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I. INTRODUCTION

The discovery of the extraordinary electrical conduction and sensor properties of graphene, for which Geim and Novoselov were awarded the Nobel Prize in physics in 2010, has focused attention on Dirac materials. Throughout the world, all disciplines of science and engineering are heavily involved in research of these materials for their potential to succeed silicon as the material of choice for the next generation of electronic devices and computers. Graphene and the other Dirac materials are characterized by low energy spectra that mimic that of relativistic electrons/positrons, having Hamiltonians that are linearly proportional to momentum. These materials include silicene, topological insulators, group VI dichalcogenides, and others, as well as graphene. In addition to the enormous commercial potential of the Dirac materials, their similarity to relativistic particles intensifies intellectual interest in their low energy phenomenology. In this work, because of the importance of a magnetic field as a probe of the properties of matter (and as an agent modifying them) and considering the increasing importance of nanostructures, we focus on the role of a quantizing magnetic field involving a superlattice of quantum antidots in Group VI dichalcogenides using a Krönig–Penney type model.

In Sec. II, we describe the system dynamics in terms of its Green’s function, which we solve explicitly for dynamical development along the axis of the lattice, determining this Green’s function in terms of the corresponding “no-lattice” dichalcogenide Green’s function in a perpendicular, Landau-quantizing magnetic field. In Sec. III, we examine the dispersion relation for the energy spectrum of this system and solve it, explicitly tracing the formation of Landau minibands for the “relativistic” dichalcogenide carriers with weak lattice coupling. Section IV reviews our conclusions with a discussion of energy parameters and our approximate solution for the spectrum of dichalcogenide Landau minibands.
in frequency(ω) representation. Here, \( G_0(x_1, x_2; y_1, y_2; \omega) \) represents the two dimensional infinite-space matrix Green’s function of the dichalcogenides in a normal quantizing magnetic field in the absence of the superlattice of antidot potential barriers, which we model as a one-dimensional row of Dirac-delta functions on the x-axis, similar to the non-relativistic Kröning-Penney model.\(^\text{17}\) The dichalcogenide Green’s function is actually an \( 8 \times 8 \) block-diagonal matrix composed of four 2 \times 2 blocks, each of which is characterized by a given set of values of its spin(\( s_z = \pm 1 \)) and valley (\( v = \pm 1 \)) indices. Such 2 \times 2 blocks are referred to as the “Green’s function” in this work,

\[
U(\vec{r}) = U(x, y) = a \sum_{n=-\infty}^{\infty} \delta(x-nd)\delta(y). \quad (2)
\]

\( \alpha \equiv U_0a^2 \) is essentially the product of the antidot potential barrier height and its cross-sectional area \( a^2 \), and \( d \) is the lattice period. Accordingly, we have (suppress \( \omega \))

\[
G(x_1, x_2; y_1, y_2) = G_0(x_1, x_2; y_1, y_2) + a \sum_{n=-\infty}^{\infty} G_0(x_1, nd; y_1, 0)G(nd, x_2; y_2). \quad (3)
\]

To solve, we need \( G(nd, x_2; 0, y_2) \) at the discrete points \( x = nd \), and its determination may be obtained by setting \( x_1 = md \) and \( y_1 = 0 \) on the left of Eq. (3), whence

\[
G(md, x_2; 0, y_2) = G_0(md, x_2; 0, y_2) + a \sum_{n=0}^{\infty} G_0(md, nd; 0, 0)G(nd, x_2; 0, y_2). \quad (4)
\]

The “no-lattice” 2D Dirac-type 2 \times 2 matrix “relativistic” Green’s function \( G_0 \) in a magnetic field [for given valley (\( v = \pm 1 \)) and spin (\( s_z = \pm 1 \)) indices of the dichalcogenides] has the form\(^\text{18,19} \)

\[
\hat{G}_0(\vec{r}, \vec{r}'; t, t') = \hat{C}(\vec{r}, \vec{r}')G_0(\vec{r} - \vec{r}', t - t'), \quad (5)
\]

where \([\phi(\vec{r})] \) is an arbitrary gauge potential

\[
C(\vec{r}, \vec{r}') = \exp\left[\frac{ie}{2} \vec{r} \times (\vec{r}' - \phi(\vec{r}) + \phi(\vec{r}'))\right]. \quad (6)
\]

