Oscillons in Interacting Relativistic Bose-Einstein Condensates

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In this paper we study a mean field model for the dynamics of an interacting Bose-Einstein condensate in two dimensional pseudo-relativistic materials. This model is relatively simple, but contains stable solutions called oscillons which are absent in non-relativistic condensates. We report on a variety of scenarios including interactions between pairs of oscillons and oscillons propagating across an inhomogeneous material boundary. Hitherto relativistic oscillons have been studied only in high energy physics and cosmology and their relevance has not been highlighted so far in condensed matter physics.

I. INTRODUCTION

Many decades after the theoretical prediction of Bose and Einstein, Bose-Einstein condensates (BECs) were experimentally detected in laser-cooled, magnetically-trapped ultracold bosonic atomic clouds. More recently, BECs have also been seen in fermionic atomic gases as a result of fermions pairing into bosons. An interesting and widely studied example of fermions pairing are the excitonic bound states of electron and holes in semiconductors. The possibility for semiconductor excitons to undergo Bose-Einstein condensation has been suggested long ago, at the beginning of the sixties. As the critical temperature for elementary boson condensation scales as the inverse of the boson mass, it was thought that exciton condensation could be obtained at 100 K or even at room temperature, the exciton mass being much less than the free electron mass. The experimental search for the condensed phase, however, turned out to be challenging mostly due to the fact that excitons are not an elementary but a composite boson with a finite lifetime. However it is known that excitons and exciton-polaritons show a BEC-like insulating phase, that has recently been the subject of promising theoretical and experimental investigation mainly in graphene-like real and synthetic lattices. Due to the pseudo-relativistic behavior of low energy quasiparticles in a honeycomb lattice one may wonder what are the relevant properties of the dynamics in the condensed phase. Moreover the relevance of relativistic BECs has been recently pointed out in gases with both electron and hole pairing. Relativity comes into play as those two composite bosons form a particle antiparticle pair.

In this paper, starting from the dispersion of excitons in Dirac-like materials, we derive and investigate a simple, but flexible mean field model that can describe the dynamics of the condensed phase in different physical scenarios. Central to this model is a relativistic generalisation of the Gross-Pitaevskii equation, i.e a nonlinear Klein-Gordon equation. In Section II we derive the exciton dispersion relation, using a two particle model. In section III we study the condensate phase of the exciton and derive the mean field model. In Section IV we investigate the properties of a non-stationary, but localised solution of the model, known as an oscillon. In Sections V and VI we study the oscillon dynamics in more complicated scenarios: when they interact with each other and with a localized defect, and, when two materials with different energy gap are in contact. Until now such oscillon solutions of field theories have been studied only in high energy physics and cosmology, in particular for self-interacting scalar fields and in the SU(2) Higgs model. Different types of non-relativistic oscillon solutions have been found in coupled BECs and in traps with oscillating wall.

II. EXCITON DISPERSION IN DIRAC MATERIALS

The Hamiltonian describing the low energy behavior of Dirac quasi-particles reads

\[ H_1 = \begin{pmatrix} \Delta/2 & v_{pe} e^{i\theta} \\ v_{pe}^{-1} e^{-i\theta} & -\Delta/2 \end{pmatrix}, \]

where \( \Delta \) is the energy gap and \( v \) the Fermi velocity, \( p = \hbar k \) the modulus of the electron momentum and \( \theta = \arctan(p_y/p_x) \). Such dispersion is appropriate to describe low energy electrons in gapped graphene and, with certain limitations, transition metal dichalcogenides (TMDs). Assuming zero center of mass momentum for excited \( e-h \) pairs, the two particle Hamiltonian, without Coulomb interaction is given by the tensor product

\[ H_2 = H_1 \otimes I_2 - I_2 \otimes (TH_1 T^{-1}), \]

with \( I_2 \) the \( 2 \times 2 \) identity matrix and \( T \) the time reversal operator. It reads

\[ H_2 = \begin{pmatrix} 0 & v_{pe} e^{i\theta} & v_{pe}^{-1} e^{i\theta} & 0 \\ v_{pe}^{-1} e^{-i\theta} & \Delta & 0 & v_{pe} e^{-i\theta} \\ v_{pe} e^{i\theta} & 0 & -\Delta & v_{pe}^{-1} e^{i\theta} \\ 0 & v_{pe}^{-1} e^{-i\theta} & v_{pe} e^{-i\theta} & 0 \end{pmatrix}, \]

and this matrix has four eigenvalues: \( \pm 2\sqrt{v^2 p^2 + \Delta^2/4} \) and a doubly degenerate zero eigenvalue. The zero-energy eigenstates correspond to from the cases when the system has a single electron or a hole with its complementary particle in the negative energy sector.
III. THE EXCITON CONDENSATE STATE

