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DERIVATION OF GROSS-PITAEVSKII VERSION OF NONLINEAR SCHROEDINGER EQUATION FROM SCALE INVARIANCE

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Abstract. It is known that in the usual 3-D space, the Schroedinger equation can be derived from scale-invariance. In view of the fact that, according to modern physics, the actual dimension of proper space may be different from 3, it is desirable to analyze what happens in other spatial dimensions D. It turns out that while for $D \geq 3$ we still get only the Schroedinger's equation, for $D = 2$, we also get the Gross-Pitaevskii version of a nonlinear Schroedinger equation that describes a quantum system of identical bosons, and for $D = 1$, we also get a new nonlinear version of the Schroedinger equation.

Keywords: scale-invariance, nonlinear Schroedinger equation, Gross-Pitaevskii equation, system of identical bosons.

1. Formulation of the Problem

Schroedinger's equation: a brief reminder. In non-relativistic quantum mechanics, a state of a particle is described by a complex-valued wave function $\psi(x,t)$. The observational meaning of the wave function is that for each spatial location region Ω, the probability to find the particle in this region is equal to $\int_\Omega |\psi(x,t)|^2\,\mathrm{d}x$; see, e.g., [1].

The dynamics of the wave function is described, in the non-relativistic approximation, by the Schroedinger equation

$$\mathrm{i}\cdot\hbar\cdot\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\cdot\nabla^2\psi + V(x,t)\cdot\psi(x,t),$$

where:

- $\mathrm{i} \stackrel{\text{def}}{=} \sqrt{-1}$,
- $\hbar$ is Planck's constant,
- m is the particle's mass,
- $\nabla \stackrel{\text{def}}{=} \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \ldots, \frac{\partial}{\partial x_D}\right)$, and

- $V(x,t)$ is the potential energy of the particle at location x.

This equation can be derived from the minimum action principle. Namely, the Schroedinger equation is equivalent to requiring that the field $\psi(x,t)$ minimizes the action $S \stackrel{\text{def}}{=} \int L(x,t)\,\mathrm{d}x\,\mathrm{d}t$, where the function L – called the *Lagrange function* – has the form

$$L = \mathrm{i}\cdot\hbar\cdot\left(\psi\cdot\frac{\partial\psi^*}{\partial t} - \psi^*\cdot\frac{\partial\psi}{\partial t}\right) + \frac{\hbar^2}{2m}\cdot(\nabla\psi\cdot\nabla\psi^*) - V\cdot\psi\cdot\psi^*,$$

where:

- ψ^* means complex conjugation, and
- for every two vectors $\vec{a}=(a_1,\ldots,a_D)$ and $\vec{b}=(b_1,\ldots,b_D)$, the notation $\vec{a}\cdot\vec{b}$ describes their dot (scalar) product $\vec{a}\cdot\vec{b}=\sum\limits_{i=1}^{D} a_i\cdot b_i$.

Schroedinger's equation can be derived from scale invariance. In modern physics, the notions of symmetry play a fundamental role; see, e.g., [1, 6]. This makes perfect sense, since:

- the main purpose of science is to make predictions, and
- the only way we can make predictions about new situations in when we find some similarity (symmetry) between the new situations and situations that have been previously observed – and for which we know what happened.

One of the simplest symmetries comes from the fact that while physical equations deal with the numerical values of the physical quantities, these numerical values depend on the choice of the corresponding measuring units. If we use a new measuring unit which is λ times smaller than the previously used one, then all the numerical values of the corresponding quantity get multiplied by λ: $x \to x' = \lambda\cdot x$. For example, if we replace 1 m with 1 cm as the unit of length, then instead of 2 m, we get $200\cdot 2 = 200$ cm.

It is reasonable to require that the fundamental physical equations should not change if we simply re-scale the numerical values by changing the measuring units. It turns out that many fundamental physical equations – including Maxwell's equation for electrodynamics, Einstein's equation for General Relativity, and Schroedinger's equation of quantum mechanics – can be derived from this requirement of scale-invariance – plus a few other reasonable symmetries; see, e.g., [2, 3, 7, 8].