Equation (6) is equally valid in both time- and frequency-representations. It is important to note that \( \hat{G}_0(\vec{r} - \vec{r}', t - t') \) on the right of Eq. (5) is effectively spatially translationally invariant. As our concern is focused on the carrier quantum dynamics along the axis of the lattice, we set \( y \equiv 0 \), in which case \( \vec{r} = x\vec{a} \) and \( \vec{r}' = x'\vec{a} \) are parallel, so \( C(\vec{r}, \vec{r}') \equiv 1 \) in the perpendicular magnetic field (choosing the arbitrary gauge phase to vanish: \( \phi \equiv 0 \)). The resulting structure of \( G_0(md, nd, 0, 0) \) is that of a translationally invariant matrix

\[
G_0(md, nd, 0, 0) = G_0([m - n]d, 0, 0), \quad (7)
\]

which we indicate by an overhead dot on \( G_0 \) on the right of Eq. (7). Invoking lattice periodicity, we proceed defining the Fourier series \( (r \text{ are integers below}) \)

\[
\hat{G}(p) = \sum_{r=-\infty}^{\infty} e^{ip\vec{r}d} G(rd) \quad (8)
\]

with

\[
G(rd) = \frac{d}{2\pi} \int_{-\pi/d}^{\pi/d} dp \; e^{-ipd} \hat{G}(p) \quad (9)
\]

and

\[
\hat{G}_0([m - n]d) = \frac{d}{2\pi} \int_{-\pi/d}^{\pi/d} dp \; e^{-ipd} \hat{G}_0(p). \quad (10)
\]

Substituting into Eq. (4), we obtain

\[
\hat{G}(p) = \hat{G}_0(p) + a \hat{G}_0(p) \sum_{n=-\infty}^{\infty} e^{ipn(n+1)d} G(nd) = \hat{G}_0(p) + a \hat{G}_0(p) \int_{-\pi/d}^{\pi/d} dq \left( \sum_{n=-\infty}^{\infty} e^{ipnqd} \right) \hat{G}_0(q), \quad (11)
\]

and the use of the Poisson sum formula as

\[
\sum_{n=-\infty}^{\infty} e^{ipnqd} = \frac{2\pi}{d} \sum_{m=-\infty}^{\infty} \delta(p - q - 2\pi nm/d)
\]

yields

\[
\hat{G}(p) = \hat{G}_0(p) + a \hat{G}_0(p) \int_{-\pi/d}^{\pi/d} dq \delta(p - q - 2\pi nm/d) \hat{G}_0(q) \quad (12)
\]

or

\[
\hat{G}(p) = \hat{G}_0(p) + a^{\hat{G}_0}(p) \hat{G}(p) \quad (13)
\]

since the \( q \)-integration is only over the first Brillouin zone alone. Restoring \( x_2 \) and \( \omega \), the solution for the \( 2 \times 2 \) matrix dichalcogenide Green’s function describing Landau quantized carrier dynamics along the axis of the antidot lattice (\( y \equiv 0 \)) is given by Eq. (13) as

\[
G(p; x_2; 0, 0; \omega) = \left[1 - a(\hat{G}_0(p; 0, 0; \omega))\right]^{-1} \hat{G}_0(p; x_2; 0, 0; \omega), \quad (14)
\]

and employing Eqs. (3) and (9), we have

\[
G(x_1, x_2; 0, 0) = G_0(x_1, x_2; 0, 0) + a \sum_{n=0}^{\infty} G_0(x_1, nd; 0, 0) \frac{d}{2\pi} \int_{-\pi/d}^{\pi/d} dp \times e^{-ipd} \left[1 - a(\hat{G}_0(p; 0, 0; \omega))\right]^{-1} \hat{G}_0(p; x_2; 0, 0; \omega) \quad (15)
\]

for the 2D Kröning-Penney type “relativistic” model at hand, with a high magnetic field.

