A density-wave mechanism with a continuously variable wave vector

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The origin of density waves is a vital component of our insight into electronic quantum matters. Here, we propose a novel, independent DW mechanism to a higher-dimensional lattice model in the presence of a magnetic field. Therefore, to locate the optimal DW wave vector, we can, in turn, look for the magnetic field strength that minimized the energy of the corresponding higher-dimensional system. Such an argument is unrelated to the FSN and remains relevant even when the DW strength is no longer weak in comparison with the bandwidth. Here, we focus on a specific set of two-dimensional (2D) models, namely, the Peierls transition has successfully described the properties of various quasi-1D DW materials [5–10], its extensions to higher dimensions have witnessed many difficulties [5]. Other mechanisms based upon electron-phonon coupling [11, 12] and exciton condensation [13–16] offer consistent explanations on the CDW origin and physical properties of a series of materials such as NbSe2, TaSe2 and CeTe3 without FSN. Besides, Overhauser’s theory pointed out the importance of electron interaction and correlations in the formation of DW in certain 2D materials [22, 24].

The existing theories do well in and only in their respective sphere of applications. Some of them are based upon perturbative analysis and become less controlled for stronger coupling [12, 24]. In addition, most theories cater to preferential DW wave vectors that are discrete and special to the band structures and/or the auxiliary degrees of freedom. Still, the origin of various CDWs, e.g., the 3D CDW states in M3Ir4Sn13 (e.g. Ca3Ir4Sn3 and Sr3Ir4Sn3) [25, 26], the CDW in cuprate materials [27], remain controversial to a degree. For instance, the charge modulation in some cuprate materials exhibits a dependence on the spectral gap [27] with its wave vector spanning a continuous spectrum [28–30]. Therefore, our overall understanding of the DW mechanism has not, by far, reached a complete picture yet.

Here, we propose a novel, independent DW mechanism from a Dirac-fermion Landau levels (LLs) energetics perspective. We note that a model with DW is equivalent to a magnetic field. Here, we propose an additional mosaic to the existing mechanisms such as Fermi-surface nesting, electron-phonon coupling, and exciton condensation. In particular, we find that certain 2D density-wave systems are equivalent to 3D nodal-line systems in the presence of a magnetic field, whose electronic structure takes the form of Dirac-fermion Landau levels and allows a straightforward analysis on its optimal filling. The subsequent minimum-energy wave vector varies over a continuous range and shows no direct connection to the original Fermi surfaces in 2D. Also, we carry out numerical calculations where the results on model examples support our theory. Our study points out that we have yet attained a complete story on our understanding of emergent density wave formalism.

INTRODUCTION

The origin of density waves (DWs) [1–4], relevant to various physical phenomena in electron and spin quantum matter, has been a fundamental yet controversial problem in condensed matter physics for several decades. In the Peierls theory of charge density waves (CDWs), the Fermi surface nesting (FSN) in the 1D chain gives rise to a spatially periodic re-distribution of charge density [5–8] with a 2π/qn period, commonly accompanied by a distortion of the lattice structure and a metal-insulator transition, where qn = 2kF is the nesting vector between the two Fermi points. Though the Peierls transition has been a fundamental yet controversial problem in condensed matter physics for several decades. In the Peierls theory of charge density waves (CDWs), the Fermi surface nesting (FSN) in the 1D chain gives rise to a spatially periodic re-distribution of charge density [5–8] with a 2π/qn period, commonly accompanied by a distortion of the lattice structure and a metal-insulator transition, where qn = 2kF is the nesting vector between the two Fermi points. Though the Peierls transition has successfully described the properties of various quasi-1D DW materials [5–10], its extensions to higher dimensions have witnessed many difficulties [5]. Other mechanisms based upon electron-phonon coupling [11, 12] and exciton condensation [13–16] offer consistent explanations on the CDW origin and physical properties of a series of materials such as NbSe2, TaSe2 and CeTe3 [17–21] without FSN. Besides, Overhauser’s theory pointed out the importance of electron interaction and correlations in the formation of DW in certain 2D materials [22, 24].