What if we take into account that the dimension of proper space may be different from 3? The above derivations deal with the usual 4-dimensional space-time, in which the proper space is 3-dimensional. However, according to modern physics, the actual dimension D of proper space may be different from 3; see, e.g., [4].

It is therefore desirable to analyze what happens if we look for scale-invariant equations and Lagrange functions in spatial dimensions $D \neq 3$.

What we do in this paper. In this paper, we show that for dimensions $D \geq 3$, we still get only the Schroedinger equation, but for $D = 2$ and $D = 1$, we also get additional nonlinear versions of Schroedinger's equations:

- For $D = 2$, we also get the Gross-Pitayevsky equation

$$\mathrm{i} \cdot \hbar \cdot \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \cdot \nabla^2 \psi + V(x,t) \cdot \psi(x,t) + \frac{c}{m} \cdot |\psi|^2 \cdot \psi,$$

  where c is a constant. This equation describes a quantum system of identical bosons; see, e.g., [5,9,10]. This equation corresponds to the Lagrange function

$$L = \mathrm{i} \cdot \hbar \cdot \left(\psi \cdot \frac{\partial \psi^*}{\partial t} - \psi^* \cdot \frac{\partial \psi}{\partial t}\right) + \frac{\hbar^2}{2m} \cdot (\nabla \psi \cdot \nabla \psi^*) - V \cdot \psi \cdot \psi^* + \frac{f}{m} \cdot |\psi|^4.$$

- For $D = 1$, we also get the following new nonlinear version of the Schroedinger's equation

$$\mathrm{i} \cdot \hbar \cdot \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \cdot \nabla^2 \psi + V(x,t) \cdot \psi(x,t) + \frac{c}{m} \cdot |\psi|^4 \cdot \psi.$$

  This equation corresponds to the Lagrange function

$$L = \mathrm{i} \cdot \hbar \cdot \left(\psi \cdot \frac{\partial \psi^*}{\partial t} - \psi^* \cdot \frac{\partial \psi}{\partial t}\right) + \frac{\hbar^2}{2m} \cdot (\nabla \psi \cdot \nabla \psi^*) - V \cdot \psi \cdot \psi^* + \frac{f}{m} \cdot |\psi|^6.$$

2. Analysis of the Problem

Lagrange function for non-relativistic quantum mechanics: a general description. We want to obtain a Lagrange function describing the dynamics of a particle of mass m, described by a (complex-valued) wave function $\psi(x,t)$, in a field with a potential energy function $V(x,t)$. Since the Lagrange function must be real-valued, it can also depend on the complex conjugate values $\psi^*(x,t)$.

This Lagrange function should be rotation-invariant. There is one more invariance specific for non-relativistic quantum mechanics. Namely, it is known that in quantum mechanics, we can add a constant phase to all the values of $\psi(x,t)$ without changing the physical meaning. Thus, the Lagrange function should be *phase-invariant*, i.e., invariant with respect to the transformation

$$\psi(x,t) \to \exp(\mathrm{i} \cdot \alpha) \cdot \psi(x,t)$$

for any real constant α.

In general, a Lagrange function depends both on the fields and on their derivatives. Let us, as usual, denote the time derivative by $\dot{\psi}$, and the derivative with respect to x_k by $\psi_{,k}$.

Definition 1. *By a* Lagrange function L for non-relativistic quantum mechanics, *we mean a phase-invariant rotation-invariant real-valued analytical function of the* *mass m, its inverse m^{-1}, fields $\psi(x,t)$, $\psi^*(x,t)$, and $V(x,t)$, and their derivatives of arbitrary orders with respect to time and spatial coordinates:*

$$L(m, m^{-1}, \psi(x,t), \psi_{,k}(x,t), \dot{\psi}(x,t), \ldots, \psi^*(x,t), \psi^*_{,k}(x,t), \dot{\psi}^*(x,t), \ldots,$$