### III. Green’s function analysis of the Landau quantized dichalcogenide antidot lattice dispersion relation

For a given set of spin (\( s_z = \pm 1 \)) and valley (\( v = \pm 1 \), referring to the \( K, K' \) points) indices, the “no-lattice” dichalcogenide carrier Green’s function

\[
G_0(\vec{r}_1, \vec{r}_2; \omega) = G(\vec{r}_1, \vec{r}_2; \omega) \quad (16)
\]

in a quantizing magnetic field in the absence of a lattice is a \( 2 \times 2 \) matrix with diagonal elements \( G_{11}, G_{22} \) collectively denoted as \( G^\text{Diag}_{22} \) [notation: \( G^\text{Diag}_{22} \rightarrow G^\text{Diag}_{11}(R, \omega) \rightarrow G^\text{Diag}_{11}(R) \), suppressing \( \omega \), and \( R = r_1 - r_2 = (X, Y) = (x_1 - x_2, y_1 - y_2) \)]. These spatially translation-
ally invariant elements of the Green's function have been recently determined as
\[
G'_{12}(R, \omega) = \frac{eB}{2\pi} \omega \exp\left(-\frac{eB}{4} [X^2 + Y^2]\right)
\]
\[
\times \sum_{n=0}^{\infty} L_n \left(\frac{eB}{2} [X^2 + Y^2]\right) D_{n,\omega,\nu,k},
\]
(16)
where \( G_{11}, G_{22} \) correspond to the upper, lower of alternative (+, -) signs and
\[
D_{n,\omega,\nu,k} \equiv 2g_{\nu,\omega} - \epsilon_{n,\nu,k}^2.
\]
(17)
Here, \( \omega_{\pm} = \omega \pm E_{\nu,\nu} \pm \epsilon_{n,\nu,k}^2 = \left[2n + 1 \mp 1\right] \gamma eB \left(1_{\nu} = \pm 1 \text{ for } v = \pm 1 \right) \) \((\Delta' \text{ is the energy gap, } E_{\nu,\nu} = s_{\nu} k/2 \) \((\lambda \text{ is the spin splitting), } L_n \text{ are the Laguerre polynomials, and the upper or lower of alternative signs correspond to } G_{11} \text{ or } G_{22}, \text{ respectively. Furthermore, the off-diagonal elements were discussed along with the diagonal ones in Ref. 29.) \( \text{They are given by}
\]
\[
G'_{12}(R, \omega) = \frac{\gamma(yeB)^2}{2\pi} \left[(X + Y)[1 \mp 1_\nu] e^{-\frac{eB}{2} X^2} \sum_{n=0}^{\infty} \left(\frac{eB^2}{2}\right)^n D_{n,\omega,\nu,k}\right] + \frac{\gamma(yeB)^2}{2\pi} \left[(X + Y)[1 + 1_\nu] e^{-\frac{eB}{2} X^2} \sum_{n=0}^{\infty} \left(\frac{eB^2}{2}\right)^n D_{n,\omega,\nu,k}\right]
\]
(18)
From Eq. (15), it is clear that the superlattice-induced energy spectrum is determined by the dispersion relation
\[
\text{det}\left[1 - \alpha \Gamma_{\nu}(p, 0, 0; \omega)\right] = 0
\]
or
\[
1 = a \left[ \hat{G}_{11}(p) + \hat{G}_{22}(p) \right] - a^2 \left[ \hat{G}_{11}(p) \hat{G}_{22}(p) - \hat{G}_{21}(p) \hat{G}_{12}(p) \right].
\]
(19)
The diagonal elements are given by Eqs. (16) and (8) as
\[
\hat{G}_{11}^{\text{Diag}}(p) = \sum_{n=0}^{\infty} \frac{\omega_n N_n}{D_{n,\omega,\nu,k}}
\]
with
\[
N_n = \frac{eB}{2\pi} \sum_{r=-\infty}^{\infty} e^{ipr} e^{-\frac{eB^2}{2} [r^2] L_n \left(\frac{eB^2}{2}\right) r},
\]
(20)
and the off-diagonal elements are
\[
\hat{G}_{12}(p) = \sum_{n=0}^{\infty} \frac{M_n}{D_{n,\omega,\nu,k}},
\]
(21)
where we have defined
\[
M_n = \frac{\gamma(yeB)^2}{2\pi} \sum_{r=-\infty}^{\infty} e^{ipr} e^{-\frac{eB^2}{2} [r^2]} \left(\frac{1 \mp 1_\nu}{2} \left[ L_n \left(\frac{eB^2}{2}\right)^n r\right] + L_{n-1} \left(\frac{eB^2}{2}\right) r\right)
\]
(22)
The energy (frequency, \( h \to 1 \)) denominators may be written as
\[
D_{n,\omega,\nu,k} = \omega_n^2 \mp 2g_{\nu,\omega} - \epsilon_{n,\nu,k}^2 = (\Omega_k - R_{n,\omega,\nu,k})(\Omega_k + R_{n,\omega,\nu,k})
\]
(23)
and
\[
\frac{1}{D_{n,\omega,\nu,k}} = \frac{1}{2R_{n,\omega,\nu,k}} \sum_{n'=0}^{\infty} \frac{\tau^1}{\omega_n \pm \frac{\tau}{\omega_n} R_{n,\omega,\nu,k}},
\]
(24)
where we use the notation (bear in mind \( \omega_{\pm} = \omega - E_{\nu,\nu} \pm \epsilon_{n,\nu,k}^2 \)
\[
\Omega_k \equiv [\omega_n \pm g_{\nu,\omega}^2] \text{ and } R_{n,\omega,\nu,k} = \sqrt{\omega_{\pm} + \epsilon_{n,\nu,k}^2}.
\]
(25)
Of course, the “no-lattice” energy levels are given by the zeros of \( D_{n,\omega,\nu,k} = 0 \) or \( \Omega_k = \pm \frac{\tau}{\omega_n} R_{n,\omega,\nu,k}. \)

