APPLICATION DIRECT METHOD CALCULUS OF VARIATION FOR KLEIN-GORDON FIELD

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Graphical abstract

Abstract

Klein-Gordon field is often used to study the dynamics of elementary particles. The Klein–Gordon equation was first considered as a quantum wave equation by Schrödinger in his search for an equation describing de Broglie waves. The equation was found in his notebooks from late 1925, and he appears to have prepared a manuscript applying it to the hydrogen atom. Yet, because it fails to take into account the electron’s spin, the equation failed to predict the fine structure of the hydrogen atom, and overestimated the overall magnitude of the splitting pattern energy. This paper will describe in detail using the Direct Method of Calculus Variation as an alternative to solve the Klein-Gordon field equations. The Direct Method simplified the calculation because the variables are calculated and expressed in function of energy. The result of the calculation of Klein-Gordon Field provided the existence of the minimizer, i.e. $\tilde{\phi} = \phi_0 + u$ with $u \in W^{1,p}_0$ and $\phi_0 \in W^{1,p}$. Explicit form of the minimizer was calculated by the Ritz method through rows of convergent density.

Keywords: Direct method, density functional theory, klein-gordon field

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1.0 INTRODUCTION

The Klein–Gordon equation was first considered as a quantum wave equation by Schrödinger in his search for an equation describing de Broglie waves as evident from his notebooks from the late 1925, and he appears to have prepared a manuscript applying it to the hydrogen atom. Yet, because it fails to take into account the electron’s spin, the equation incorrectly predicted the fine structure of the hydrogen atom, including overestimating the overall magnitude of the splitting pattern energy level. Since the sine-Gordon equation is not integrable when the singular potential term is present, no exact solution is available and no exact value of the critical parameter is available as well. There are many unknown properties of the solution behaviors in this case [1–5]. A similar phenomenon has been also found with the non-linear Schrodinger equations [6, 7]. For example, in [6, 8] the singular potential term perturbs the soliton propagation and similar phenomena of particle pass, particle capture and particle-reflection were observed for some critical parameters.

The Density Functional Theory (DFT) for quantum systems is an inexact theory or idea about the problem of many particles, to study the behaviors of the ground state electron systems via the variation principle. Although formally exact, the general functional is unknown. Nevertheless, there are various approaches that work well for a variety of electronic systems [9, 10].

In practical terms, this theory is very reliable to use in studying the structural stability of the system, elasticity, vibration behavior and determine the equilibrium state. Thus, DFT also has drawbacks, among which include uncontrolled approximation.
However, with DFT, it is possible to study the behavior of the system through the massive range of density that depends only on four variables x, y, z, and t. It is certainly easier for researchers than having to seek answers to the Schrödinger equation that depends on the variables of each particle making up the system, as in the Hartee-Fock method. Thus, DFT offers a fairly simple method for calculation.

2.0 DIRECT METHOD CALCULUS VARIATION

The typical problem of the calculus of variations is to minimize an integral of the form

$$F(u) := \int_{\Omega} f(x, u(x), Du(x))dx$$

(1)

where $\Omega$ is some open subset in $\mathbb{R}^d$ (in most cases, $\Omega$ is bounded), among function

$$u: \Omega \rightarrow \mathbb{R},$$

which belongs to some suitable class of functions and satisfying a boundary condition. For example, a Dirichlet boundary condition is as follows:

$$u(y) = g(y) \text{ for } y \in \partial \Omega$$

for $g: \partial \Omega \rightarrow \mathbb{R}$ given.

Thus, the problem is

$$F(u) \rightarrow \min, \quad u \in \mathcal{C},$$

where $\mathcal{C}$ is some space of functions. The strategy of the direct method is very simple, i.e. to take a minimizing sequence where

$$(u_n)_{n \in \mathbb{N}} \subset \mathcal{C} \text{ minimization},$$

$$\lim_{n \rightarrow \infty} F(u_n) = \inf_{u \in \mathcal{C}} F(u),$$

(2)

and show that a subsequence of $(u_n)$ converging to a minimizer $u \in \mathcal{C}$. To solve several problem about minimization, several conditions must be fulfilled:

1. Some compactness condition has to hold so that a minimizing sequence contains a convergent subsequence. This requires the careful selection of a suitable topology on $\mathcal{C}$.
2. The limit $u$ of such a subsequence should be contained in $\mathcal{C}$. This is a closedness condition on $\mathcal{C}$.
3. Some lower semi-continuity condition of the form

$$F(\rho) \leq \liminf_{n \rightarrow \infty} F(u_n)$$

if $u_n$ converges to $u$.

