Modified Kortweg-de Vries equation approach to zero-energy states of graphene

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Abstract – We utilize the relation between soliton solutions of the modified Kortweg-de Vries (mKdV) and the combined mKdV-KdV equation and the Dirac equation to construct electrostatic fields which yield exact zero-energy states in graphene. The examples considered here are fairly general and it has also been shown that some of these examples reproduce the previously known results when parameters are chosen suitably.

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Introduction. – The relation between the solutions of nonlinear evolution equations and the nonrelativistic Schrödinger equation is well known. For example, the soliton solutions of the KdV equation

\[ u_t + uu_x + 6u_{xx} = 0, \]

where the subscripts \( t \) and \( x \) indicate the time and space derivatives, respectively, can be used to construct reflectionless potentials of the one-dimensional Schrödinger equation [1–4]. There is also a similar relation between the soliton solutions of the mKdV and combined mKdV-KdV equation and the Dirac equation [2,5–9]. However this relation has been exploited to a lesser extent to find out electrostatic fields admitting exact solutions of the Dirac equation [10].

It may be recalled that the dynamics of electrons in graphene is governed by the (2 + 1)-dimensional massless Dirac equation with the exception that the velocity of light \( c \) is replaced by the Fermi velocity \( v_F = c/300 \) [11]. In graphene one of the important problems is to confine or control the motion of the electrons. Such confinement can be achieved, for example, by using various types of magnetic fields [12]. Moreover, it is generally believed that because of Klein tunneling [13] electrostatic confinement is relatively more difficult compared to magnetic confinement. However, it has been shown recently that certain types of electrostatic fields can indeed produce confinement [14] and zero-energy states, which were earlier found using various magnetic fields [15] can also be found using electrostatic fields [16–18].

In this paper it will be shown that the Dirac equation of the graphene model is closely related to nonlinear evolution equations, namely the mKdV equation and the combined KdV-mKdV equation [7]. To be more specific, the soliton solutions of the above-mentioned equations actually act as electrostatic potentials of the Dirac equation for the charge carriers in graphene. Here our objective is to use this correspondence to obtain several electrostatic field configurations which admit exact zero-energy solutions of the graphene system.

Zero-energy states in graphene. – The motion of electrons in graphene in the presence of an electrostatic field or potential is governed by the equation

\[
\begin{align*}
\psi(x) &= e^{ik_y y} \left( \begin{array}{c} \psi_A \\ \psi_B \end{array} \right),
\end{align*}
\]

Then from eq. (1) we obtain

\[
\begin{align*}
(\psi_A - \epsilon) \psi_A - i \left( \frac{d}{dx} + k_y \right) \psi_B &= 0, \\
(\psi_B - \epsilon) \psi_B - i \left( \frac{d}{dx} - k_y \right) \psi_A &= 0,
\end{align*}
\]

where \( V(x) = U(x)/\hbar v_F \) and \( \epsilon = E/\hbar v_F \).

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It is interesting to note that eqs. (3) and (4) are invariant under the following transformations:

\[ k_y \rightarrow -k_y, \quad \psi_A \rightarrow \psi_B. \quad (5) \]

This means that if the spinor \( \psi = e^{ik_y y}(\psi_A, \psi_B)^T \) is a solution for \( k_y \), then \( \psi = e^{-ik_y y}(\psi_B, \psi_A)^T \) is a solution for \( -k_y \) (here “*” means transpose). That is, eigenstates with opposite signs of \( k_y \) are spin-flipped.

Here we shall consider \( k_y \neq 0 \), since for \( k_y = 0 \) the wave function \( \psi(x) \) is normalizable only in a finite region if \( V(x) \) is real.

Defining \( \psi_{1,2} = (\psi_A \pm \psi_B) \) we obtain from eqs. (3) and (4)

\[
\begin{align*}
(V(x) - \epsilon - i \frac{d}{dx}) \psi_1 + i k_y \psi_2 &= 0, \quad (6) \\
(V(x) - \epsilon + i \frac{d}{dx}) \psi_2 - i k_y \psi_1 &= 0. \quad (7)
\end{align*}
\]