In the regime of strong Coulomb interactions, materials with a purely relativistic, gapped dispersion undergo a phase transition to a BEC-like state. Coulomb interactions can be included in a system with Dirac-like dispersion by deriving a set of renormalised Dirac-Bloch equations. The related electron-hole Dirac problem can be solved giving the excitons energies and wavefunction. The energy levels of the exciton series are given by

\[ E_{n,j} = \frac{\Delta}{\sqrt{1 + \frac{\alpha^2}{(n+\gamma)^2}}} \],

where \( n \) is the principal quantum number and \( \gamma = \sqrt{\beta^2 - \alpha^2} \) with \( j = m + 1/2 \) being the eigenvalue of the pseudospin-angular momentum. The constant \( \alpha \) is the dimensionless Coulomb coupling strength and the spinor wavefunction is of the form

\[ \tilde{\Psi}(q) = \left( \begin{array}{c} \varphi(q) \\ \pm \chi(q) \end{array} \right). \]

If the coupling constant exceeds the critical value (\( \alpha_c = \frac{1}{2} \)), the ground state energy becomes imaginary and a phase transition to an excitonic insulator occurs. This excitonic insulator state is a BEC-like condensate of excitons, i.e. a coherent superposition of the non-interacting ground-state and all exciton states with vanishing real part of the lowest energy level \( E_0 \). In what follows we derive the mean field model that describes the dynamics of the condensate state. The system Hamiltonian in the exciton operators picture can be written as

\[ H = \sum_p [\mathcal{E}_{ex}(p) - \mu_{ex}] \hat{c}^\dagger_p \hat{c}_p + \frac{1}{2A} \sum_{k,q,p} U_{ex-ex}(p,q,k) \hat{c}^\dagger_p \hat{c}^\dagger_q \hat{c}_{k} \hat{c}_{p-k}, \]

where \( \mathcal{E}_{ex}(p) = 2\sqrt{v^2 p^2 + \Delta^2/4} \), \( \mu_{ex} \) is the exciton chemical potential, \( A \) the area of the layer. The exciton creation operator is defined as,

\[ \hat{c}^\dagger_p = \sum_q (\varphi(q) - i\chi(q)) \hat{a}^\dagger_{p+q} \hat{b}^\dagger_{p-q} \]

here \( \{\hat{a}^\dagger, \hat{b}^\dagger, \hat{a}, \hat{b}\} \) are ladder operators for electrons and holes. Note that in the Hamiltonian (Eq. 5) we are including \( X^0 \)-type excitons only, i.e. with spin and pseudospin both equal to zero. To simplify our treatment we approximate the exciton-exciton interaction with a hard sphere potential.

\[ U_{ex-ex}(p,q,k) = U_0 = \frac{4\pi \hbar^2 a_B}{m L_{eff}}, \]

where \( m = (\partial^2 \mathcal{E}_{ex}(p))/\partial p^2 \)^{-1} = \( \Delta/(4v^2) \) is the exciton effective mass, \( a_B \) is the exciton Bohr radius and \( L_{eff} \) the effective thickness of the monolayer. Within this approximaion we can write Eq. (5) in position space as

\[ H = \frac{1}{2} \int d^2x \left[ \frac{\hbar^2}{2m} \nabla^2 \hat{\phi}^2 + \frac{\hbar^2}{m} (\nabla \hat{\phi})^2 + mv^2 \hat{\phi}^2 + 2U_0 \hat{\phi}^4 \right], \]

with \( \hat{\phi}(r,t) \) being a real scalar field describing a relativistic spinless and uncharged boson.