The lower semi-continuity condition becomes easier if the topology of $\mathcal{C}$ is more restrictive, because the stronger the convergence of $u_n$ to $u$, the easier that condition is satisfied. That is at variance, however, with the requirement of (1) since for too strong a topology, sequences do not always contain convergent subsequences. Therefore, the researchers expect that the topology for $\mathcal{C}$ to be carefully chosen so as to balance the various requirements.

3.0 LOWER SEMI-CONTINUITY

The researchers believe that a topological space $X$ satisfies the first axiom of countability if the neighbourhood system of each point $x \in X$ has a countable base, i.e. there exists a sequence $(U_n)_{n \in \mathbb{N}}$ of open subsets of $X$ and $x \in U_n$, with the property that for every open set $U \subset X$ with $x \in U$ there exists $n \in \mathbb{N}$ with $U_n \subset U$.

$X$ satisfies the second axiom of countability if its topology has a countable base, i.e. there exists a a family $(U_n)_{n \in \mathbb{N}}$ of open subsets of $X$ with the property that for every open subset $V$ of $X$, there exists $n \in \mathbb{N}$ with $U_n \subset V$.

The researchers note that separable metric spaces $X$ satisfy the second axiom of countability. If $(x_n)_{n \in \mathbb{N}}$ can be a dense subset of $X$, and $(r_n)_{n \in \mathbb{N}}$ be dense in $\mathbb{R}^+$, then,

$$U(x_n, r_n) := \{x \in X: d(x, x_n) < r_n\}$$

(3)

where $d(\cdot, \cdot)$ is the distance function of $X$ that forms a countable base for the topology.

If the first countability axiom is satisfied, topological notions usually admit sequential characterizations. For example, if $(x_n)_{n \in \mathbb{N}} \subset X$ is a sequence in a topological space $X$ satisfying the first axiom of countability, then any accumulation point of $(x_n)$ (i.e. any $x \in X$ with the property that for every neighbourhood $U$ of $x$ and any $m \in \mathbb{N}$, there exists $n \geq m$ with $x_n \in U$) can be obtained as the limit of some subsequence of $(x_n)$.

Definition 1: Let $X$ be a topological space. A function $F: X \rightarrow \mathbb{R} := \mathbb{R} \cup \{\pm \infty\}$ is called lower semi-continuous (lsc) at $x$ if

$$F(x) \leq \liminf_{n \rightarrow \infty} F(x_n)$$

for any sequence $(x_n)_{n \in \mathbb{N}} \subset X$ converging to $x$. $F$ is called lower semi-continuous if it is lsc at every $x \in X$.

Lemma 2:

(i). If $F: X \rightarrow \mathbb{R}$ is lsc $\lambda \geq 0$, then $\lambda F$ is lsc.

(ii). If $F, G: X \rightarrow \mathbb{R}$ is lsc, and if their sum $F + G$ is well defined (i.e. there is no $x \in X$ for which one of the values $F(x), G(x)$ is $+\infty$ and the other one is $-\infty$), then $F + G$ is also lsc.

(iii). If $F, G: X \rightarrow \mathbb{R}$, $\inf \{F, G\}$ is also lsc.

(iv). If $(F_i)_{i \in I}$ is a family of lsc functions, then $\sup_{i \in I} F_i$ is also lsc.

Definition 3:

(i). Let $X$ be a normed space, with norm $\| \cdot \|$. $F: X \rightarrow \mathbb{R}$ is weakly proper, if for every sequence $(x_n)_{n \in \mathbb{N}} \subset X$ with $\|x_n\| \rightarrow \infty$, we have $F(x_n) \rightarrow \infty$ for $n \rightarrow \infty$.

(ii). Let $X$ be a topological space. $F: X \rightarrow \mathbb{R}$ is coercive if every sequence $(x_n)_{n \in \mathbb{N}} \subset X$ with $F(x_n) \leq \text{constant}$ (independent of $n$) has an accumulation point.