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Here, we propose a novel, independent DW mechanism from a Dirac-fermion Landau levels (LLs) energetics perspective. We note that a model with DW is equivalent to a higher-dimensional lattice model in the presence of a magnetic field. Therefore, to locate the optimal DW wave vector, we can, in turn, look for the magnetic field strength that minimized the energy of the corresponding higher-dimensional system. Such an argument is unrelated to the FSN and remains relevant even when the DW strength is no longer weak in comparison with the bandwidth. Here, we focus on a specific set of two-dimensional (2D) models, namely, the Peierls transition has successfully described the properties of various quasi-1D DW materials [5–10], its extensions to higher dimensions have witnessed many difficulties [5]. Other mechanisms based upon electron-phonon coupling [11, 12] and exciton condensation [13–16] offer consistent explanations on the CDW origin and physical properties of a series of materials such as NbSe2, TaSe2 and CeTe3 [17–21] without FSN. Besides, Overhauser’s theory pointed out the importance of electron interaction and correlations in the formation of DW in certain 2D materials [22, 24].

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We organize the rest of the paper as follows: In the next section, we introduce the Dirac-fermion LLs perspective for density wave tendencies, including the duality between a 2D DW system and a 3D system with a magnetic field, and the optimal DW wave vector in terms of the energetics on filling the Dirac-fermion LLs. In section III, we showcase the emergent DW in a benchmark 2D model and compare the numerical results on the optimal DW wave vectors with our theoretical expectations from the Dirac-fermion LL perspective. We also summarize the approximations enlisted in our theory and their potential impacts. We conclude our discussions with a summary of our theory and models, the implications, and what we can do in the next stage.
A DIRAC-FERMION LANDAU-LEVEL PERSPECTIVE FOR DENSITY-WAVE TENDENCIES

Let’s consider a category of model systems where our theoretical analysis can semi-quantitatively determine the preferential wave vector of an emergent density wave.

**Equivalence between a 2D DW system and a 3D system with a magnetic field**—A 2D system with an incommensurate density wave:

$$\hat{H}_{2D} = \hat{H}_0 + \sum_{\vec{r}=(x,y)} V_q \cos(\vec{q} \cdot \vec{r} + \phi) \hat{c}^\dagger \hat{c},$$  \hspace{1cm} (1)

where $\hat{H}_0$ includes the translation-invariant terms, $\hat{c}_\vec{r}$ is the electron annihilation operator at site $\vec{r}$, and $\vec{q} = (q_x, q_y)$ is the DW wave vector, is equivalent to a 3D system $\hat{H}_{3D} = \sum_{\vec{r},\vec{s},\vec{z}} \hat{H}_{\vec{r}, \vec{s}, \vec{z}}$:

$$\hat{H}_{\vec{r}, \vec{s}, \vec{z}} = \hat{H}_{0,\vec{r},k_z} + \sum_{\vec{r}=(x,y)} V_q \cos(\vec{q} \cdot \vec{r} + k_z) \hat{c}^\dagger_{\vec{r},k_z} \hat{c}_{\vec{r},k_z},$$ \hspace{1cm} (2)

with a magnetic field $\vec{B} = (q_y, -q_x, 0)$ corresponding to the vector potential $\vec{A} = (0, 0, q_y \cdot \vec{r})$, and $k_z = \phi$ is a good quantum number. We have applied the convention that the lattice spacing is 1 and $\epsilon = \hbar = 1$. We aim to determine the optimal $\vec{q}$ with the lowest energy given the rest of the model parameters, in analogy to the search for the Peierls transition in a mean-field treatment of the electron-phonon couplings, etc. For an incommensurate $\vec{q}$, the physics of $\hat{H}_{2D}$ is independent of $\phi = k_z$, which is sometimes denoted as a ‘sliding symmetry.’ Therefore, $\hat{H}_{2D}$ is equivalent to $\hat{H}_{3D}$ up to a constant factor of $N_z$, the number of sites of the 3D system in the $\hat{z}$ direction, and we can analyze the former with the help of the latter (or vice versa). The above equivalence relation offers a clear physical picture when the zero-field electronic structure around the Fermi energy takes the form of NLs in the 3D system, which we will discuss next.

