Derivation of Gross-Pitaevskii Version of Nonlinear Schroedinger Equation from Scale Invariance

Olga Kosheleva and Vladik Kreinovich

University of Texas at El Paso
500 W. University
El Paso, Texas 79968, USA
olgak@utep.edu, vladik@utep.edu

1. Schroedinger's Equation: A Brief Reminder

- In non-relativistic quantum mechanics, a state of a particle is described by a complex-valued wave f-n $\psi(x,t)$.
- The observational meaning: for each spatial region Ω, the probability P to find the particle in Ω is

$$P = \int_\Omega |\psi(x,t)|^2 \, \mathrm{d}x.$$

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

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

- This equation can be derived from the minimum action principle $S \stackrel{\text{def}}{=} \int L(x,t)\,\mathrm{d}x\,\mathrm{d}t \to \min$, where

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

2. Scale Invariance

- In modern physics, the notions of symmetry play a fundamental role; this makes perfect sense:
- The main purpose of science is to make predictions.
- 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.

3. Scale Invariance (cont-d)

- In general:
  - 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.
- Many fundamental physical equations can be derived from scale-invariance, including Schroedinger's.

4. What We Do

- The above derivations deal with the usual 4-dimensional space-time.
- However, according to modern physics, the actual dimension D of proper space may be different from 3.
- We show that for dimensions $D \geq 3$, we still get only the Schroedinger equation.
- For $D = 2$, we also get the Gross-Pitayevsky equation that describes a quantum system of identical bosons:

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

- This equation corresponds to the Lagrange function

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

5. What We Do (cont-d)

- For $D = 1$, we also get a 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

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

6. Analysis of the Problem

- 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.
- Also, in quantum mechanics:
  - we can add a constant phase to all the values of $\psi(x,t)$
  - without changing the physical meaning.

7. Analysis of the Problem (cont-d)

- Thus, the Lagrange function should be *phase-invariant*, i.e., invariant with respect

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

- 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 $\psi_{,k}$.

8. What Is a Lagrange function L for Non-Relativistic Quantum Mechanics: Definition

- By L, we mean a phase-invariant rotation-invariant real-valued analytical function of:
  - the mass m and its inverse m^{-1}, and
  - fields $\psi(x,t)$, $\psi^*(x,t)$, and $V(x,t)$, and their derivatives of arbitrary orders w.r.t. t and x_i:

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

9. What Does Scale Invariance Mean

- We can 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?
- In quantum measurements, 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 $L \to L' = \lambda^{-D} \cdot \mu^{-1} \cdot L$.
- Invariant action is energy $\times$ time, so energy $V(x,t)$ transforms as $V \to V' = \mu^{-1} \cdot V$.

10. What Does Scale Invariance Mean (cont-d)

- 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 invariant.
- So, $|\psi|^2 \sim 1/\text{length}^D$, hence, $|\psi|^2 \to \lambda^{-D} \cdot |\psi|^2$, and $\psi \to \psi' = \lambda^{-D/2} \cdot \psi$.

11. When Is L Scale-Invariant

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

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

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

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

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

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

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

- We say that L is *scale-invariant* if for all $\lambda > 0$ and $\mu > 0$, these expressions coincide.

12. Main Results: Formulation

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

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

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

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

- For $D = 1$, every scale-invariant Lagrange function has the form

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

13. Proof

- Let us consider only transformations which preserve m, i.e., transformations for which $\mu = \lambda^2$.
- For these transformations, the expression-to-coincide have the form

$$L_1 = \lambda^{-(D+2)} \cdot L(m, m^{-1}, \psi(x,t), \psi_{,k}(x,t), \dot{\psi}(x,t), \ldots,$$

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

$$L_2 = L(m, m^{-1}, \lambda^{-D/2} \cdot \psi, \lambda^{-D/2-1} \cdot \psi_{,k}, \lambda^{-D/2-2} \cdot \dot{\psi}, \ldots,$$

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

$$\lambda^{-2} \cdot V, \lambda^{-3} \cdot V_{,k}, \lambda^{-4} \cdot \dot{V}, \ldots).$$

14. Proof (cont-d)

- Since L is an analytical function, both expressions L_i are analytical in λ^{-1}.
- So, each L_i is a (possibly infinite) sum of monomials.
- So, all the coefficients at the corresponding monomials must coincide.
- All the monomials in L_1 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 multiplies by λ^{-1}.

15. Proof (cont-d)

- Thus, we must have

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

  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 S and, thus, do not contribute to the equations.

- Thus, we must have $n_\psi \geq 1$.

16. Proof (cont-d)

- 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 $n_\psi - 2 \geq 0$, thus $2 = \dfrac{D}{2} \cdot (n_\psi - 2) + 2n_V + n_S + 2n_T$.
- 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, then $n_\psi - 2 \geq 2$ and $(D/2) \cdot (n_\psi - 2) \geq D \geq 3$.
- 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 $n_\psi - 2 \geq 2$ and $(D/2) \cdot (n_\psi - 2) \geq D > 2$.

17. Proof (cont-d)

- 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 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.

18. Proof (cont-d)

- 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.

19. 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 $(\psi \cdot \psi^*)^2 = |\psi|^4$.

20. 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 L 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 to be ≥ 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 $n_V = n_S = n_T = 0$.
- The only phase-invariant real-valued term of sixth order in ψ and ψ^* is the term $(\psi \cdot \psi^*)^3 = |\psi|^6$.

21. 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, ... should depend on m, and
  - describe the requirement that the resulting formula be scale-invariant.
- This enables us to find the exact dependence of all the coefficients on m.
- The theorems are proven.

22. Acknowledgments

This work was supported in part:

- by the National Science Foundation grants:
  - HRD-0734825 and HRD-1242122 (Cyber-ShARE Center of Excellence) and
  - DUE-0926721, and
- by an award from Prudential Foundation.