Employing Eqs. 20–25 to construct the terms of the dispersion relation [Eq. (19)] for given \( s_2 \) and \( v \) values, we have (abbreviate: \( R_{n,\omega,\nu,k} \to R_{n,\omega,\nu,k}; D_{n,\omega,\nu,k} \to D_{n,\omega,\nu,k} \))
\[
\hat{G}_{11}(p) + \hat{G}_{22}(p) = \sum_{n=0}^{\infty} \sum_{\pm} \sum_{\pm} \frac{N_n \omega_n}{\Omega_n \pm \frac{\tau}{\omega_n} R_{n,\omega,\nu,k}}
\]
(26)
where \( \Omega_k \equiv \omega_n \pm g_{\nu,\omega}^2 \) and \( R_{n,\omega,\nu,k} = \sqrt{\omega_{\pm} + \epsilon_{n,\nu,k}^2}. \)

The multitude of simple frequency poles in the trace \( Tr\hat{G} = \hat{G}_{11}(p) + \hat{G}_{22}(p) \) imply the existence of a multitude of states corresponding to the roots of the dispersion relation [Eq. (19)], which are in turn shifted by the coincident set of simple poles in the product \( \hat{G}_{11}(p) \hat{G}_{22}(p) \) in Eq. (27). The last term of Eq. (27) for \( \hat{G}_{11}(p) \hat{G}_{22}(p) \) also introduces second order poles, which bifurcate the spectrum of states introduced by the simple poles already discussed. This bifurcation of states, even in the absence of off-diagonal elements, is to be expected since the dispersion relation of Eq. (19) then factorizes into
\[
[1 - a \hat{G}_{11}(p)] [1 - a \hat{G}_{22}(p)] = 0,
\]
(28)
with two distinct bifurcated branches,
\[
[1 - a \hat{G}_{11}(p)] = 0 \text{ and } [1 - a \hat{G}_{22}(p)] = 0.
\]
(29)
These branches of the bifurcated spectrum as well as the underlying "simple pole" solutions approximated by
\[
1 - a \hat{G}_{11}(p) + \hat{G}_{22}(p) = 0
\]
(30)
are further shifted by off-diagonal contributions associated with the dispersion relation term \( \hat{G}_{21}(p) \hat{G}_{12}(p) \) in Eq. (19). (This bifurcated
multiplicity of the spectrum is a manifestation of its pseudospin feature, as in the case of ordinary spin-1/2, for example. (To the extent that the bifurcation results in identical mode energies, it adds to their degeneracy.)