**Dirac-fermion LLs for a NL system**—Without loss of generality, we consider a 3D model with a magnetic field:

$$\hat{H}_{3D} = \sum_{\vec{r},\vec{s},\vec{z},\vec{z}'} t_{\vec{r},\vec{s}} e^{iA(\vec{r}',\vec{r})} \hat{c}_{\vec{r}',\vec{s},\vec{z},\vec{z}'}^\dagger \hat{c}_{\vec{r},\vec{s},\vec{z},\vec{z}'} + h.c.$$ \hspace{1cm} (3)

where the first (second) line is the intra-layer (inter-layer) hopping between different $x \times y$ planes, $\vec{z}' = \vec{z}$ for $\vec{r}'$ and $\vec{r}$, and $\sigma^l$ and $\sigma^m$ for $l, m = x, y, z, l \neq m$ are the Pauli matrices on the spin (or pseudo-spin) $s, s'$. $A = (0, 0, q_x + q_y y)$ is the magnetic vector potential of a magnetic field $\vec{B} = (q_y, -q_x, 0)$. In this gauge, we can diagonalize the Hamiltonian in the $k_z$ basis:

$$\hat{H}_{3D}(k_z) = \sum_{\vec{r},\vec{s}} t_{\vec{r},\vec{s}} e^{iA(\vec{r},\vec{r})} \hat{c}_{\vec{r},\vec{s},\vec{z},\vec{z}}^\dagger \hat{c}_{\vec{r},\vec{s},\vec{z},\vec{z}} + h.c.$$ \hspace{1cm} (4)

V($\vec{r}_{xy}, k_z$) = $t'_{\vec{z}} \cos(\vec{q} \cdot \vec{r}_{xy} - k_z) - t''_{\vec{y}} \sin(\vec{q} \cdot \vec{r}_{xy} - k_z),$

where $t'_{\vec{z}}$ ($t''_{\vec{y}}$) is the real (imaginary) part of $t_z$ and $\vec{r}_{xy} = (x, y)$. $\hat{H}_{2D} \propto \hat{H}_{3D}(k_z)$ reflects a 2D DW system and is our focus in this work. To understand the preferential DW wave vector $\vec{q}$ in such a 2D system, we can analyze the preferential magnetic field amplitude and direction in the equivalent 3D system in Eq. 3.

Without the magnetic field, the 3D Hamiltonian $\hat{H}_{3D}$ can be diagonalized in the $\vec{k}$ space given its fully restored translation symmetry:

$$h_{3D}(\vec{k}) = \epsilon(\vec{k}_{xy}) \sigma^l + 2|t'_{\vec{z}} \cos(k_z) + t''_{\vec{y}} \sin(k_z)| \sigma^m, \hspace{1cm} (5)$$

where $\vec{k}_{xy} = (k_x, k_y)$, and $\epsilon(\vec{k}_{xy})$ represents the in-plane terms in Eq. 3. The Hamiltonian has a nodal line wherever $\epsilon(\vec{k}_{xy}) = 0$ and $t'_{\vec{z}} \cos(k_z) + t''_{\vec{y}} \sin(k_z) = 0$, which is illustrated in Fig. 1. We note that all the nodes on the nodal line are at the same energy in this specific model example, which simplifies our upcoming discussion but can be relaxed to some extent as long as there is little mixing between the zeroth and higher LLs once the magnetic field is present.

![FIG. 1](image-url)

In the presence of the magnetic field $\vec{B}$, the momentum $k_{\parallel}$ parallel to the magnetic field is a good quantum number that labels the different perpendicular cross-sections. Each cross-section may possess pairs of Dirac nodes, as shown in Fig. 1, which develop into discrete
LLs $\epsilon_n \propto \pm \sqrt{nB}$, $n = 0, 1, 2 \ldots$ in the presence of the magnetic field - the zeroth Landau level exists at the energy of the Dirac nodes, while the rest of the LLs are either above or below with a gap $\propto \sqrt{B}$. Summing over $k_\parallel$, we obtain a large zeroth LL degeneracy proportional to the number of Dirac nodes intersected - the NLs' projection along $k_\parallel$, see Fig. 2. The counting works for both strong (large $t_z$) and weak (small $t_z$) DWs.

