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

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1. 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: for each spatial region \( \Omega \), the probability \( P \) to find the particle in \( \Omega \) is

\[
P = \int_{\Omega} |\psi(x, t)|^2 \, dx.
\]

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

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

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

\[
L = i \cdot \hbar \cdot \left( \psi \cdot \frac{\partial \psi^*}{\partial t} - \psi^* \cdot \frac{\partial \psi}{\partial t} \right) + \frac{\hbar^2}{2m} \cdot (\nabla \psi \cdot \nabla \psi^*) - V \cdot \psi \cdot \psi^*.
\]
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 \( \lambda \) times smaller than the previously used one,
  - then all the numerical values of the corresponding quantity get multiplied by \( \lambda \): \( x \rightarrow x' = \lambda \cdot x \).

- 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:

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

• This equation corresponds to the Lagrange function

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

- For $D = 1$, we also get a new nonlinear version of the Schrödinger’s equation

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

- This equation corresponds to the Lagrange function

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

  \[ \psi(x, t) \rightarrow \exp(i \cdot \alpha) \cdot \psi(x, t). \]

- 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 $x^i \rightarrow x'^i = \lambda \cdot x^i$ and a unit of time $t \rightarrow t' = \mu \cdot t$.

• 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 $S = \int L(x,t) \, dx \, dt$ must be invariant with respect to scale transformations.

• Hence, $L(x,t)$ (which is action/(volume×time)) must transform as $L \rightarrow L' = \lambda^{-D} \cdot \mu^{-1} \cdot L$.

• Invariant action is energy × time, so energy $V(x,t)$ transforms as $V \rightarrow V' = \mu^{-1} \cdot V$. 
10. What Does Scale Invariance Mean (cont-d)

- Energy is mass × velocity$^2$.
- We know how energy is transformed and how velocity is transformed.
- Therefore, for mass, we get $m \rightarrow m' = \lambda^{-2} \cdot \mu \cdot m$.
- The transformation law for the wave function $\psi(x, t)$ can be deduced from its physical meaning.
- The integral $\int |\psi|^2 \, dx$ is a probability and is therefore invariant.
- So, $|\psi|^2 \sim 1/\text{length}^D$, hence, $|\psi|^2 \rightarrow \lambda^{-D} \cdot |\psi|^2$, and $\psi \rightarrow \psi' = \lambda^{-D/2} \cdot \psi$. 


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

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

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

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

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

$$i \cdot b \left( \psi \cdot \frac{\partial \psi^*}{\partial t} - \psi^* \cdot \frac{\partial \psi}{\partial t} \right) + \frac{c}{m} (\nabla \psi \cdot \nabla \psi^*) + d \cdot V \cdot \psi \cdot \psi^* + \frac{f}{m} |\psi|^6 + L_0.$$
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 $\lambda^{-1}$.

- 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:
  - $\psi$ is multiplied by $\lambda^{-D/2}$,
  - $V$ is multiplied by $\lambda^{-2}$,
  - spatial differentiation leads to multiplication by $\lambda^{-1}$, and
  - temporal differentiation multiplies by $\lambda^{-1}$. 
15. Proof (cont-d)

- Thus, we must have

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

where:

- \( n_\psi \) is the total number of terms \( \psi, \psi^* \), 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 \( \psi \) 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 $\psi$ or in its derivatives are not phase-invariant.

- So, we must have $n_\psi$ even and $n_\psi \geq 2$, hence $n_\psi - 2 \geq 0$, thus $2 = \frac{D}{2} \cdot (n_\psi - 2) + 2n_V + n_S + 2n_T$.

- 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 $\psi$ and $\psi^*$.

- 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 $\psi$.
- Due to the requirement that $L$ is real-valued, one of them must be $\psi$, and another one $\psi^*$.
- 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 $\psi$ and $\psi^*$ 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 $\psi$ and $\psi^*$ 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 $\geq 2$.

- 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 $\psi$ and $\psi^*$ 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.
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