$$V(x,t), V_{,k}(x,t), \dot{V}(x,t), \ldots)$$

What does scale invariance mean for non-relativistic quantum mechanics? In relativistic physics, there is a direct connection between units of space and time. In contrast, in the non-relativistic case, there is no such direct connection, so we can independently change the unit for space $x^i \to x'^i = \lambda \cdot x^i$ and a unit of time

$$t \to t' = \mu \cdot t.$$

How do L, $\psi(x,t)$, and $V(x,t)$ change under these transformations? A specific feature of quantum measurements is that simple experiments enable us to obtain a unit of action $\hbar$; therefore action $S = \int L(x,t)\,\mathrm{d}x\,\mathrm{d}t$ must be invariant with respect to scale transformations. Hence, $L(x,t)$ (which is action/(volume$\times$time)) must transform as $L \to L' = \lambda^{-D} \cdot \mu^{-1} \cdot L$, where D is the spatial dimension.

Similarly, since action is energy $\times$ time, and action is invariant, the potential energy $V(x,t)$ must transform as $V \to V' = \mu^{-1} \cdot V$.

Energy is mass $\times$ velocity^2. We know how energy is transformed and how velocity is transformed. Therefore, for mass, we get $m \to m' = \lambda^{-2} \cdot \mu \cdot m$.

The transformation law for the wave function $\psi(x,t)$ can be deduced from its physical meaning: the integral $\int |\psi|^2\,\mathrm{d}x$ is a probability and is therefore independent (invariant) on the choice of length or time units, i.e. invariant. So, $|\psi|^2 \sim 1/\text{length}^D$, hence, $|\psi|^2 \to \lambda^{-D} \cdot |\psi|^2$, and $\psi \to \psi' = \lambda^{-D/2} \cdot \psi$.

If we change the units, then we get the new expression for L

$$L'(x,t) = \lambda^{-D} \cdot \mu^{-1} \cdot L(m, m^{-1}, \psi(x,t), \psi_{,k}(x,t), \dot{\psi}(x,t), \ldots,$$

$$\psi^*(x,t), \psi^*_{,k}(x,t), \dot{\psi}^*(x,t), \ldots, V(x,t), V_{,k}(x,t), \dot{V}(x,t), \ldots). \quad (1)$$

On the other hand, if we change the units in the original expression, we get

$$L' = L(\lambda^2 \cdot \mu^{-1} \cdot m, \lambda^{-2} \cdot \mu \cdot m^{-1}, \lambda^{-D/2} \cdot \psi, \lambda^{-D/2-1} \cdot \psi_{,k}, \lambda^{-D/2} \cdot \mu \cdot \dot{\psi}, \ldots,$$

$$\lambda^{-D/2} \cdot \psi^*, \lambda^{-D/2-1} \cdot \psi^*_{,k}, \lambda^{-D/2} \cdot \mu \cdot \dot{\psi}^*, \ldots,$$

$$\mu^{-1} \cdot V, \lambda^{-1} \cdot \mu^{-1} \cdot V_{,k}, \mu^{-2} \cdot \dot{V}, \ldots). \quad (2)$$

Definition 2. *We say that a Lagrange function is* scale-invariant *if for all $\lambda > 0$ and $\mu > 0$, the expressions* (1) *and* (2) *coincide.*

Now, we are ready to present our main results.

3. Main Results

Theorem 1. *For $D \geq 3$, every scale-invariant Lagrange function has the form*

$$L = \mathrm{i} \cdot b \cdot \left(\psi \cdot \frac{\partial \psi^*}{\partial t} - \psi^* \cdot \frac{\partial \psi}{\partial t} \right) + \frac{c}{m} \cdot (\nabla \psi \cdot \nabla \psi^*) + d \cdot V \cdot \psi \cdot \psi^* + L_0, \quad (2)$$

where b, c, and d are real constants, and L_0 is an expression which does not contribute to variational equations.