**Magnetic field for optimal filling**—For a system with a fixed electron density $n_e = 1 + \delta n_e$, $\delta n_e \ll 1$, the optimal filling is to fill the zeroth LLs and leave all the higher LLs empty. When $|\vec{B}| < |\vec{B}|_{\text{opt}}$, the electrons will be forced into the higher LLs, leading to an excitation in an incompressible system and an increase in the systematic energy; when $|\vec{B}| > |\vec{B}|_{\text{opt}}$, on the other hand, while the zeroth LLs fully accommodating the electrons above half-filling provide no further energy reduction, the Fermi sea sees an uncompensated energy rise due to the larger magnetic field. Such energy dependence versus the external magnetic field or LL filling constitutes the premise of quantum oscillations $[36, 37]$, e.g., the dHvA effect. Therefore, quantitatively, the electron density above half-filling should match half of the zeroth LL degeneracy:

$$(N-1)L_\parallel S_\perp = \int n_D(k_\parallel)dk_\parallel |q_{\text{opt}}|_{S_\perp} \frac{1}{2\pi}$$
$$\Rightarrow N - 1 = \frac{n_D |q_{\text{opt}}|}{2\pi},$$

where $L_\parallel$ ($S_\perp$) is the length (area) of the system parallel (perpendicular) to the magnetic field, $|\vec{B}|/2\pi = |\vec{q}|/2\pi$ is the LL degeneracy over unit space, $n_D(k_\parallel)$ denotes the number of Dirac nodes in the cross-section at $k_\parallel$, and $|q_{\text{opt}}| = \int n_D(k_\parallel)dk_\parallel/2\pi$ is its average over all $k_\parallel$. With $n_D$, the expression for optimal $|q_{\text{opt}}|$ resembles the one-dimensional case in Ref. 38 yet $n_D$ is a continuous variable instead of an integer just like $n_D(k_\parallel)$.

A similar analysis yields the favorable $\vec{q} \equiv \vec{B}$ direction: we note that under the circumstance of the filling of the zeroth Landau level, $\vec{B}$, and thus the energy penalty to the Fermi sea is minimal when $n_D$ is maximum, which depends on the geometry of the nodal lines and favors the direction with the largest projection. In Fig. 2 we illustrate an example of a simple-loop NL and the direction to maximize the span of the projection $|\vec{k}_1 - \vec{k}_2|$ parallel to $\vec{B}$ and thus $n_D = |\vec{k}_1 - \vec{k}_2|/\pi$.

**Our approximations**—Our arguments are valid when the magnetic field is small enough to treat the Dirac nodes of the same $k_\parallel$ independently. Otherwise, quantum tunneling kicks in and gaps the Dirac nodes out, which happens if the separation between them $|\Delta k_\parallel| \lesssim |l_B^{-1}|$, where $l_B = \sqrt{\hbar/eB}$ is the magnetic length $[39, 40]$. Those zeroth LLs split beyond the nonzero LLs should not count in Eq. 6. As we can see in Fig. 3, there are always regions where pairs of Dirac nodes get arbitrarily close and violate the condition $|\Delta k_\parallel| \gg |l_B^{-1}|$. Fortunately, the splitting $\propto B$ is generally smaller than the spacing between the zeroth and nonzero LLs $\propto \sqrt{B}$ for small $B$. On the other hand, even the Dirac nodes have pairwise-annihilated and developed a mass, as the points $\iota$ and $\jmath$ in Fig. 1, the original zeroth LLs may have not yet shifted beyond the first LLs, leading to an underestimated (over-estimation) of $n_{3D} (q_{\text{opt}})$ following Eq. 6. We find the latter effect more dominant in our examples and provide a detailed numerical analysis of these effects in the Appendix. Also, we have assumed that the energy of the Fermi sea depends monotonically on the strength of the magnetic field and is insensitive to its direction, for which we show supporting numerical results in the Appendix.