The above equations can be easily decoupled and the equations satisfied by the components \( \psi_{1,2} \) can be obtained as

\[
\begin{align*}
-\frac{d^2}{dx^2} - (V(x) - \epsilon)^2 - i \frac{dV}{dx} + k_y^2 \psi_1 &= 0, \quad (8) \\
-\frac{d^2}{dx^2} - (V(x) - \epsilon)^2 + i \frac{dV}{dx} + k_y^2 \psi_2 &= 0. \quad (9)
\end{align*}
\]

Note that eqs. (8) and (9) can be interpreted as a pair of Schrödinger equations with energy-dependent potentials which for \( \epsilon = 0 \) read

\[
\begin{align*}
V_1(x) &= -V^2(x) - i \frac{dV}{dx} + k_y^2, \quad (10) \\
V_2(x) &= -V^2(x) + i \frac{dV}{dx} + k_y^2. \quad (11)
\end{align*}
\]

It is also interesting to note that when \( V(x) \) is an even function the potentials in eqs. (8) or (9) are \( PT \) symmetric [19]. It will now be shown that the equations for graphene’s zero-energy states are related to solutions of nonlinear evolution equations.

**mKdV equation.** – The mKdV equation for a real field \( u(x,t) \) is given by

\[ u_t + 6u^2 u_x + u_{xxx} = 0, \quad (12) \]

This equation is the compatibility condition of a set of linear equations [2,7]

\[
\begin{align*}
v_{1x} + i \zeta v_1 &= u v_2, \\
v_{2x} - i \zeta v_2 &= -u v_1. \quad (13)
\end{align*}
\]

for certain functions \( v_{1,2} \).

It is seen that the transformations

\[
\begin{align*}
v_1 &\leftrightarrow i\psi_B, \quad v_2 \leftrightarrow \psi_A, \\
\zeta &\leftrightarrow -i k_y, \quad u(x) \leftrightarrow V(x). \quad (14)
\end{align*}
\]

map eqs. (3) and (4) into (16) and (17), and vice versa for \( \epsilon = 0 \). Accordingly, the transformation

\[
\begin{align*}
\phi_1 &= -iv_1 + v_2, \\
\phi_2 &= iv_1 + v_2, \quad (15)
\end{align*}
\]

changes eq. (13) into

\[
\begin{align*}
-\frac{d^2}{dx^2} - u^2 - i u_x - \zeta^2 \phi_1 &= 0, \quad (16) \\
-\frac{d^2}{dx^2} - u^2 + i u_x - \zeta^2 \phi_2 &= 0. \quad (17)
\end{align*}
\]

Comparing the two sets of eqs. (16), (17) and (8) and (9), one finds that they are identical for \( \epsilon = 0 \) with the identification \( V(x) \leftrightarrow u(x) \), \( \psi_{1,2} \leftrightarrow \phi_{1,2} \) and \( k_y \leftrightarrow -\zeta^2 \). Now the connection of graphene’s zero-energy states and solutions of mKdV equation is clear. By choosing the parameters including the time \( t \) appropriately, one can make the solution of the mKdV equation an even function of \( x \), i.e., \( u(x) = u(-x) \). This function \( u(x) \) then furnishes a potential \( V(x) = u(x) \) of the original Dirac equation (1) admitting exactly known zero energy states.

The soliton solutions of the mKdV equation can be obtained by the inverse scattering method. For the boundary conditions \( u(x,t) \rightarrow 0 \) as \( |x| \rightarrow \infty \), the \( N \)-soliton solution is given by [6,7]

\[ u(x,t) = -2 \frac{\partial}{\partial x} \tan^{-1} \left[ \frac{\text{Im} \det(I + A)}{\text{Re} \det(I + A)} \right], \quad (18) \]

where \( I \) is the \( N \times N \) unit matrix, and \( A \) denotes the \( N \times N \) matrix with elements

\[ A_{mn}(x,t) = -\frac{d_n}{\zeta_n + \zeta_m} \exp[i(\zeta_n + \zeta_m)x], \quad (19) \]

\[ m, n = 1, 2, \ldots, N, \]

\[ \zeta_n = i\eta_n, \quad \eta_n > 0, \]

\[ d_n(0) = d_n(0) \exp(8i\eta^2_n). \]

Here \( d_n(0) \) and \( \eta_n \) are real, and without loss of generality one can take

\[ \eta_1 < \eta_2 < \cdots < \eta_N. \quad (20) \]

**One- and two-soliton potentials.** – We shall present some examples of solutions of the mKdV equation that provide exactly solvable potentials for the graphene’s problem. Only the solutions \( u(x) \) which correspond to the confining potential \( V(x) = u(x) \) are presented.

