New Magnetic Field Dependence of Landau Levels in a Graphenelike Structure

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We consider a tight-binding model on the honeycomb lattice in a magnetic field. For special values of the hopping integrals, the dispersion relation is linear in one direction and quadratic in the other. We find that, in this case, the energy of the Landau levels varies with the field B as $\epsilon_n(B) \sim [(n+\gamma)B]^{2/3}$. This result is obtained from the low-field study of the tight-binding spectrum on the honeycomb lattice in a magnetic field (Hofstadter spectrum) as well as from a calculation in the continuum approximation at low field. The latter links the new spectrum to the one of a modified quartic oscillator. The obtained value $\gamma = 1/2$ is found to result from the cancellation of a Berry phase.

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Introduction.—The recent discovery of graphene has boosted the study of the physical properties of the honeycomb lattice, especially in a magnetic field [1]. Among the peculiarities of the electronic dispersion relation, the spectrum in the band center ($\epsilon = 0$) is linear, exhibiting the so-called Dirac spectrum around two special points at the corners $\boldsymbol{K}$ and $\boldsymbol{K}'$ of the Brillouin zone. Near these points the density of states varies linearly [2]. In a magnetic field [3], the energy levels around $\epsilon = 0$ vary with the field B as $\epsilon_n(B) \sim \pm[nB]^{1/2}$, with a twofold valley degeneracy corresponding to the two points $\boldsymbol{K}$ and $\boldsymbol{K}'$. This spectrum has to be contrasted with the familiar field dependence of Landau levels $\epsilon_n(B) = (n+1/2)eB/m$ for electrons in a quadratic band with mass m. This square-root dependence has been observed experimentally [4,5].

Here we present an example where the field dependence of the Landau levels (LLs) is neither linear nor a square root, but reveals a new power law, namely, a $[(n+\gamma)B]^{2/3}$ behavior, with $\gamma = 1/2$. This is obtained for tight-binding electrons on the honeycomb lattice, the same problem as for graphene, but with special values of the hopping integrals between nearest neighbors which, contrarily to the case of graphene, are not taken to be equal. We find that around a special point of the reciprocal space, the zero-field spectrum is linear in one direction and quadratic in the other. This ''hybrid'' spectrum leads to a new field dependence of the Landau levels, described by a quartic oscillator $V(X) = X^4 + 2X$. The value $\gamma = 1/2$ is found to result from the cancellation of a Berry phase.

The model.—We consider the tight-binding model on the honeycomb lattice with the possibility that one of the three hopping elements between nearest neighbors may take a different value t' from the two others t (Fig. 1) [6]. This problem has been studied recently both in zero field [7] and in a magnetic field [8], where the authors mention the special interest of the case $t' = 2t$, with a square-root energy dependence of the density of states at the band center [7], and they compute the evolution of the Hofstadter spectrum when t' varies between t and $2t$ [8]. Here, we emphasize the new and peculiar character of the LLs around $\epsilon = 0$, which has not been foreseen in previous works.

The tight-binding Hamiltonian couples sites of different sublattices named A and B. The eigenvectors are Bloch waves of the form

$$|\boldsymbol{k}\rangle = \frac{1}{\sqrt{N}} \sum_j (c_{\boldsymbol{k}}^A |\boldsymbol{R}_j^A\rangle + c_{\boldsymbol{k}}^B |\boldsymbol{R}_j^B\rangle) e^{i\boldsymbol{k}\cdot\boldsymbol{R}_j}, \tag{1}$$

where $|\boldsymbol{R}_j^A\rangle$, $|\boldsymbol{R}_j^B\rangle$ are atomic states. The sum runs over vectors of the Bravais lattice. The eigenequations read

$$\begin{aligned} \epsilon c_{\boldsymbol{k}}^A &= -[te^{i\boldsymbol{k}\cdot\boldsymbol{a}_1} + te^{i\boldsymbol{k}\cdot\boldsymbol{a}_2} + t']c_{\boldsymbol{k}}^B, \\ \epsilon c_{\boldsymbol{k}}^B &= -[te^{-i\boldsymbol{k}\cdot\boldsymbol{a}_1} + te^{-i\boldsymbol{k}\cdot\boldsymbol{a}_2} + t']c_{\boldsymbol{k}}^A, \end{aligned} \tag{2}$$