**MODEL EXAMPLE AND NUMERICAL RESULTS**

**2D model example**—For demonstration purpose, let’s consider the model $\hat{H}_{2D} = \hat{H}_0 + \hat{H}_{DW}$ as follows:

$$\hat{H}_0 = \sum_{\vec{r},\vec{s},s,s'} t_{\vec{r},\vec{s},s,s'} \hat{c}_{\vec{r},s,s}^\dagger \hat{c}_{\vec{s},s,s'}^\dagger \sigma_3^{s,s'} (\vec{e} \cdot \sigma)_{s,s'} + h.c.$$  
$$\hat{H}_{DW} = - \sum_{\vec{r},\vec{s},s,s'} [2V \cos(\vec{q} \cdot \vec{r} + \phi_0)] \hat{c}_{\vec{r},s,s}^\dagger \hat{c}_{\vec{s},s,s'} + 2\lambda \sin(\vec{q} \cdot \vec{r} + \phi_0) \hat{c}_{\vec{r},s,s}^\dagger \hat{c}_{\vec{s},s,s'}]$$  

where $\sigma = (\sigma^x, \sigma^y, \sigma^z)$ are the Pauli matrices, $\vec{e} = (\epsilon_1, 0, \epsilon_0)$ are the onsite potentials, and $t_{\vec{r}} = t$ for $\vec{r} = \vec{x}, \vec{y}$ and $t_{\vec{r}} = it'$ for $\vec{r} = \vec{x} + \vec{y}, \vec{x} - \vec{y}$ are the hopping parameters. The dispersion of the translation invariant Hamiltonian $\hat{H}_0$: 

$E_k^0 = \pm 2 \sqrt{\epsilon_1 + t (\cos k_x + \cos k_y) + 2t' \sin k_x \cos k_y}^2 + \epsilon_0^2,$  

$E_k = \pm 2 \sqrt{\epsilon_1 + t (\cos k_x + \cos k_y) + 2t' \sin k_x \cos k_y}^2 + \epsilon_0^2.$  

![FIG. 2](image-url) The optimal direction of the magnetic field $\vec{B}$ for an anisotropic nodal line in the $k_x$-$k_y$ plane is to maximize the range $|\vec{k}_1 - \vec{k}_2|$ parallel to $\vec{B}$, which yields the largest $n_D = |\vec{k}_1 - \vec{k}_2|/\pi$. 

![Diagram](image-url)
In the presence of the magnetic field, the Dirac nodes—For an incommensurate $\tilde{q}$, the 2D model in Eq. 7 is equivalent to a 3D system with a magnetic field. Without the magnetic field, the 2D model in Eq. 7 shows shows a $4\epsilon_0$ gap between the two bands. $t = 1$, $t' = 0.1$, $\epsilon_0 = 0.5$, $\epsilon_1 = -2.15$. (b) The Fermi surface of (a) at Fermi energy $E_F = 1.3$ slightly above half-filling shows no sign of FSN.

is shown in Fig. 3b, where the Fermi surface slightly above half-filling, as shown in Fig. 3a, is rather circular and shows no obvious FSN. However, we will show that to minimize energy, the model prefers a DW, characterized by the mean-field $H_{DW}$, with a preferential wave vector $\tilde{q}_{\text{opt}}$ that shows a continuous range and nothing to do with FSN.

3D nodal-line system and LLs—For an incommensurate $\tilde{q}$, the 2D model in Eq. 7 is equivalent to a 3D system with a magnetic field. Without the magnetic field, the 3D system $(\hat{a}_{\xi,\uparrow}^\dagger, \hat{a}_{\xi,\downarrow}^\dagger)h_{3D}(\tilde{k})(\hat{a}_{\xi,\uparrow}, \hat{a}_{\xi,\downarrow})^T$ in the momentum space:

$$h_{3D}(\tilde{k}) = [2\epsilon_1 - 2\lambda \sin k_z + 2t(\cos k_x + \cos k_y) + 4t' \sin k_x \cos k_y] \sigma^x + [2\epsilon_0 - 2V \cos k_z] \sigma^z,$$

may possess NLs where the $\sigma^z$ coefficient in Eq. 9 vanishes on the $k_z = \pm \arccos(\epsilon_0/V)$ planes. We show a couple of examples in Fig. 4.