When the bosons are in a condensate state, it is then possible to describe the dynamics of the condensate at the mean-field level by performing the substitution \( \hat{\phi}(r,t) \rightarrow \phi(r,t) \); the order parameter \( \phi \) satisfies then the classical equation

\[ \Box \phi - \mu^2 \phi - U_0 \phi^3 = 0, \]

with \( \mu = mv/\hbar, U_0 = mU_0/h^2 \) and we adopted the standard definition for the flat space box operator

\[ \Box = -\frac{1}{v^2} \partial^2 + \nabla^2, \]

with the Fermi velocity \( v \). This equation, in 2 + 1-dimensions has non-stationary localised solutions called oscillons which we explore in the following sections.

IV. OSCILLONS IN RELATIVISTIC BECS

We now solve numerically equation (9) and study the localised solutions. To do so we introduce a system of scaled space and time variables given by

\[ \xi = \frac{x}{x_0}, \eta = \frac{y}{y_0}, \tau = \frac{t \Delta}{\hbar}, \]

and define \( r_0 = \sqrt{x_0^2 + y_0^2} \). \( x_0 \) and \( y_0 \) are chosen appropriately for the initial conditions of the problem and for our purposes we always choose \( x_0 = y_0 \). In these variables equation (9) reads

\[ \partial^2_\tau \psi - \beta (\partial^2_\xi + \partial^2_\eta) \psi + \psi + \psi^3 = 0, \]

where \( \beta = 8[\hbar v/(r_0 \Delta)]^2 \), and the dimensionless field \( \psi(\xi,\eta,\tau) \) is defined as

\[ \psi = \frac{8\hbar v}{\Delta} \sqrt{\frac{\pi a_B}{L_{eff}}} \phi. \]

Equation (12) has been solved using both a pseudospectral implicit method and a finite difference leapfrog algorithm. In what follows we present the results for a gapped graphene sample \( \Delta = 0.2 \text{eV}, v = c/300 \) and \( \beta = 1 \), which implies \( r_0 = 20 \text{nm} \). Figure 1 shows the modulus square of the field \( \psi \) when the initial state comprises a uniform condensate background with a gaussian shaped hole at the origin, i.e.

\[ \psi(\xi,\eta) = A_0 \left( 1 - e^{-x^2+y^2/a_0^2} \right), \]
with $A_0 = 1$ and $\sigma = 2.86$ which is chosen so that the oscillon solution is maximally stable. This means that in this configuration the nonlinearity best compensates the dispersion.

In figure 1 we show the dynamics of the square modulus of the oscillon’s field, after subtracting the background ($A_0$), we can see after one period the original peak is fully recovered. These oscillating dynmics are quite resilient, as we can see in figure 2(a), even if it suffers from a weak breathing effect due to the non-integrability of the system. In contrast in figure 2(b) we can see the propagation of a dispersive solution ($A_0 = 1$ and $\sigma = 1$). It is interesting to study the effect of the dispersion on the dynamics of the oscillon, by varying the width of the initial gaussian hole. In figure 3 we can see how the dispersion mostly affects the early stage of the dynamics. When we increase $r_0$ the dispersion term becomes less important and the formation of the oscillon is considerably delayed, as we can clearly see from figure 3(b) and 3(c). In figure 3(d) the dynamics completely changes, as the dispersion becomes completely negligible, and the field at $(0,0)$ oscillates only slightly around the minimum ($\psi = 0$) - note the axis scale change. The oscillations of the background instead are driven by the amplitude of the field only, as expected in the strong nonlinear limit (see figure 4).

In figure 4 we can see that the oscillon’s frequency increases with the strength of the initial field, that also defines the strength of the nonlinearity. This is a well known nonlinear effect called self-phase modulation.
FIG. 5: Scattering of two oscillons of initial amplitude $A_0 = 1$, $\sigma = 2.86$ and initial speed $v_0 = 0.5$. (a) Initial state of the oscillon (b) separation of positive and negative energies, (c) collision time, (d) final state after collision. Here with $\tilde{\psi}$ we indicate the field after subtracting the background.