The researchers can now formulate the following general existence theorem for minimizers

Theorem 4: Let $X$ be a separable reflexive Banach space, $F: X \rightarrow \mathbb{R}$ weakly proper and lower semi-continuous with respect to weak convergence. Then there exists a minimize $x_0$ for $F$, i.e.

$$F(x_0) = \inf \{F(x): (\rightarrow -\infty)\}$$

Proof: Let $(x_n)_{n \in \mathbb{N}} \subset X$ be a minimizing sequence for $F$, i.e.

$$\lim_{n \rightarrow \infty} F(x_n) = \inf \{F(x): (\rightarrow -\infty)\}$$

Since $F$ is weakly proper, $\|x_n\|$ is bounded. Since $X$ is reflexive, after selection of a subsequence, $x_n$ converges weakly to some $x_0 \in X$. Since there is lower semi-continuity of $F$,

$$F(x_0) \leq \lim_{n \rightarrow \infty} F(x_n) = \inf \{F(x): (\rightarrow -\infty)\}$$

and since $x_0 \in X$, equality must be achieved. Also, since $F$ assumes only finite values by assumption, this implies that
Remark. The argument of the preceding proof also shows that in a separable reflexive Banach space $F: \rightarrow $ is a weakly lower semi-continuous functional with respect to the weak topology.

**Definition 5:** Let $V$ be a convex subset of a vector space $F: V \rightarrow \mathbb{R}$ be a vectorial set. If for any $x, y \in V$, $0 \leq t < 1$, $F(tx + (1-t)y) \leq tF(x) + (1-t)F(y)$, then $F$ is called convex if $V$ is convex. Convexity of $V$ means that $tx + (1-t)y \in V$ whenever $x, y \in V$, $0 \leq t < 1$.

**Lemma 6:** Let $V$ be a convex subset of a separable reflexive Banach space $F: V \rightarrow \mathbb{R}$ and $L$, lower semi-continuous, then $F$ is also lower semi-continuous with respect to weak convergence.

**Proof:** Let $(x_n)_{n \in \mathbb{N}} \subset X$ converge weakly to $x \in V$. Assume that $F(x_n)$ converges to some $\kappa \in \mathbb{R}$. For every $m \in \mathbb{N}$ and every $\epsilon > 0$, a convex combination may be found,

$$y_m := \sum_{n=m}^N \lambda_n x_n \quad (\lambda_n > 0, \sum_{n=m}^N \lambda_n = 1)$$

with

$$\|y_m - x\| \leq \epsilon.$$

Since $F$ is convex,

$$F(y_m) \leq \sum_{n=m}^N \lambda_n F(x_n).$$

(4)

Given $\epsilon > 0$, we choose $m = m(\epsilon) \in \mathbb{N}$ so large that for all $n \geq m$,

$$F(x_n) \leq \kappa + \epsilon.$$

Letting $\epsilon$ approaches 0, and from (4) the following is obtained

$$\limsup_{m \rightarrow \infty} F(y_m) \leq \kappa.$$

Since $F$ is lsc,

$$F(x) \leq \liminf_{m \rightarrow \infty} F(y_m) \leq \limsup_{m \rightarrow \infty} F(y_m) \leq \kappa = \lim F(x_n).$$

This shows weak lower semi-continuity of $F$.

### 4.0 The Existence of Minimizers for Convex Variational Problems

**Lemma 7:** Let $\Omega \subset \mathbb{R}^d$ be open, $f: \Omega \times \mathbb{R}^d \rightarrow \mathbb{R}$, then $f(., v)$ measurable for all $v \in \mathbb{R}^d$, $f(., .)$ continuous for all $x \in \Omega$, and

$$f(x, v) \geq -a(x) + b|v|^p$$

for all $x \in \Omega$, and all $v \in \mathbb{R}^d$, with $a \in L^1(\Omega)$, $b \in \mathbb{R}$, $p \geq 1$. Then,

$$\Phi(v) := \int_{\Omega} f(x, v(x)) \, dx$$

is a lower semi-continuous functional on $L^p(\Omega)$, $\Phi: L^p(\Omega) \rightarrow \mathbb{R} \cup \{\infty\}$.