In the presence of the magnetic field, the Dirac nodes along the nodal lines exhibit themselves as Dirac-fermion NLs. While the $n \neq 0$ LLs depend on Fermi-velocity details and form continuum, the zeroth Landau levels remain (nearly) degenerate at zero energy and are separated from the rest of the Landau bands with large gaps due to the LL spacings. For example, we show in Fig. 5 the density of states (DOS) of the models with the NLs in Fig. 4 in a magnetic field $|\tilde{q}| \ll 2\pi$, where the contributions from the zeroth LLs are clearly visible between the red dashed lines.

**Optimal DW wave vectors**—We calculate the energy of $H_{2D}$ in Eq. 7 numerically via exact diagonalization on system size $L_x = 1000$ along $\tilde{q}$ and $L_z = 200$ values of $k_z$ in the perpendicular direction. We discuss our setup for $\tilde{q}$ along directions other than $\tilde{x}$ and $\tilde{y}$ in the Appendix. The results on the average energy per electron $\bar{E}$ versus the DW wave vector $\tilde{q}$ for the model parameters in Figs. 4 and 5 is shown in Fig. 6. The optimal wave vector $|\tilde{q}_{\text{opt}}| \sim 0.15$ is approximately consistent with our theoretical expectation of $|\tilde{q}_{\text{theory}}| \sim 0.17$ according to Eq. 6. In addition, the DWs in the $\tilde{q} = \tilde{x}, \tilde{y}$ directions yield the lowest energy overall with negligible difference, consistent with our analysis and the fact that the NLs projection $|k_1 - k_2|$ and subsequently $\bar{n}_D$ are largest along these two directions. In comparison, the average electron energy without the DW $H_{DW}$ is $\Delta E_0 \sim 0.29$ above these minima, suggesting that the DW formation is indeed favorable energetically.

Also, the dependence of $\bar{E}$ with $|\tilde{q}|$ is consistent with our expectation: the optimal $|\tilde{q}_{\text{opt}}|$ allows all the electrons above charge neutrality to be accommodated by the degenerate zeroth LLs; when $0 < |\tilde{q}| < |\tilde{q}_{\text{opt}}|$, the filling goes to some of the higher LLs leading to higher energy; when $|\tilde{q}| > |\tilde{q}_{\text{opt}}|$, on the other hand, the electron Fermi sea suffers an energy penalty due to the higher magnetic field. We discuss more detailed results and analysis on energetics in the Appendix.

More generally, the value of $\tilde{q}_{\text{opt}}$ versus the DW amplitude $\lambda$ as a tuning parameter is summarized in Fig.
6. Different colors denote results for $\vec{q}$ filling. The system has a $V_\lambda$ tour and grows with $\lambda$ intuitively, when $\epsilon$ their respective $\Delta$ obtained by comparing the energy for different $q$ theory versus the DW strengths. The former is $\overline{\nu}_D$, we compare the two in the inset of Fig. 4. Overall, we note that the DWs wave vectors change continuously with the DW strengths, in sharp contrast to the behaviors descending from the FSN, electron-phonon coupling, or exciton condensation, where the DW wave vector is generally fixed by the Fermi surface geometry or a momentum specially meaningful to the bosonic degrees of freedom.

**CONCLUSIONS**

In summary, we put forward a novel perspective to understand the DW tendency in 2D systems from the energetics of a 3D NL system. Our setup is parallel to the Peierls transition yet does not require any apparent FSN to begin with. Correspondingly, the optimal DW wave vector depends on the geometry of the 3D NLs and may vary continuously with respect to the model parameters. Also, our numerical results on benchmark models fit with our analysis consistently. Such continuous variations of the DW wave vectors are present in materials such as various cuprates [27–30], where a purely FSN interpretation is unlikely. While we do not intend to relate our analysis to these materials directly, our perspective kindles the theoretical possibility of a variable DW wave vector from more generic origins.