V. OSCILLON INTERACTIONS

We now study how oscillons interact. First we show the collision of two identical oscillons moving along the diagonal. As shown in figure 5, the soliton-like behaviour of the solution is preserved after the collision. It is also interesting to see how the oscillons interact with a defect of the condensate. This can be simulated by adding a loss term, proportional to the first time-derivative of the field. Equation (12) is modified as follows

$$\partial^2_\tau \psi - \beta (\partial^2_\xi + \partial^2_\eta) \psi + \psi + \psi^3 + \Gamma(\xi,\eta) \partial_\tau \psi = 0,$$

(15)

and we consider a gaussian defect of the form

$$\Gamma(\xi,\eta) = \Gamma_0 \exp\left(-\frac{(\xi - \xi_d)^2}{\sigma_d^2} - \frac{(\eta - \eta_d)^2}{\sigma_d^2}\right),$$

(16)

where $\Gamma_0$ is the strength of the damping and $\{\xi_d, \eta_d\}$ the coordinates of the defect. In figure 6 we observe that the oscillon is resilient even to non-perturbative damping ($\Gamma_0 \gg 1$).

VI. CONDENSATES IN HETEROLAYERS

We now investigate BECs spanning two connected Dirac material slabs with different energy gaps ($\Delta_1$ and $\Delta_2$) requiring an adapted version of equation (12),

$$\partial^2_\tau \psi - \beta (\partial^2_\xi + \partial^2_\eta) \psi + \gamma^2(\xi) \psi + \gamma(\xi) \psi^3 = 0$$

$$\psi(\xi,\eta,0) = \psi_0(\xi,\eta)$$

(17)

with $\beta = 8[\hbar v/(r_0 \Delta_1)]^2$, the scaled time is given by $\tau = t\Delta_1/\hbar$ and the scaled field $\psi$ is defined as in equation (13) with $\Delta = \Delta_1$. The space dependent coefficient $\gamma(\xi)$ is defined as follows

$$\begin{cases} 
\gamma(\xi) = 1 & \xi < 0, \\
\gamma(\xi) = \frac{\Delta_2}{\Delta_1} & \xi > 0.
\end{cases}$$

(18)

We take first the simplest case of a constant background, $\psi_0(\xi,\eta) = \psi_0$. As we can see from figure 7, travelling waves are generated by scattering at the boundary between the two layers and propagate throughout the two sides of the condensate. This dynamics of these waves is straightforwardly understood using a multiple scale perturbative analysis of equation (17) limited to one side of the heterolayer (See the Appendix for details).

In figure 8 we show the motion of an oscillon located initially in the condensate with energy gap $\Delta_1$. The stability of the oscillon dynamics in not particularly influenced by the presence of the second condensate after the splitting of positive and negative energies. The oscillon moves through the second condensate and starts oscillating with a higher frequency proportional to the second gap $\Delta_2$ as we show in figure 9. From figure 9 we can compute the frequency (in eV) of the first harmonics of the oscillons on both sides of the condensate. We get $\omega_1 = 0.04$ eV and $\omega_2 = 0.07$ eV. Those values are significantly lower than the two energy gap ($\Delta_1$ and $\Delta_2$) in the two sides of the heterolayer, this is because we are studying the dynamics of the system at a relatively early stage, between $\tau = 10$ and $\tau = 200$, when the combined effect of the dispersion and the nonlinearity is still
strong. For long time propagation the value of the frequency approaches the one of the energy gap and the system behaves like a harmonic oscillator\cite{22}. In the inset we can observe the generation of third harmonics in the spectrum of the bosonic field as expected from a system with third order nonlinearity. This effect is clearly not specifically related to the heterolayer structure studied in this section and would be present also in the spectrum of time series in figures 2, 3 and 4.