**Proof:** Since $f$ is continuous in $v$, $f(x, v(x))$ is a measurable function, and also $\Phi$ is well-defined on $L^p(\Omega)$. Let $(v_n)_{n \in \mathbb{N}}$ converges to $v$ in $L^p(\Omega)$, then a subsequence converges pointwise almost everywhere to $v$. Since $f$ is continuous in $v$ (actually, it would suffice to have $f$ lower semi-continuous in $v$), i.e.

$$f(x, v(x)) - b|v_n(x)|^p \geq -a(x)$$

with $a \in L^1(\Omega)$. Based on Fatou theorem, the following can be concluded

$$\int_{\Omega} \left( f(x, v(x)) - b|v_n(x)|^p \right) \, dx \leq \liminf_{n \rightarrow \infty} \int_{\Omega} \left( f(x, v(x)) - b|v_n(x)|^p \right) \, dx$$

since $v_n$ converges to $v$ in $L^p(\Omega)$.

$$\int_{\Omega} b|v_n(x)|^p \, dx = \lim_{n \rightarrow \infty} \int_{\Omega} b|v_n(x)|^p \, dx$$

and the researchers conclude lower semi-continuity, namely,

$$\int_{\Omega} f(x, v(x)) \, dx \leq \liminf_{n \rightarrow \infty} \int_{\Omega} f(x, v_n(x)) \, dx$$

**Lemma 8:** Under the assumptions of Lemma 3.7, assume that $f(x, .)$ is a convex function on $\mathbb{R}^d$ for every $x \in \Omega$. Then $\Phi(v) := \int_{\Omega} f(x, v(x)) \, dx$ defines a convex functional on $L^p(\Omega)$.

**Proof:** $v, w \in L^p(\Omega)$, $0 \leq t \leq 1$

$$\Phi tv + (1 - t)w \rightarrow \int_{\Omega} f(x, tv(x) + (1 - t)w(x)) \, dx$$

by the convexity of $f$

$$= t\Phi(v) + (1 - t)\Phi(w).$$

The researchers may now obtain a general existence result for the minimizer of a convex variational problem.

**Theorem 9:** Let $\Omega \subset \mathbb{R}^d$ be open, and suppose $\omega \times \mathbb{R}^d \rightarrow \mathbb{R}$, satisfies

(i). $f(., v)$ w measurable for all $v \in \mathbb{R}^d$

(ii). $f(., .)$ is convex for all $x \in \Omega$

(iii). $f(x, v) \geq -a(x) + b|v|^p$ for almost all $x \in \Omega$, all $v \in \mathbb{R}^d$, with $a \in L^1(\Omega)$, $b > 0$, $p > 1$. Let $g \in H^1_p(\Omega)$, and let $A := g + H^1_p(\Omega)$. Then

$$F(u) := \int_{\Omega} f(x, Du(x)) \, dx$$

assuming its infimum on $A$, i.e. there exists $u_0 \in A$ with

$$F(u_0) := \inf_{u \in A} F(u).$$

**Proof:** By Lemma 7, $F$ is lower semi-continuous with respect to $H^1_p(\Omega)$ convergence. By Lemma 3.7 $F$ then is also lower semi-continuous with respect to $H^1_p(\Omega)$ convergence, since $H^1_p(\Omega)$ is separable and reflexive for $p > 1$, then minimization from sequence $(u_n)_{n \in \mathbb{N}}$ in $A$, i.e.

$$\lim_{n \rightarrow \infty} F(u_n) = \inf_{u \in A} F(u).$$

Since

$$\int_{\Omega} |Du_n|^p \leq \frac{1}{b} F(u_n) + \frac{1}{b} \int_{\Omega} a(x) \, dx$$

$Du_n$ is bounded in $L^p(\Omega)$, hence $(u_n)_{n \in \mathbb{N}} \subset g + H^1_p(\Omega)$ is bounded in $g + H^1_p(\Omega)$ by the Poincare inequality. Since $H^1_p(\Omega)$ is a separable reflexive Banach space, after selection of a sequence, $(u_n)_{n \in \mathbb{N}}$ converges weakly to some $u_0 \in A$ (A is closed under weak convergence). Since $F$ is convex by Lemma 3.8 and lower semicontinuous by Lemma 7, E it is also lower semicontinuous w.r.t. weak $H^1_p(\Omega)$ convergence, so
5.0 KLEIN-GORDON FIELD