On the other hand, our study points out that our current understanding of the DW origin is still primitive and a universal understanding is not yet available. Our current study has focused on models with rather specific constructions. While such a setup facilitates the theoretical analysis and its controllability, it also limits the generalization of the mechanism and its application in practice. It will be interesting to probe the generalization of the current mechanism beyond its model limits and its connection with FSN and other DW mechanisms in interpolating models for further physical intuition.

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Appendix

Beyond approximations of independent, massless Dirac nodes

To account for the potential impact of Dirac fermion mass, pair separation, and the magnetic field strength, we consider a simple 2-bands model:

\[ \hat{H}_D = (m - k_x^2)\sigma^x + k_y\sigma^y, \]

where \( m \) is a parameter. The model has 2 Dirac-fermions at \((±\sqrt{m}, 0)\) for \( m > 0 \), and massive Dirac-fermions with a mass \( \sim |m| \) for \( m < 0 \). Therefore, we can use this model to simulate the low-energy scenarios at different \( k_y \) cross-sections in Fig. 1 in the main text. In the presence of a magnetic field \( \vec{B} = (0, 0, B) \) with gauge \( \vec{A} = (0, Bx, 0) \), we can express the momentum as:

\[ k_x = \frac{1}{\sqrt{2|B|}} (\hat{a} + \hat{a}^\dagger) \]
\[ k_y + \frac{eBx}{\hbar} = i \frac{1}{\sqrt{2|B|}} (\hat{a} - \hat{a}^\dagger), \]

where \( \hat{a} \) and \( \hat{a}^\dagger \) are ladder operators defined upon the LL number space. In turn, we can re-write the Hamiltonian as:

\[ \hat{H}'_D = (m - \frac{1}{\sqrt{2|B|}} (\hat{a} + \hat{a}^\dagger))^2)\sigma^x + i \frac{1}{\sqrt{2|B|}} (\hat{a} - \hat{a}^\dagger)\sigma^y, \]

which we solve for the dependence of the low-lying LLs on \( B \), as in Fig. 8.

When two Dirac nodes are farther apart, they behave independently, and their zeroth LLs contribute to the zero-energy DOS in the magnetic field. However, as their separation \( |\Delta k_\perp| \ll l_B^{-1} \) gets smaller in comparison with the magnetic length, the quantum tunneling between the Dirac nodes leads to splittings between the Landau levels [39, 40], which gradually deviates from the zero energy as \( B \) increases. This process is illustrated in Fig. 8 for \( m = 0.01 \). Fortunately, such splitting is relatively small in comparison with the LL spacings, especially between the \( n = 0 \) and \( n = 1 \) LLs (see the red curves in Fig. 8 for \( n = 1 \) LLs), at small to moderate magnetic field, and does not deflect much of our reasoning.

On the other hand, even when the Dirac nodes have annihilated in pairs and no NL is present, similar to the \( i \) and \( j \) points in Fig. 1, the resulting LLs depend on the actual values of their masses and may still be relatively close to zero energy. For instance, we present the zeroth LL for \( m = -0.01 \) in Fig. 8 which are closer to zero energy than the generic first LLs. By counting only the NLs, we may underestimate the contribution from such (slightly) massive Dirac-fermion LLs to the DOS around zero energy. Still, the NLs offer a good starting point for the counting, as the LLs for most massive fermion LLs, e.g., \( m = -0.25 \), are too far away from zero energy to actually contribute, and our neglect is small.