where $\boldsymbol{a}_1 = a(\frac{3}{2}, \frac{\sqrt{3}}{2})$, $\boldsymbol{a}_2 = a(\frac{3}{2}, -\frac{\sqrt{3}}{2})$ are elementary vectors of the Bravais lattice, a is the interatomic distance, and t, t' are shown in Fig. 1(a). When $t' = t$, the energy vanishes at two points $\boldsymbol{D}$ and $\boldsymbol{D}'$ located at the corners $\boldsymbol{K}$ and $\boldsymbol{K}'$ of the Brillouin zone ($\boldsymbol{K} = 2\boldsymbol{a}_1^*/3 + \boldsymbol{a}_2^*/3$, $\boldsymbol{K}' = \boldsymbol{a}_1^*/3 + 2\boldsymbol{a}_2^*/3$, where $\boldsymbol{a}_1^*$ and $\boldsymbol{a}_2^*$ are reciprocal lattice vectors). As t' increases, the two points $\boldsymbol{D}$ and $\boldsymbol{D}'$ approach each other (their distance varies as $\overrightarrow{DD'} = \frac{3}{\pi}\overrightarrow{KK'} \arctan\sqrt{4t^2/t'^2 - 1}$) and merge into a single point $\boldsymbol{D}_0 = (\boldsymbol{a}_1^* + \boldsymbol{a}_2^*)/2$ when $t' = 2t$ (for $t' > 2t$, a gap opens between the two subbands). An expansion $\boldsymbol{k} = \boldsymbol{D} + \boldsymbol{p}$ around these two points gives the low-energy spectrum, solution of the two equations ($a = 1$ for shorter notations)

$$\epsilon c_{\boldsymbol{k}}^A = \left[-\frac{3}{2} it' p_x \pm \sqrt{3} t'' p_y + \frac{3}{8} t'(3p_x^2 + p_y^2) + \frac{3\sqrt{3}}{2} t'' p_x p_y \right] c_{\boldsymbol{k}}^B$$

with $t'' = \sqrt{t^2 - t'^2/4}$ and a similar expression for $\epsilon c_{\boldsymbol{k}}^B$ with $(i \to -i)$. The $\pm$ sign denotes the vicinity of the two points $\boldsymbol{D}$ and $\boldsymbol{D}'$.

We now consider the case $t' = 2t$. In the vicinity of the single point $\boldsymbol{D}_0$, keeping the leading terms in each direction, we find

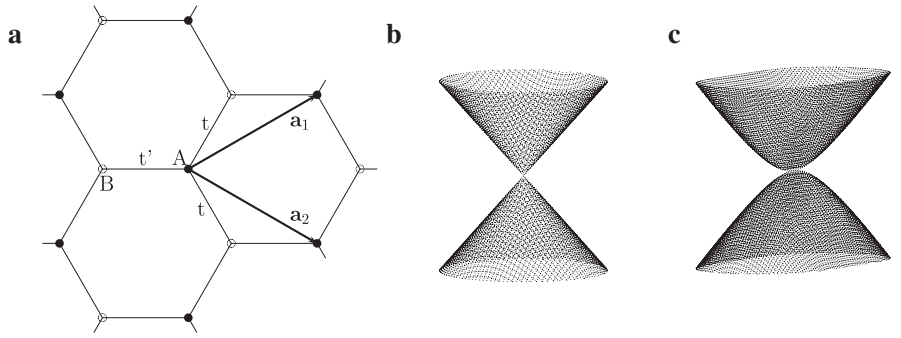

FIG. 1. (a) Honeycomb lattice with hopping integrals t and t', and elementary vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ discussed in the text. (b),(c) Low-energy spectrum for the cases $t' = t$ (b) and $t' = 2t$ (c).

$$\epsilon c_{\boldsymbol{k}}^A = ta\left(-3ip_x + \frac{3}{4}ap_y^2\right)c_{\boldsymbol{k}}^B \tag{3}$$

and a similar equation with $(A \rightarrow B,\ i \rightarrow -i)$, so that the Hamiltonian can be written in the form

$$H = \begin{pmatrix} 0 & -icp_x + \frac{p_y^2}{2m} \\ icp_x + \frac{p_y^2}{2m} & 0 \end{pmatrix} \tag{4}$$

where we have defined the velocity $c = 3ta$, an effective mass $m = 2/(3ta^2)$, and a "mass energy" $mc^2 = 6t$ (we fix $\hbar = 1$). The eigenvalues read

$$\epsilon = \pm\left(c^2p_x^2 + \frac{p_y^4}{4m^2}\right)^{1/2}. \tag{5}$$

Remarkably, the spectrum is linear in one direction, quadratic in the other [Figs. 1(b) and 1(c)]. It has been noticed [7] that such a dispersion relation leads to a square-root dependence of the density of states, that can be written in the form $\rho(\epsilon) \propto \frac{\sqrt{m}}{c}\sqrt{\epsilon}$ which is unusual in 2D. One may expect that this peculiar behavior leads to a new repartition of LLs.

