}$ we arrive at the corresponding Lagrangian

$$L = \int dx \left[\frac{1}{2\hbar}\phi[\hbar^2 c^2\Delta + m^2 c^4]^{1/2}\phi + \frac{\hbar}{2}\dot{\phi}[(\hbar^2 c^2\Delta + m^2 c^4)^{1/2}]^{-1}\dot{\phi} \right], \tag{41}$$

and the corresponding Lagrangian equations for real functions $\phi(t, x)$

$$\frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2} = \Delta\phi - \left(\frac{mc}{\hbar}\right)^2\phi \tag{42}$$

This is the Klein–Gordon equation for the real field $\phi(t, x)$.

4 Summary

In summary, we have developed the Lagrangian formalism for the abstract linear Schrödinger equation on a complex Hilbert space of a quantum system. For a given Hamiltonian operator $\hat{H} = \hat{H}^R + i\hat{H}^I$ the Lagrangian system is expressed in terms of the operators $\hat{H}^R$, $\hat{H}^I$ and $(\hat{H}^R)^{-1}$, and is given by a second order equation on a real space. The operator $(\hat{H}^R)^{-1}$, which is crucial for construction of the Lagrangian formulation, exists provided that the spectrum of $\hat{H}$ is bounded away from zero. If this is not the case, than the Schrödinger equation is in fact equivalent to a constrained

Hamiltonian system, with the corresponding singular Lagrangian formulation. A simple example illustrating the failure of the procedure that might occur in a singularly chosen basis is provided. The general formulation of the Lagrangian system is also illustrated in the eigenbasis of a Hamiltonian with a discrete spectrum and in the coordinate representation. The Klein–Gordon equation is seen as the Lagrangian system corresponding to the Schrödinger equation of a relativistic free particle.

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