![FIG. 8. Selected LLs of Eq.12 versus the magnetic field \( B \) for massless (\( m = 0.01 \)) and massive (\( m = -0.01 \), \( m = -0.25 \)) Dirac-fermion cases dictate the possible contributions to the DOS around zero energy.](image)

![FIG. 9. The (relative) average energy \( E_r \) \( E_0 \) of the electrons in the Fermi sea at half-filling \( n_e = 1 \) depends monotonically on the largeness of \( \vec{q} \); yet little on the direction of \( \vec{q} \). We have applied the same parameter setting as in Figs. 4a and 5a in the main text.](image)

**Energy cost of magnetic field on the Fermi sea**

We calculate the energy of the Fermi sea, i.e., the average energy of the electrons at half-filling \( n_e = 1 \) for the model in Figs. 4a and 5a in the main text in a magnetic field \( B \), and summarize the results in Fig. 9. The energy increases monotonically with respect to the amplitude of the magnetic field (DW wave vector) and is relatively insensitive to the direction of the magnetic field (DW wave vector). Therefore, we cannot arbitrarily increase \( |q_{opt}| \) after reaching the complete filling of zeroth LLs due to the associated energy cost.
For a DW vector $\vec{q} = |q_0|\left(\frac{1}{\sqrt{1+p^2}}, \frac{p}{\sqrt{1+p^2}}\right)$ on the 2D square lattice, we change the basis from $\hat{x}, \hat{y}$ to $\hat{x}', \hat{y}'$ so that we can utilize the translation symmetry along the $\hat{y}'$ direction.

**Numerical method for systems with a tilted magnetic field**

Generally, density waves may arise in any direction, and we need to consider the case where $\vec{q} = (q_x, q_y)$ is tilted from the $\hat{x}$ or $\hat{y}$ directions for the most energetically favorable condition. Here is the method we used to compute the dispersion of the model in Eq. 7 with $\vec{q}$ in any direction.

While our theoretical analysis based upon 3D NLs is a low-energy effective theory that can apply to $\vec{q}$ along any direction, the numerical calculations require that $\vec{q} = (q_x, q_y)$ points to a commensurate direction, $\frac{q_x}{q_y} = \frac{m}{n}, m, n \in \mathbb{Z}, \gcd(m, n) = 1$. Without loss of generality, we limit ourselves to:

$$\vec{q} = |q_0|\left(\frac{1}{\sqrt{1+p^2}}, \frac{p}{\sqrt{1+p^2}}\right),$$

(13)

for simplicity, so that there will not be additional sublattices. Here, $|q_0|$ is the norm of the wave vector, and $p \in \mathbb{Z}$ determines the direction of $\vec{q}$.

This wave vector in the 2D DW system corresponds to a magnetic field $\vec{B} = |q_0|\left(-\frac{p}{\sqrt{1+p^2}}, -\frac{1}{\sqrt{1+p^2}}, 0\right)$ in the 3D system, whose electromagnetic vector potential takes the form of $\vec{A} = (0, 0, \vec{q} \cdot \vec{r})$. Consequently, neither $k_x$ nor $k_y$ is good quantum number. Instead, we can take a new basis:

$$\hat{x}' = (1, 0)$$
$$\hat{y}' = (-\frac{p}{\sqrt{1+p^2}}, \frac{1}{\sqrt{1+p^2}}),$$

(14)

so that there remains translation symmetry along the $\hat{y}'$ direction, and $k_{y'}$ is a good quantum number, see Fig. 10 for illustration.

The Hamiltonian $\hat{H}_{2D} = \hat{H}_0 + \hat{H}_{DW}$ in the new basis takes the same form as Eq. 7 in the main text and can be solved in a similar fashion, with the following changes to the model settings:

$$\vec{\delta} = \vec{x}, \vec{y} \Rightarrow \vec{\delta} = \hat{x}', \hat{y}'$$
$$\vec{\delta} = \vec{x} + \vec{y}, \vec{x} - \vec{y} \Rightarrow \vec{\delta} = (p+1)\hat{x}' + \hat{y}', (1-p)\hat{x}' - \hat{y}'$$
$$\vec{\delta} \cdot \vec{r} \Rightarrow q_x x = \frac{|q_0| x}{\sqrt{1+p^2}}.$$

(15)

Finally, we apply a polynomial fit to the resulting $E_0(|\vec{q}|)$ to get rid of the fluctuations in data, mainly caused by the limited system and step sizes, for a smoother display.