Effect of the magnetic field, new Landau levels.—To describe qualitatively the effect of a weak magnetic field, we start with a simple semiclassical argument. The quantization condition for energy levels in a field B has the form $S(\epsilon) = 2\pi(n + \gamma)eB$ where $S(\epsilon)$ is the area of an orbit of energy ϵ in reciprocal space and γ is a constant $0 \leq \gamma < 1$ [9]. From Eq. (5), one finds easily [10]

$$S(\epsilon) = \beta\frac{\sqrt{m}}{c}\epsilon^{3/2} \quad \rightarrow \quad \epsilon_n = \left(\frac{2\pi ec}{\beta\sqrt{m}}\right)^{2/3}[(n + \gamma)B]^{2/3} \tag{6}$$

with $\beta = 2\Gamma(1/4)^2/(3\sqrt{\pi}) \simeq 4.9442$. This new behavior has to be contrasted with the usual case of free massive particles where $S(\epsilon) = 2\pi m\epsilon$, so that $\epsilon_n = \omega_c(n + \gamma)$ or with the case of Dirac particles where $S(\epsilon) = \pi\epsilon^2/c^2$, leading to a square-root magnetic field dependence $\epsilon_n = \pm c\sqrt{2eB(n + \gamma)}$ of the energy levels. The phase factor γ cannot be obtained from such semiclassical argument.

We now come to the numerical calculation of the spectrum of the tight-binding problem in a magnetic field (the so-called Hofstadter spectrum [11]) for the honeycomb lattice (Fig. 2). It has first been calculated by Rammal for the case $t' = t$ and more recently for $t' = 2t$ [8,12]. The procedure to obtain this spectrum is described at length in Ref. [12]. The fractal structure results from the competition between magnetic field and lattice effects. For a commensurate reduced flux $f = p/q$, the spectrum exhibits $2q$ subbands. It is a periodic function of the reduced flux $f = Ba^2 3\sqrt{3}/(2\phi_0)$ through one plaquette in units of the flux quantum ϕ_0. At low field, the lattice effects are negligible, and we expect to recover the results of a continuum limit. The linear dependence of the LLs is clearly seen on the top

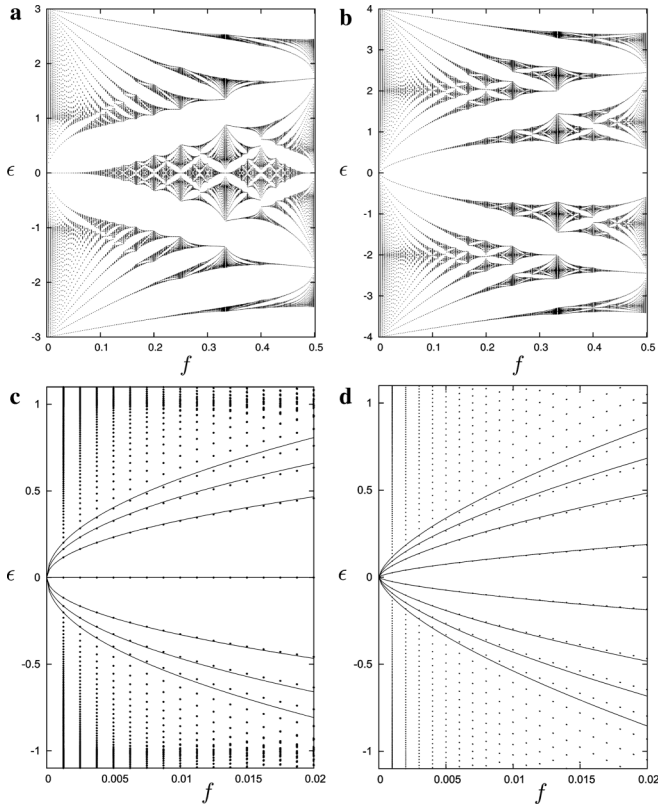

FIG. 2. (a) Hofstadter-Rammal spectrum in the case $t' = t$. (b) Spectrum for the case $t' = 2t$. (c) Low-field behavior in the case $t' = t$. The low-field bands are well fitted by the analytical expansion $\epsilon_n = \pm t\sqrt{2\pi 3^{1/2}nf}$. (d) In the case $t' = 2t$, the low-field spectrum is well fitted by Eq. (12). Deviations at higher field or higher energy are due to lattice effects.

and bottom of the spectrum (Fig. 2). For $t' = t$, the square-root dependence of the levels is observed around $\epsilon = 0$. For $t' = 2t$, the levels exhibit the new magnetic field dependence which is well fitted by a power law $B^{2/3}$ [Fig. 2(d)]. In order to derive the low-field spectrum analytically, we now calculate the magnetic field effect in the continuum approximation around $\epsilon = 0$.

