Spin echo dynamics under an applied drift field in graphene nanoribbon superlattices

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We investigate the evolution of spin dynamics in graphene nanoribbon superlattices (GNSLs) with armchair and zigzag edges in the presence of a drift field. We determine the exact evolution operator and show that it exhibits spin echo phenomena due to rapid oscillations of the quantum states along the ribbon. The evolution of the spin polarization is accompanied by strong beating patterns. We also provide detailed analysis of the band structure of GNSLs with armchair and zigzag edges.

Manipulation of electron spins using gate potentials in low dimensional semiconductor nanostructures is of interest, among other things, in that it provides a promising approach for the practical realization of robust qubit operations1–10. In recent years, experimental and theoretical research has sought a better understanding of the underlying physics of electrostatically defined quantum dots formed in two-dimensional electron gases for applications to solid state based quantum computing11–12. In these devices, the spin-orbit interaction gives rise to decoherence due to the coupling of the electron spins to lattice vibrations. Hyperfine interactions between electron and nuclear spins are also a factor in some systems. Much work has focused on III-V systems although Si quantum dots are also of interest because of their relatively long decoherence times due to weak spin-orbit and hyperfine interactions,10–19. In another promising approach, experimentalists have succeeded in fabricating and testing a low operation voltage organic field effect transistor using graphene as the gate electrode placed over a thin polymer gate dielectric layer19. Graphene is promising because it exhibits extremely weak spin orbit coupling and hyperfine interactions,20–23. In this paper, we present a theoretical investigation of the spin echo phenomena in GNSLs under an externally applied drift field. We find that the spin echo is accompanied by a strong beating pattern in the evolution of spin dynamics along the GNSLs with armchair and zigzag edges. We show that with a particular choice of the period and drift field, the spin polarization can be controlled to propagate on the surface of the Bloch sphere in a desired fashion.

The effective mass Hamiltonian for single layer GNSLs elongated along either armchair or zigzag direction (see Fig. 1) near the K point of the Brillouin zone can be written as: $H = v_F \sigma \cdot p + \Delta \sigma_z + U(r,t)$. Here $v_F$ is the Fermi velocity, $\Delta$ is the miniband width, $\sigma_i (i=x,y,z)$ are the Pauli spin matrices and $U(r,t)$ is the confining potential.

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For GNSLS with zigzag edge, we consider $U(r,t) = U_0(y + y(t))^2 / \ell_0^2$ and the wave function of the above Hamiltonian $H$ is $\psi(x,y) = \exp(ik_x x) \psi(y)$ (see Ref. 23 for details). Now, we define the relative coordinate $Y = y - y(t)$ and relative momentum $P_Y = p_y - p_y(t)$ and formulate the total Hamiltonian in the form: $H = H(P_Y,Y) + H_{qz}$. Here,

$$H(P_Y,Y) = v_F \sigma_y P_Y + U_0 Y^2 / \ell_0^2,$$

$$H_{qz} = C_1 \sigma_x + C_2 \sin(k_z a) \sigma_y + \Delta \sigma_z,$$

where $C_1 = \hbar v_F k_x$ and $C_2 = v_F m y_0 a_0$. Under an externally applied drift field $E_D$, we write the equation of motion for $k_x$ as: $\hbar \partial_t k_x(t) = eE_D$ (see Ref. 23 for details). Thus we can write $k_x(t) = \alpha_0 t$ with $\alpha_0 = eE_D / \hbar$. In (2), we have written the quasi momentum $p_y(t) =$

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FIG. 1. (Color online) Schematic diagram of graphene sheet with armchair along x-axis and zigzag along y-axis. Spin orientation shown by arrow sign in Fig. 1(a) and (b) move rapidly between $-x_0$ and $+x_0$ for armchair and between $-y_0$ and $+y_0$ for zigzag GNSLS that induce spin echo under an externally applied drift field.

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FIG. 2. (Color online) Band structure of GNSLs with zigzag edge. Localized and edge states wave function squared are plotted in Fig. 2(b) and (c) at $k = 0.1 \text{nm}^{-1}$. Here we chose $U_0 = +60 \text{ meV}$ for electron-like state and $U_0 = -60 \text{ meV}$ for hole-like state. Also we chose $\Delta = 60 \text{ meV}$, $v_p = 10^4 \text{ cm/s}$, $E_D = 10^6 \text{ V/cm}$, $y_0 = 100 \text{ nm}$, $\ell_0 = 150 \text{ nm}$, $m = 0.007m_e$ and $a = 5 \text{ nm}$.

$\dot{y} = -my_0a_0a \sin (k_z(t)a)$. We have used the Finite Element Method and solved the corresponding eigenvalue problems for (1) and (2) and plotted the band structures of GNSLs with zigzag edge in Fig. 2(a). In addition to the localized states (Fig. 2(b)), we also see the presence of edge states (Fig. 2(c)) in GNSLs.