Klein-Gordon equations for real scalar field (position on the space)

\[ (\partial^2 - m^2) \phi(x) = 0 \]

To get Lagrangian density, we can calculate

\[ 0 = \int_0^L d\tau \int \frac{1}{2} \left( \frac{\partial \phi}{\partial \tau} \right)^2 - \frac{1}{2} \left( \frac{\partial \phi}{\partial \tau} \right)^2 - \frac{1}{2} \nabla^2 \phi^2 - \frac{1}{2} m^2 \phi^2 \]

with operation integral partial, boundary condition \( \delta \phi(t_1) = \delta \phi(t_2) = 0 \) and \( \phi \) convergence to infinite, then Lagrangian density Klein-Gordon Field is obtained [12]

\[ L(\phi, \partial_\tau \phi) = \frac{1}{2} \partial^2 \phi_\tau \phi_\tau - \frac{1}{2} \nabla^2 \phi^2 \]

6.0 APPLICATION DIRECT METHOD OF CALCULUS VARIATION FOR EXISTENCE MINIMIZER

The Lagrangian density functional form to Klien-Gordon Field is

\[ E(\phi) = \int L(\phi, \partial_\tau \phi) d\tau \]

\[ E(\phi) = \int \left( \frac{1}{2} \partial^2 \phi_\tau \phi_\tau - \frac{1}{2} \nabla^2 \phi^2 \right) d\tau \]

Where \( d\tau \) is Lebesgue measure on \( \mathbb{R}^3 \), for \( \rho \in W \), with

\[ \{\phi|\phi \geq 0, \phi \in L^1\}. \]

7.0 MINIMIZER CONSTRUCTION

Rayleigh-Ritz method is the direct variational method for minimizing a functional which has been given. A ‘jump’ here means the solution to variations exist without involving differential equations derived from the Euler-Lagrange. This method was first conveyed by Rayleigh in 1877 and expanded by the Ritz in 1909.

Without prejudice to the generality, suppose that the functional form

\[ I(\phi) = \int F(x, y, \phi, \phi_x, \phi_y) dS \]

Since the aim is to minimize the integral, Rayleigh-Ritz method was selected with linearly independent set consisting of functions that are called expansion functions [basis functions] \( u_n \) and construct a solution approach in equation [11], which satisfy some boundary conditions.

The solution proposed in the form of infinite series

\[ \phi_N = \sum_{n=1}^N a_n u_n + u_0 \]

with \( u_0 \) requirement the inhomogeneous boundary condition, whereas \( u_n \) satisfy homogeneous boundary. Coefficient \( a_n \) is the expansion coefficient to be determined and \( \phi_N \) is the solution approach \( \phi \) (exact solution). If equation (12) substituted to (11), integral \( I(\phi) \) viewed as a function consisting of \( N \) with coefficients \( a_1, a_2, a_3, \ldots, a_N \).
The minimum value of this function is obtained if the function is derived for each coefficient is equal to zero:
\[
\frac{\partial l}{\partial a_1} = 0, \quad \frac{\partial l}{\partial a_2} = 0, \quad \frac{\partial l}{\partial a_n} = 0,
\]
\[
\frac{\partial l}{\partial a_n} = 0 \quad n = 1, 2, 3, \ldots N
\]
The set of \( N \) simultaneous equations is thus obtained. A system of linear algebraic equations are solved to obtain \( a_n \), the results are incorporated into the solution equation approach (12). Approximation solution equation (12), if \( \Phi_N \rightarrow \Phi \), with \( N \rightarrow \infty \) as the result is said to converge to the exact solution to the (13).