Theorem 2. *For $D = 2$, every scale-invariant Lagrange function has the form*

$$L = \mathrm{i} \cdot b \cdot \left(\psi \cdot \frac{\partial \psi^*}{\partial t} - \psi^* \cdot \frac{\partial \psi}{\partial t} \right) + \frac{c}{m} \cdot (\nabla \psi \cdot \nabla \psi^*) + d \cdot V \cdot \psi \cdot \psi^* + \frac{f}{m} \cdot |\psi|^4 + L_0, \quad (3)$$

where b, c, d, and f are real constants, and L_0 is an expression which does not contribute to variational equations.

Theorem 3. *For $D = 1$, every scale-invariant Lagrange function has the form*

$$L = \mathrm{i} \cdot b \cdot \left(\psi \cdot \frac{\partial \psi^*}{\partial t} - \psi^* \cdot \frac{\partial \psi}{\partial t} \right) + \frac{c}{m} \cdot (\nabla \psi \cdot \nabla \psi^*) + d \cdot V \cdot \psi \cdot \psi^* + \frac{f}{m} \cdot |\psi|^6 + L_0, \quad (4)$$

where b, c, and d are real constants, and L_0 is an expression which does not contribute to variational equations.

Comment. Thus, we indeed get the desired equations: only Schroedinger for $D \geq 3$, Gross-Pitaevskii for $D = 2$, and a new nonlinear equation for $D = 1$.

Proof of Theorems 1–3.

General analysis. Let us first fix m and consider only transformations which preserve m, i.e., transformations for which $\mu = \lambda^2$. For these transformations, the formula (1) takes the form

$$L'(x,t) = \lambda^{-(D+2)} \cdot L(m, m^{-1}, \psi(x,t), \psi_{,k}(x,t), \dot{\psi}(x,t), \ldots,$$
$$\psi^*(x,t), \psi^*_{,k}(x,t), \dot{\psi}^*(x,t), \ldots, V(x,t), V_{,k}(x,t), \dot{V}(x,t), \ldots), \quad (5)$$

while the formula (2) takes the form

$$L' = L(m, m^{-1}, \lambda^{-D/2} \cdot \psi, \lambda^{-D/2-1} \cdot \psi_{,k}, \lambda^{-D/2-2} \cdot \dot{\psi}, \ldots,$$
$$\lambda^{-D/2} \cdot \psi^*, \lambda^{-D/2-1} \cdot \psi^*_{,k}, \lambda^{-D/2-2} \cdot \dot{\psi}^*, \ldots,$$
$$\lambda^{-2} \cdot V, \lambda^{-3} \cdot V_{,k}, \lambda^{-4} \cdot \dot{V}, \ldots). \quad (6)$$

The expressions (5) and (6) must coincide. Since L is an analytical function, it is a (possibly infinite) sum of monomials. Since the two analytical functions of λ^{-1} coincide, this means that all the coefficients at the corresponding monomials must coincide.

Each monomial depends on λ^{-1}. All the monomials in the expression (5) multiply by $\lambda^{-(D+2)}$. Thus, in the right-hand side, we can only have the monomials which are similarly multiplied. Here:

- ψ is multiplied by $\lambda^{-D/2}$,
- V is multiplied by λ^{-2},
- spatial differentiation leads to multiplication by λ^{-1}, and
- temporal differentiation leads to multiplication by λ^{-1}.

Thus, we must have

$$D + 2 = \frac{D}{2} \cdot n_\psi + 2n_V + n_S + 2n_T, \tag{7}$$

where:

- n_ψ is the total number of terms ψ, ψ^*, and their derivatives,
- n_V is the total number of V and its derivatives,
- n_S is the total number of spatial differentiations, and
- d_T is the total number of differentiations with respect to time.

Terms not depending on ψ do not affect the action and, thus, do not contribute to the equations; all these terms go directly to L_0. Thus, we must have $n_\psi \geq 1$.