FIG. 3. (Color online) Quasi-eigen energy of GNSLs with zigzag and armchair edges. The material parameters are chosen to be the same as in Fig. 2 but $E_D = 10^6 \text{ V/cm}$.

FIG. 4. (Color online) Fidelity, $F = |\langle \chi_- | \chi(t) \rangle|$, vs time in GNSLs with zigzag edge. Here we chose $y_0 = 100 \text{ nm}$, $a = 3 \text{ nm}$ and $\Delta = 10 \text{ meV}$.

FIG. 5. (Color online) Components of the evolution operator (exact results) for zigzag GNSLs under an applied drift field $E_D = 1 \text{ mV/nm}$. The material constants are chosen to be the same as in Fig. 4.

FIG. 6. (Color online) Spin-flip transition probability vs time in both zigzag and armchair GNSLs at $a = 1 \text{ nm}$ (solid lines with circles) and $a = 3 \text{ nm}$ (solid lines). The material constants are chosen to be the same as in Fig. 4.

The Hamiltonian $H (P_Y, Y)$ associated to the relative coordinates and relative momentum does not couple to the lowest spin states. Only the quasi-Hamiltonian $H_{qz}$ induces Bloch oscillations in the evolution of spin dynamics in GNSLs. For convenience, we write Eq. (2) as:

$$H_{qz}(t) = Cs_+ + C^\star s_- + 2\Delta s_z,$$

where $C = C_1 - iC_2 \sin(k_z(t)a)$, $C^\star = \text{conj}(C)$ and $s_\pm = s_x \pm is_y$. The band structures of quasi electron-hole states described by the Hamiltonian (3) can be written as

$$\delta = \pm \left(|C|^2 + \Delta^2\right)^{1/2}.$$

The band structure of electron and hole states in the first Brillouin zone $[-\pi/a, \pi/a]$ with the specific choice of the parameters is shown in Fig. 3.

We construct a normalized orthogonal set of eigen-spinors of the quasi-Hamiltonian (3) as:

$$\chi^\pm(t) = \frac{\delta - \Delta}{|C|^2 + (\delta - \Delta)^2}^{1/2} \left(\frac{C}{\delta - \Delta}\right),$$

where $C = C_1 - iC_2 \sin(k_z(t)a)$, $C^\star = \text{conj}(C)$ and $s_\pm = s_x \pm is_y$. The band structures of quasi electron-hole states described by the Hamiltonian (3) can be written as

$$\delta = \pm \left(|C|^2 + \Delta^2\right)^{1/2}.$$
tor (7) can be written as:
\[ U = \operatorname{conj}(P_{\alpha \beta \gamma}) \] due to the fact that \( \langle \chi_{s}^\pm | \chi_{r}^\pm \rangle = 1 \) and \( \langle \chi_{s}^\pm | \chi_{r}^\pm \rangle = 0 \).

With the use of the Feynman disentangling technique, the exact evolution operator of Hamiltonian (3) can be written as (see also supplementary material):
\[ U(t, 0) = T \exp \left\{ -\frac{i}{\hbar} \int H(t) dt \right\} \]
\[ = \exp(\alpha(t) s_+ \alpha) \exp(\beta(t) s_0 \beta) \exp(\gamma(t) s_- \gamma), \]
where \( T \) is the time ordering operator. At present, the time dependent functions \( \alpha, \beta, \gamma \) are unknown and can be found by the Feynman disentangling scheme as discussed below.

For a spin-1/2 particle, the exact evolution operator (10) can be written as:
\[ U(t) = \left( \exp \left\{ \frac{\alpha}{2} \right\} + \alpha \exp \left\{ -\frac{\alpha}{2} \right\} \right) \left( \exp \left\{ \frac{\beta}{2} \right\} + \beta \exp \left\{ -\frac{\beta}{2} \right\} \right) \]
\[ \left( \exp \left\{ \frac{\gamma}{2} \right\} + \gamma \exp \left\{ -\frac{\gamma}{2} \right\} \right), \]

which can be seen to satisfy \( U_{22} = \operatorname{conj}(U_{11}) \) and \( U_{12} = -\operatorname{conj}(U_{21}) \) due to the fact that \( U(t) \) is unitary.

At \( t = 0 \), we use the initial condition \( \chi^\pm_2(0) = (0 1)^T \), where \( T \) denotes transpose and write \( \chi^\pm_2(t) = U(t, 0)\chi^\pm_2(0) \) as
\[ \chi_2^\pm(t) = (\alpha \exp \{-\beta/2\} \exp \{-\beta/2\})^T. \]

Next, we find the functional form of \( \alpha(t), \beta(t), \) and \( \gamma(t) \) of GNSLs with zigzag edge by utilizing the Feynman disentangling scheme.