By taking \( \zeta = i\eta, \eta > 0 \), one obtains a one-soliton solution of the mKdV equation

\[ u(x) = -2\eta \text{sech}(2\eta x). \quad (21) \]

This gives an exactly solvable potential \( V(x) = u(x) \) admitting one zero-energy bound state with \( k_y^2 = \eta^2 \). The case \( \eta = 1/2 \) correspond to the reflectionless potential with one bound state, which is a special case of the example considered in [16,18].
A periodic solution for the mKdV equation also furnishes a periodic potential of the graphene system that admits a zero-energy bound state with \( k^2 = \eta^2 \).

In the limit \( m \to 1 \), \( \eta \to a/2 \), and \( u(x) \to -a \text{sech} \ ax \), which is just the 1-solution case in eq. (21).

Other periodic potentials can be obtained from the examples given in [21,22]. As two examples, let us take [22]

\[
\begin{align*}
 u(x) &= -m \eta \text{cn} (\eta x, m), \quad \eta \equiv \sqrt{\frac{a}{2m^2 - 1}},
\end{align*}
\]

and

\[
\begin{align*}
 u(x) &= -m \eta \text{dn} (\eta x, m), \quad \eta \equiv \sqrt{\frac{a}{2 - m^2}}.
\end{align*}
\]

Here \( \text{cn}(x,m) \) and \( \text{dn}(x,m) \) are the Jacobi elliptic functions with modulus \( m \) and \( a > 0 \) is a constant. These two solutions of the mKdV equation provide another two periodic potentials of the graphene system admitting a zero-energy bound state with \( k^2 = \eta^2 \), where \( \eta \) are given by eqs. (27) and (28) respectively. In the limit \( m \to 1 \), both \( \text{cn}(x,m) \), \( \text{dn}(x,m) \) \( \to \text{sech} \ ax \), and eqs. (27) and (28) reduce to eq. (21).

In figs. 2 and 3 we present visual representations of the potentials (24) and (27) for different parameter values.

**Combined KdV and mKdV equation.** – The above observation can be extended to other soliton equations. For instance, consider the combined KdV and mKdV equation [7,20]

\[
\begin{align*}
 u_t + 6\alpha au_x + 6\beta u^2 u_x + u_{xxx} = 0, \quad \beta > 0. \quad (29)
\end{align*}
\]

and the scale

\[
\eta \equiv \frac{1}{2} \left[ (a - c)(a + b + c) \right]^{\frac{1}{2}}.
\]
For illustration we present the one-soliton solution of a problem or experiment there are actually enough here are quite general and depending on the specific needs we would like to mention that the potentials considered between the solutions of nonlinear evolution equations, namely, the mKdV equation and combined mKdV and KdV equation to find a large number of potentials admitting exact zero-energy solutions. Figure 4 shows that the potential (31) is a single-well one of eq. (29) are known [7].

The N-soliton solutions \( u(x) \) of eq. (29) are known [7]. For illustration we present the one-soliton solution

\[
\begin{align*}
V(x) &= \sqrt{\beta} u(x) + \gamma, \quad \gamma = \frac{\alpha}{2\sqrt{\beta}}; \\
k^2_0 &= \eta^2 + \gamma^2. 
\end{align*}
\]

(30)

The N-soliton solutions \( u(x) \) of eq. (29) are known [7]. For illustration we present the one-soliton solution

\[
\begin{align*}
u(x) &= V(x) = \frac{2\eta}{\sqrt{\beta}} \frac{\sin \theta}{\cos \theta + \cosh 2\eta x}; \\
\cos \theta &= \alpha (\alpha^2 + 4\eta^2 \beta)^{-1/2}. 
\end{align*}
\]

(31)

Figure 4 shows that the potential (31) is a single-well one and the depth of the potential can be increased or decreased by choosing the parameters suitably.

Summary. – In this letter we have utilized the relation between the solutions of nonlinear evolution equations, namely, the mKdV equation and combined mKdV and KdV equation and the Dirac equation to find a large number of potentials admitting exact zero-energy solutions. We would like to mention that the potentials considered here are quite general and depending on the specific needs of a problem or experiment there are actually enough scope to tune the various potential parameters to model the potentials. There are of course many other solutions of the aforementioned equations [23] and some of these may also serve the purpose.

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