VII. CONCLUSIONS

In this paper we derived a simple mean field model to investigate the dynamics of Bose Einstein condensates for quasi-particle with pseudo-relativistic low energy dispersion. This approach is based on a generalisation of the Gross-Pitaevskii equation. We applied this model to the exciton dispersion of gapped Dirac material, such as doped or strained graphene and TMDs. We remark, however, that the interest of this model is not limited to these materials but could be applied to other physical systems. Magnons in TiCuCl\textsubscript{3}\cite{24}, for example, have been proven to show a BEC phase with a relativistic dispersion relation. It could be also be generalised by including the polarisation degree of freedom, to exciton-polariton condensates in synthetic honeycomb-like photonic lattices. We studied the properties of a non-stationary, but localised solution of the model, known as an oscillon. We detailed the dynamics of the two oscillons interaction and proved that this solution is also resilient to the interaction with impurities of the background. Until now the relevance of oscillon solutions of field theories has been highlighted only in high energy physics in both 2+1 and 3+1 dimension and they have not been considered in condensed matter physics. It is important to note that oscillon solutions of this kind are not allowed in non-relativistic BECs because the Gross-Pitaevskii is first order in time. They are tightly related to the pseudo-relativistic dispersion of Dirac quasiparticles. Materials that show a BEC phase with pseudo-relativistic dispersion relation could represent an interesting optical analogue platform to experimentally mimic field theories.
Appendix: Multiple scale perturbation theory for the NLKGE

In this appendix we introduce the multiple scale method for the nonlinear Klein-Gordon equation to show how the travelling waves propagates in a heterolayer condensate since the dynamics is the same on both sides.

\[ \partial^2_t \psi - (\partial^2_\xi + \partial^2_\eta) \psi + m^2 \psi + \psi^3 = 0, \]  \hspace{1cm} (19)

with initial conditions

\[ \psi(\xi, \eta, 0) = \psi_0(\xi, \eta), \]
\[ \psi_\tau(\xi, \eta, 0) = \psi_1(\xi, \eta), \]  \hspace{1cm} (20)

we set a slow space-time scale \( \xi_1 = \epsilon \xi, \eta_1 = \epsilon \eta, \) and \( \tau_1 = \epsilon \tau. \) We can now make the following ansatz of a perturbation series for the solution

\[ \psi(\xi, \eta, 0) = \sum_n \epsilon^{n+1} \Psi_n(\xi, \xi_1, \eta, \eta_1, \tau, \tau_1, \tau_2). \]  \hspace{1cm} (21)

Modifying the derivatives accordingly to the slow scale transformations and inserting the ansatz, the wave equation \([19], up to the second order, becomes (we will implicitly assume that initial conditions must be met at each order)

\[ \epsilon \mathcal{L}_{KG}(\Psi_0) + \epsilon^2 [\mathcal{L}_{KG}(\Psi_1) - 2 \Psi_{0, \tau_1 \tau} + 2 \Psi_{0, \xi \xi} \epsilon^2] + O(\epsilon^3) = 0 \]  \hspace{1cm} (22)

where \( \mathcal{L}_{KG} = \Box - m^2 \) is the linear Klein-Gordon operator.

The order \( \epsilon \) gives \( \mathcal{L}_{KG}(\Psi_0) = 0, \) that is solved by a function of the form

\[ \Psi_0(\xi, \xi_1, \eta, \eta_1, \tau, \tau_1) = A(\xi_1, \eta_1, \tau)e^{i(k_1 \xi + k_2 \eta - \omega \tau)} + c.c. \]  \hspace{1cm} (23)

with the dispersion relation \( \omega(k) = \sqrt{k^2 + m^2} \), \( k = (k_1, k_2). \) Proceeding to the following order we get

\[ \mathcal{L}_{KG}(\Psi_1) = 2i(\omega A_\tau + k_1 \partial_{\xi_1} A + k_2 \partial_{\eta_1} A) e^{i(k_1 \xi + k_2 \eta - \omega \tau)} + c.c., \]  \hspace{1cm} (24)

this term has the same structure as the solution to the homogeneous problem, it thus represents a secularity and needs to be eliminated. This leads to the following condition on the amplitude \( A(\xi_1, \eta_1, \tau) \)

\[ \omega A_\tau + k_1 \partial_{\xi_1} A + k_2 \partial_{\eta_1} A = 0, \]  \hspace{1cm} (25)

and a solution of this equation is a unidirectional travelling wave of the form \( A = A(\rho_1 - v_1 \tau) \) where \( \rho_1 = (\xi_1, \eta_1) \) and \( v = (v_\xi, v_\eta) \) is the group velocity vector. This explains the behaviour in figure [7] and [8] where we see unidirectional waves propagating along the \( \xi \) direction only, since the initial momentum along \( \eta \) is set to zero.
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