The exact evolution operator of Hamiltonian (3) can be written as:
\[ U(t) = \exp \left\{ \alpha(t) s_+ \right\} \exp \left[ -\frac{i}{\hbar} \int_0^t \left\{ (C - x) s_+ + C^* s_- + 2\Delta s_0 \right\} dt' \right], \]
where
\[ \alpha(t) = -\frac{i}{\hbar} \int_0^t x(t) dt', \]
\[ s_\mu'(t) = \exp(-\alpha s_+) s_\mu \exp(\alpha s_+). \]

Differentiating Eq. (12) with respect to \( \alpha \), we find
\[ \frac{ds_\mu'}{d\alpha} = -\exp(-\alpha s_+) (s_+ s_\mu - s_\mu s_+) \exp(\alpha s_+). \]

By utilizing initial condition \( s_\mu'(0) = s_\mu \), the primed operators are determined
\[ s_\mu' = s_\mu, \quad s_0' = s_0 + \alpha, \quad s_- = s_- + \alpha^2 s_\mu - 2s_0\alpha. \]

By substituting Eq. (14) in Eq. (10) and equating the coefficient of \( s_+ \) to zero, we find the following Riccatti equation:
\[ \frac{d\alpha}{dt} = -\frac{i}{\hbar} \left\{ C - C^* \alpha^2 + 2\Delta \alpha \right\}. \]

Hence the dependence on \( s_+ \) in (10) has been disentangled. By following the above procedure and by disentangling \( s_0 \) and \( s_- \), another set of the Riccatti equations for the time dependent functions \( \beta(t) \) and \( \gamma(t) \) can be written as
\[ \frac{d\beta}{dt} = -\frac{2i}{\hbar} \left\{ \Delta - C s_+ \alpha \right\}, \]
\[ \frac{d\gamma}{dt} = -\frac{i}{\hbar} C^* \exp \{ \beta \}. \]

In a similar way, for armchair GNSLs, we write the total Hamiltonian \( H = H(P_X, X) + H_{qa} \), where
\[ H(P_X, X) = v_x \sigma_x P_x + U_0 X^2 / \delta^2, \]
\[ H_{qa} = -C_2 \cos(k y) (\alpha \sigma_x + C_1' \sigma_y + \Delta \sigma_z). \]

Here \( C_1' = \hbar v_x k y(t) \) and \( C_2' = v_x m x_0 y_0 \alpha \alpha \). We construct a normalized orthogonal set of eigenspinors of the quasi-Hamiltonian (10) as:
\[ \chi^a_2(t) = \frac{\delta - \Delta}{|C'|^2 + (\delta - \Delta)^2} \left( \frac{C_1'}{\Delta \delta} \right), \]
\[ \chi^a_2(t) = \frac{\delta - \Delta}{|C'|^2 + (\delta - \Delta)^2} \left( \frac{C_2'}{\Delta \delta} \right), \]
\[ \chi^a(0) = \frac{\delta - \Delta}{|C'|^2 + (\delta - \Delta)^2} \left( \frac{C_1'}{\Delta \delta} \right), \]
and find $\chi^a(t) = U(t,0)\chi^a(0)$. The three coupled Riccati equations for the quasi-Hamiltonian of GNSLs with armchair edge can be written as

$$\frac{d\alpha}{dt} = -\frac{i}{\hbar} \left\{ \tilde{C} - \tilde{C}^* \alpha^2 + 2\Delta \alpha \right\}, \quad (23)$$

$$\frac{d\beta}{dt} = -\frac{2i}{\hbar} \left\{ \Delta - \tilde{C}^* \alpha \right\}, \quad (24)$$

$$\frac{d\gamma}{dt} = -\frac{i}{\hbar} \tilde{C}^* \exp \{ \beta \}, \quad (25)$$

where $\tilde{C} = -iC'$. We have solved the three coupled Riccati equations for zigzag and armchair GNSLs numerically and found the exact evolution operator (see Eq. 6 and 9), with the analytical solutions (see Eqs. 6 and 9), with the increasing magnitude of the drift field. The components of the spin waves in both kinds of superlattices travel with different velocities. Note that the Hahn echo patterns in GNSLs with zigzag (solid line with circles) and armchair (solid lines with diamond) edges due to the fact that the spin waves in both kinds of superlattices travel with different velocities. Note that the Hahn echo patterns in GNSLs with zigzag (solid line with circles) and armchair (solid lines with diamond) edges due to the fact that the spin waves in both kinds of superlattices travel with different velocities. The Hahn echo accompanied by strong beating patterns, is observed. The authors in Ref. 19 have fabricated a field effect transistors (FET) using graphene where the gate electrode was placed over a thin polymer gate dielectric layer. Such devices show excellent output and transfer characteristics (mobility $\approx 0.1 \text{cm}^2/\text{Vs}$) for gate and drain operations (see Fig.(4b) in Ref. 19). The present work was motivated in part by these experimental studies and our results (e.g., Figs. 14) might provide useful information for the design of quantum logic gates based on the application of the externally applied drift fields in GNSLs with both the armchair and zigzag edges.