The off-diagonal contributions are given by \( \hat{G}_{21}(p) \hat{G}_{12}(p) \) as

\[
\hat{G}_{21}(p) \hat{G}_{12}(p) = \sum_{\nu = 0}^{\infty} \sum_{m,n} \frac{M_{\nu} M_m}{4R_{\nu} R_{m}} \left\{ \sum_{\nu'} \sum_{\nu''} \frac{(\nu''')^2}{\nu'' R_{\nu''} - \nu' R_{\nu'}} \right\} \left( \frac{1}{\Omega \pm' R_{\nu}} + \frac{1}{\Omega \pm'' R_{m}} \right) + \sum_{\nu'} \frac{1}{(\Omega \pm' R_{\nu})^2} \right\}.
\]

(31)

In general, the solution of the dispersion relation [Eq. (19)] requires considerable numerical work. However, in the important case of small \( \alpha = U_0 a^2 \), involving the square of the small dot diameter, one can make some progress analytically. In this context "small \( \alpha \)" means that

\[
a N_\nu \omega_\nu \ll |R_{m,n}|-|R_{n,m}| \quad \text{so that the separation of distinct "no-lattice" energy levels [on the right of Eq. (32)] is large compared to} \quad a N_\nu \omega_\nu, \quad \text{which is reasonable to expect for nanoscale dot sizes.} \quad \text{On this basis, most of the dispersion relation terms on the right of Eq. (19) are too small to match unity on its left side, except for those terms whose denominators almost vanish, such that}
\]

\[
\Omega \pm' R_{n,m} \sim O(\alpha). \tag{33}
\]

Employing Eq. (30) as a first approximation provides an estimate in which the root is so close to a particular simple pole that it is determined by that pole-term alone as

\[
\Omega \pm' R_{n,m} \approx \pm a N_\nu \omega_\nu (\mp' 1); \quad \Omega \approx \mp' (R_{n,m} + \pm a N_\nu \omega_\nu), \tag{34}
\]

to the neglect of contributions of all other poles that are small in conformance with Eq. (32). Of course each simple pole in the dispersion relation produces a mode/root of its own, relatively unaffected by the other simple poles, which provide corrections of higher order in \( \alpha \). Similar considerations of the simple pole terms of \( \hat{G}_{11}(p) \hat{G}_{22}(p) \) show that they too provide only corrections/shifts of higher order in \( \alpha \). In the same way for the simple pole terms of \( \hat{G}_{21}(p) \hat{G}_{12}(p) \). However, the second-order pole terms in \( \hat{G}_{11}(p) \hat{G}_{22}(p) \) and \( \hat{G}_{21}(p) \hat{G}_{12}(p) \) yield corrections of the same order in \( \alpha \) due to the bifurcation they induce, as one could surmise from Eqs. (28) and (29). To be specific about their size, these second-order poles involve terms like \( \alpha^2 (\hat{G}_{11}(p) \hat{G}_{22}(p) - \hat{G}_{21}(p) \hat{G}_{12}(p)) \)

\[
\sim \left( \frac{\nu''}{\Omega \pm' R_{\nu}} \right)^2 \sim \alpha^2 \sim 1 \quad \text{for} \quad \Omega \pm' R_{\nu} \sim O(\alpha).
\]

This is to say that even for small \( \alpha \), the second-order poles inducing bifurcation cannot be neglected.

In accordance with these considerations, the appropriate approximation for the bifurcated modes arising from the \((n, \pm')\)-pole (which is coincident with the \((n-1, -)\)-pole since \( R_{n,-} \equiv R_{n-1,-} \) and \( \epsilon_{n,-} \equiv \epsilon_{n-1,-} \)) is given to leading order in the small parameter \( \alpha \) by the quadratic equation

\[
1 = \alpha \left( \frac{\omega_{\nu} N_\nu + N_{n-1} \omega_{-n}}{2R_{n,-}(\Omega \pm' R_{\nu})} \right)^2 \sim \frac{1}{(\Omega \pm' R_{\nu})^2}
\]

(35)

which takes both diagonal and off-diagonal elements into consideration.

