Solitary Wave Interactions in Graphene Superlattices

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Abstract

Graphene superlattices (GSLs) are made of a sheet of graphene deposited on a heterostructure formed by periodically alternating nanometric layers of SiO_2 and SiC; the layers are arranged such that the hexagonal lattice of SiC{0001} was exactly under that of the graphene (Figure 1) [1]. A strong electromagnetic field (EM) incident in the GSL induce the propagation of electromagnetic waves governed by the nonlinear Klein-Gordon equation $\mathrm{u_{tt}} - \mathrm{u_{xx}} + \mathrm{V(u)} = 0$, where u is the dimensionless transversal potential of the EM field, t is time, x is the spatial direction of the superlattice axis, and $\mathrm{V}(u)$ is a nonlinear potential given by $V(\alpha) = \frac{\omega_0^2 \mathrm{b}^2 \sin\alpha}{\sqrt{1+\mathrm{b}^2(1-\cos\alpha)}}$, where ω_0 is the plasma frequency and b is a geometric parameter [2]; here on, this wave equation is referred as GSLeq.

The GSLeq has a solitary wave solution of the form $u(x,t) = \alpha(\xi)$, where $\xi = x - ct$, whose expression in integral form is omitted here for brevity. This expression corresponds to a one-dimensional topological solitary wave transiting between to consecutive multiples of 2π; it is referred to as a kink (antikink) when it is monotonically increasing (decreasing). For small enough b, the GSLeq reduces to the well-known sine-Gordon equation (sGeq). Hence, let us apply to the GSLeq the Strauss-Vazquez finite difference scheme [3], widely used for the sGeq; this scheme is given by $\frac{{u_m}^{n+1} - 2{u_m}^n + {u_m}^{n-1}}{\Delta t^2} - \frac{{u_{m+1}}^n - 2{u_m}^n + {u_{m-1}}^n}{\Delta x^2} = \frac{G({u_m}^{n+1}) - G({u_m}^{n-1})}{{\mathrm{u_m}}^{n+1} - {\mathrm{u_m}}^{n-1}}$, where u_m^n is an approximation to $u(m\Delta x, n\Delta t)$, Δx is the grid size, Δt is the time step, and $G'(u) = V(u)$. This numerical method is second-order accurate in both space and time, and nonlinearly stable since it exactly conserves a discrete energy [4].

Figures 2 and 3 show the amplitude of the solution for the interaction between an antikink and a kink with $\mathrm{b} = 0.2$ and $\mathrm{b} = 0.7$, respectively. In both figures the kink (antikink) propagates with negative (positive) speed form the left (right), colliding nearly elastically and recovering its shape, but with opposite amplitude sign, and speed after their interaction. Note that the kink (antikink) is faster for $\mathrm{b} = 0.7$ than for $\mathrm{b} = 0.2$. The ripples shown in the figures during the kink (antikink) propagation are no numerical artifacts, since the reduction of the time step Δt and the grid size Δx do not alter the results shown in Figures 1 and 2 up to the graphical resolution. In order to assess the accuracy of the numerical method the conservation of the discrete energy has been checked (the error is smaller than $12\mathrm{x}10^{-13}$). Moreover, the numerical scheme is stable under the CFL condition $\left(\frac{\Delta t}{\Delta x}\right)^2 \leq 1$. Further studies of the interactions between kinks and antikinks are required to clarify the origin of the ripples in Figures 2 and 3. Our numerical results suggest are useful for possible applications of graphene superlattices for the development of new transistors and terahertz lasers.

References

[1] Ratnikov, P. V., "Superlattice based on graphene on a strip substrate", JETP Letters, doi: 10.1134/S0021364009180143, (2009).
[2] Kryuchkov, S. V. and Kukhar', E. I., "The solitary electromagnetic waves in the graphene superlattice", Physica B: Condensed Matter, doi: 10.1016/j.physb.2012.09.052, (2012).
[3] Strauss, W. and Vazquez, L., "Numerical solution of a nonlinear Klein-Gordon equation", Journal of Computational Physics, 28, 271-278, doi:10.1016/0021-9991(78)90038-4 (1978).
[4] Guo Ben-Yu et al., "Numerical solution of the sine-Gordon equation", Applied Mathematics and Computation, doi: 10.1016/0096-3003(86)90025-1, (1986).

Figures

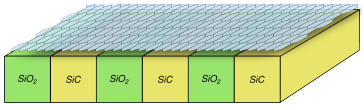

Figure 1. Graphene superlattice.

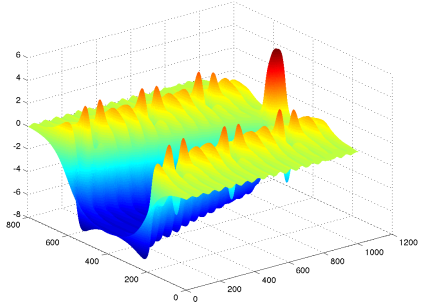

Figure 2. Kink-antikink interaction for b=0.2.

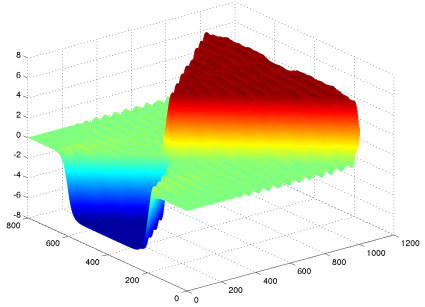

Figure 3. Kink-antikink interaction for b=0.7.