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**SUPPLEMENTARY MATERIALS:**

To verify that the evolution operator (Eq. 8) is exact, we provide an example associated with the Hamiltonian of spin-1/2 particle in an effective magnetic field having a known solution:

$$H(t) = \Omega \cos (\omega t) s_x + \Omega \sin (\omega t) s_y + \Delta s_z. \quad (26)$$

The energy eigenvalues of (20) are $\varepsilon_{\pm} = \pm \hbar \delta/2$, where $\delta = [\Delta^2 + \Omega^2]^{1/2}$. We construct a normalized orthogonal set of eigenspinors of Hamiltonian (20) as:

$$\chi_+(t) = \frac{1}{\sqrt{N}} \left( (\delta - \Delta) \exp \{i\omega t\} \right), \quad (27)$$

$$\chi_-(t) = \frac{1}{\sqrt{N}} \left( (\delta - \Delta) \exp \{-i\omega t\} \right), \quad (28)$$

where

$$N^2 = \Omega^2 + (\delta - \Delta)^2. \quad (29)$$

Since the Hamiltonian (20) is time dependent, the general time dependent Schrödinger equations can be written as

$$\partial_t a(t) = -\frac{i}{2} \left( \Delta a + \Omega \exp \{-i\omega t\} b \right), \quad (30)$$

$$\partial_t b(t) = -\frac{i}{2} \left( \Omega \exp \{i\omega t\} a - \Delta b \right). \quad (31)$$
The exact solution of time dependent Schrödinger Eqs. \((30)\) and \((31)\) can be written as
\[ a(t) = \frac{\Omega}{\sqrt{\lambda}} \left\{ \cos \left( \frac{\lambda t}{2} \right) - i \frac{\delta}{\lambda} \sin \left( \frac{\lambda t}{2} \right) \right\} \exp \left( -i \frac{\omega t}{2} \right), \]  
\[ b(t) = \frac{\delta - \Delta}{\sqrt{\lambda}} \left\{ \cos \left( \frac{\lambda t}{2} \right) - i \frac{\delta}{\lambda} \sin \left( \frac{\lambda t}{2} \right) \right\} \exp \left( i \frac{\omega t}{2} \right), \]  
where
\[ \lambda' = \sqrt{\Omega^2 + (\Delta - \omega)^2}. \]
Expressing \((32)\) and \((33)\) as a linear combination of \(|\chi_+\rangle\) and \(|\chi_-\rangle\), we have
\[
\psi(t) = \left\{ \cos \left( \frac{\lambda' t}{2} \right) - i \frac{\omega \Delta}{\lambda' \delta} \sin \left( \frac{\lambda' t}{2} \right) \right\} \exp \left( -i \frac{\omega t}{2} \right) \chi_+(t) + i \frac{\omega \Omega}{\lambda' \delta} \sin \left( \frac{\lambda' t}{2} \right) \exp \left( i \frac{\omega t}{2} \right) \chi_-(t) .
\]

FIG. 8. (Color online) Transition probability vs time. Here we choose \(\omega = 10\) THz and \(\Omega = \Delta = 1\) THz. Transition probabilities obtained from Eqs. \((36)\) and \((37)\) (solid and dashed lines, respectively) are seen to be in excellent agreement to the ones obtained from the Feynman disentangling operator scheme. The transition probabilities are given by \(|\langle \chi_+ \rangle \| U(t, 0) \chi(0)\rangle|^2\) (circles) and \(|\langle \chi_- \rangle \| U(t, 0) \chi(0)\rangle|^2\) (triangles).

where \(\lambda = \omega + \omega, \omega = \Omega (n_2 - n_1) / 2,\)
\[
n_1 = \frac{\Delta - \omega}{\Omega} + \frac{\left( (\Delta - \omega)^2 + \Omega^2 \right)^{1/2}}{\Omega}, \tag{44}\]
\[
n_2 = \frac{\Delta - \omega}{\Omega} - \frac{\left( (\Delta - \omega)^2 + \Omega^2 \right)^{1/2}}{\Omega}. \tag{45}\]

In Fig. 8, the transition probability obtained from Eqs. \((36)\) and \((37)\) (solid and dashed lines) is seen to
be in excellent agreement to the one obtained from the disentangling scheme (circles and triangles). Thus, we have demonstrated that the evolution operator obtained from the disentangling operator scheme is exact. Finding an exact unitary operator is one of the requirements for quantum computing and is one of the motivations of the present work.

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