Now we will calculate approximation for minimizer functional (5) with Ritz method. Means, will arrange a sequence that has a limit minimizer \( \Phi \). Members of suquence assumed \( \Phi_N (N = 1, 2, 3, \ldots) \), with
\[
\Phi_N = \phi_0 + \sum_{n=1}^{N} a_n \phi_n
\]
and \( \phi_0 = 0 \) and \( \phi_n = x^n(1-x) \) in order to satisfy the boundary conditions \( \phi(0) = 0 = \phi(1) \), Let \( v \) in functional \( F(\phi) \) constant, then calculation coefficient of \( a_n \) as follows:

For \( N = 1 \)
\[
\Phi_1 = a_1 x(1-x)
\]
\[
F(\Phi_1) = \int_0^1 \left( (a_1 x(1-x)) + a_1 x(1-x) v \right) dx
\]
\[
= a_1 \int_0^1 x(1-x) \frac{5}{3} dx + a_1 \int_0^1 x(1-x) v dx
\]
\[
F(\Phi_1) \text{ minimum when } \frac{\partial F(\Phi_1)}{\partial a_1} = 0 \Rightarrow \frac{5}{3} a_1 + 0.056 + 0.167 v = 0
\]
\[
a_1 = (-1.8v)^{3/2}/(1-x)
\]
\[
F(\Phi_1) = a_1 \frac{5}{3} + 0.056 + 0.167 a_1 + v = 3.1806
\]

For \( N = 2 \)
\[
\Phi_2 = a_1 \phi_1 + a_2 \phi_2
\]
\[
F(\Phi_2) = \int_0^1 \left( (a_1 x(1-x) + a_2 x(1-x)) \right)^{5/3} dx
\]
\[
= \int_0^1 \left( (a_1 x(1-x) + a_2 x(1-x)) + a_1 x(1-x) \right) v dx
\]
\[
= a_1 \frac{5}{3} \phi_1 + a_1 \frac{5}{3} \phi_2 + a_2 \phi_2 + 0.0095 + 0.167 a_1 v + 0.083 a_2 v
\]
\[
F(\Phi_2) \text{ minimum when } \frac{\partial F(\Phi_2)}{\partial a_1} = 0 \Rightarrow \frac{5}{3} a_1 + 0.033 a_1 + 0.033 a_2 + 0.167 a_1 + v = 0
\]
\[
a_1 = (-3.03v)^{3/2}/(1-x)
\]
\[
F(\Phi_2) = a_1 \frac{5}{3} + 0.033 a_1 + 0.033 a_2 + 0.167 a_1 + v = 2.9812
\]

For \( N = 3 \)
\[
\Phi_3 = a_1 x(1-x) + a_2 x(1-x) + a_3 x(1-x)
\]
\[
F(\Phi_3) = \int_0^1 \left( (a_1 x(1-x) + a_2 x(1-x) + a_3 x(1-x)) \right)^{5/3} dx
\]
\[
= a_1 \frac{5}{3} \phi_1 + a_2 \phi_2 + a_3 \phi_3 + 0.0095 + 0.167 a_1 v + 0.083 a_2 v + 0.05 a_3 v
\]
\[
F(\Phi_3) \text{ minimum when } \frac{\partial F(\Phi_3)}{\partial a_1} = 0 \Rightarrow \frac{5}{3} a_1 + 0.033 a_1 + 0.033 a_2 + 0.02 a_3 + 0.167 a_1 + v = 0
\]
\[
a_1 = (-3.03v)^{3/2}/(1-x)
\]
\[
F(\Phi_3) = a_1 \frac{5}{3} + 0.033 a_1 + 0.033 a_2 + 0.02 a_3 + 0.167 a_1 + v = 2.9812
\]

Figure 1 Graphical relation between position \( (x) \) with density \( (\phi) \).
Figure 1 shows the sequence $\tilde{\phi}_N$ converges to some expected function. Figure 2 shows the functional value $F$ for each sequence term to be monotonously decreasing over $N$.

$$\text{Figure 2} \text{ Graph relation sequence } N \text{ with functional energy } F(\tilde{\phi}_N)$$

8.0 CONCLUSION

The Direct Method of Calculus Variation is an alternative to solve the Klein-Gordon field equations. The Direct Method can simplify the calculation because the variables calculated are expressed in functional form of energy. The existence of minimizer have been proven, with minimizer $\tilde{\phi} = \phi_0 + u \in W_0^{1,p}$ and $\phi_0 \in W_1^{1,p}$. Explicit form of the minimizer was calculated by the Ritz method through rows of convergent density.

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