Terms linear (or, in general, of odd order) in ψ or in its derivatives are not phase-invariant, so we must have n_ψ even and $n_\psi \geq 2$, hence $n_\psi - 2 \geq 0$. If we subtract D from both sides of the equality (5), we conclude that

$$2 = \frac{D}{2} \cdot (n_\psi - 2) + 2n_V + n_S + 2n_T. \tag{8}$$

Case of $D \geq 3$. For odd $D \geq 3$, since the left-hand side is an integer, the difference $n_\psi - 2$ must be even. If this difference is non-zero, we must thus have $n_\psi - 2 \geq 2$. In this case, $(D/2) \cdot (n_\psi - 2) \geq D \geq 3$. However, we know that the sum of this product and several non-negative integers is equal to 2. Thus, in this case, we cannot have $n_\psi - 2 > 0$, so we must have $n_\psi - 2 = 0$ and $n_\psi = 2$.

Similarly, for even $D > 2$, if $n_\psi - 2 > 0$ then, since n_ψ is even, we must have

$$n_\psi - 2 \geq 2$$

thus $(D/2) \cdot (n_\psi - 2) \geq D > 2$, so we cannot have the sum equal to 2.

Thus, for all $D \geq 3$, we must have $n_\psi = 2$ and so,

$$2 = 2n_V + n_S + 2n_T.$$

Since all three integers n_V, n_S, and n_T are non-negative, we only have the following three options:

- $n_V = 1$, $n_S = n_T = 0$;

- $n_V = 0$, $n_S = 2$, $n_T = 0$; and
- $n_V = 0$, $n_S = 0$, $n_T = 1$.

In all these cases, we have $n_\psi = 2$.

In the first case, we get a product of V and two terms of type ψ and ψ^*; the only way to make it real-valued and phase-invariant is to have $V \cdot \psi \cdot \psi^*$. Another possibility would be $V \cdot (\psi^2 + (\psi^*)^2)$, but the corresponding term is not phase-invariant.

In the second case, we have two derivatives of two functions ψ. Due to the requirement that L is real-valued, one of them must be ψ, and another one ψ^*. Due to rotation-invariance, we have two possibilities: $\psi_{,i} \cdot \psi^*_{,i}$ and $\psi \cdot \nabla^2 \psi^*$; the second term differs from the first one by a full derivative, so we can assume that we get the first term, and add the full derivative to L_0.

In the third case, we have two functions ψ and ψ^* and one time derivative. This leads to the corresponding term in L.

Case of $D = 2$. For $D = 2$, the above equation takes the form

$$2 = (n_\psi - 2) + 2n_V + n_S + 2n_T.$$

Here, in addition to the case $n_\psi = 2$, we can also have the case when $n_\psi - 2 = 2$ and thus, $n_\psi = 4$; in this case, we have $n_V = n_S = n_T = 0$. The only phase-invariant real-valued term of fourth order in ψ and ψ^* is $(\psi \cdot \psi^*)^2 = |\psi|^4$.

Case of $D = 1$. For $D = 1$, we get

$$2 = \frac{1}{2} \cdot (n_\psi - 2) + 2n_V + n_S + 2n_T.$$

The number of spatial differentiations must be even, otherwise the Lagrange function is not rotation-invariant. Since all the terms in the above equality, except for the term

$$\frac{1}{2} \cdot (n_\psi - 2),$$

are even, this term must also be even. Thus, the only way for it to be non-zero is if this terms is ≥ 2. This term cannot be larger than 2 – then we would not be able to have 2 in the left-hand side. Thus, we must have $(1/2) \cdot (n_\psi - 2) = 2$, hence $n_\psi - 2 = 4$ and $n_\psi = 6$ – and $n_V = n_S = n_T = 0$. Similarly to the case $D = 2$, the only phase-invariant real-valued term of sixth order in ψ and ψ^* is the term $(\psi \cdot \psi^*)^3 = |\psi|^6$.

Final part of the proof. We have almost proved the theorems, except for the dependence on m. To finalize the proof, we can take the expression that we have obtained so far,

- explicitly mention that all the coefficients a, b, $\ldots$ should depend on m, and
- describe the requirement that the resulting formula be invariant with respect to the scaling transformation corresponding to all possible pairs (λ, μ).

This enables us to find the exact dependence of all the coefficients on m.

The theorems are proven.

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