### IV. CONCLUSIONS: ENERGY PARAMETERS AND APPROXIMATE SOLUTION

Pausing to reflect on the meaning of this approximate procedure in terms of energy parameters, we note that the denominators \( D_{n,m} = (\Omega - R_{n,m}) (\Omega + R_{n,m}) \) represent (squares of) energy, and the numerators in the dispersion relation Eq. (19) (e.g., \( \omega N_{n,m} \)) similarly represent the (squares of) energy associated with the interaction with the superlattice of quantum antidots. For example, considering the numerator \( \omega_{\nu} N_{\nu m} \) and restoring the factors of \( h \) (which had been set to unity), we have a measure of this lattice interaction energy (squared) for the \( n \)th energy level as

\[
\Gamma_n^2 \equiv \omega_{\nu} N_{n,m} \Rightarrow \frac{\hbar \omega_{\nu} U_0 a^2 eB}{2\pi} \rightarrow \text{(Energy)}^2. \quad \tag{36}
\]

If the antidot strength \( U_0 a^2 \) is sufficiently small so that the energy supplied by the lattice interaction is small compared to that necessary to have a carrier jump to a higher unperturbed level, i.e., \( \Gamma_n \ll R_{n,m} \pm R_{m,n} (m \neq n) \), then the dispersion relation in Eq. (19) can only be satisfied if the root is very close to the \( n \)th pole position, and is thus determined by that pole alone in the first approximation, so that (ignoring second-order poles discussed above)

\[
1 \approx \frac{\Gamma_n^2}{(\Omega_{\pm' R_{\nu}})^2} = O(\pm' R_{\nu}) \quad \text{or} \quad \Omega_{\pm' R_{\nu}} \equiv R_{n,m} + (\pm' R_{\nu}) \tag{37}
\]

(37)

(with \( \omega_{\nu} \) in \( \Gamma_n \) well approximated at the same level by \( \omega_{\nu} \equiv \pm g + R_{n,m} \)).

These considerations further support our approximation procedure in the case under consideration, with lattice interaction energy small compared to "no-lattice" energy level difference, to the effect that terms involving energy denominator products of the form \( D_{n,m} D_{m,n} \) (which occur in the products of series in \( G_{11}G_{22} \) and \( G_{21}G_{12} \)) can be neglected when they involve differing "zero-lattice" energies. This is to say that the only significant terms involving \( D_{n,m} D_{m,n} \) products of energy denominators are those with the same zero-lattice energies: The latter are second-order pole terms, whose contributions are comparable with those of the first-order poles, as exhibited in Eq. (35).

In conclusion, we present the solution of Eq. (35),

\[
\omega \pm' R_{n,m} = \left( \frac{\pm}{4R_{n,-}} \right) (N_{n m} + N_{n,-1} \omega_{-n} \pm' \frac{\pm}{4R_{n,-}} \equiv \left( \frac{\pm}{4R_{n,-}} \right) \left( N_{n m} \pm' \right) - 4(\omega_{\nu} \pm N_{n m} - M_{n,m}) \right),
\]

(38)

and note its consistency with the two branches of the bifurcated solutions of the factorized spectrum approximation of Eqs. (29).
and (30) when the off-diagonal elements of strength $M_n$ are negligible, in which case Eq. (38) reduces to

$$\omega \pm \gamma R_{n,n} \Rightarrow \pm \frac{\alpha}{2R_{n,n}} \left\{ \begin{array}{l} N_n \omega_+ \\ \text{OR} \\ N_{n-1} \omega_- \end{array} \right\}. \quad (39)$$

These solutions explicitly exhibit the formation of “relativistic” Landau minibands. In the presence of the antidot lattice, we note that the Green’s function for the quantum antidot due to bending of the underlying band structure. In contrast to the energy “linear-momentum” approximation of the Dirac-like Hamiltonian, due to bending of the underlying band structure.

The magnetotransport of an incident wave packet along the axis of the lattice, reflecting on the possibility of transport control by initial pseudospin state preparation.

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