Spectrum in the continuum approximation.—We now apply a magnetic field B and use the Landau gauge $\mathbf{A} = (0, Bx, 0)$. The substitution $p_y \rightarrow p_y - eBx$ leads to the new Hamiltonian

$$H = \begin{pmatrix} 0 & -icp_x + \frac{1}{2}m\omega_c^2\tilde{x}^2 \\ icp_x + \frac{1}{2}m\omega_c^2\tilde{x}^2 & 0 \end{pmatrix}$$

with an effective cyclotron frequency $\omega_c = eB/m = 3eBta^2/2$ which can be also written in terms of the reduced flux $f = Ba^2 3\sqrt{3}/(2\phi_0)$ through one plaquette of the lattice, namely $\omega_c = (2\pi/\sqrt{3})tf$. In $\tilde{x} = x - p_y/eB$, quantization of p_y leads to the usual degeneracy of Landau levels. The energy levels ϵ are solutions of

$$\left(c^2p_x^2 + \left(\frac{1}{2}m\omega_c^2\right)^2\tilde{x}^4 - i\frac{c}{2}m\omega_c^2[p_x, \tilde{x}^2]\right)\psi = \epsilon^2\psi.$$

Introducing new dimensionless conjugate variables X and P, we rewrite

$$\left(\frac{m\omega_c^2c^2}{2}\right)^{2/3}(P^2 + X^4 - i[P, X^2])\psi = \epsilon^2\psi. \quad (7)$$

This expression shows that the eigenvalues necessarily scale as $B^{2/3}$. Neglecting first the linear term $[P, X^2] = -2iX$, the eigenvalues of the quartic oscillator $P^2 + X^4$ can be easily estimated, at least for large n, in the WKB approximation [13] and are found to be of the form $C(n + 1/2)^{4/3}$ with $C = [3\pi\sqrt{2\pi}/\Gamma(1/4)^2]^{4/3} \simeq 2.185\,07$. Therefore, the Landau levels are given by (restoring $\hbar$)

$$\epsilon_n = \pm A(mc^2)^{1/3}[(n + 1/2)\hbar\omega_c]^{2/3}, \quad (8)$$

with $A = \sqrt{C/2^{2/3}} \simeq 1.173\,25$. This is precisely the dependence expected from the above semiclassical argument (6), with the phase factor γ now determined to be $1/2$. Replacing m and ω_c by their expressions in terms of the lattice parameters considered here, we finally obtain

$$\epsilon_n = \pm\alpha[(n + 1/2)f]^{2/3}, \quad (9)$$

where $\alpha = (2\pi)^{2/3}\sqrt{C} \simeq 5.0333$. The $f^{2/3}$ dependence of these levels is clearly seen in Fig. 2(d), and their $(n + 1/2)^{2/3}$ dependence is confirmed on Fig. 3.

It is interesting to compare Eq. (7) with the eigenequations for Dirac fermions:

$$eBc^2(P^2 + X^2 - i[P, X])\psi = \epsilon^2\psi, \quad (10)$$

with $\epsilon_n = \pm c\sqrt{2eBn}$ or for free massive particles

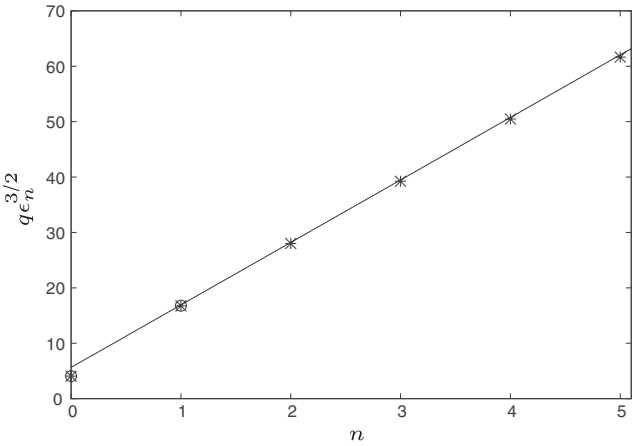

FIG. 3. For $f = 1/q$, plot of $q\epsilon_n^{3/2}$ vs n (*), and comparison with the WKB solution (9) of the quartic oscillator (straight line) and with the numerical solution of the modified quartic, $X^4 + 2X$ oscillator (o) for $n = 0$, 1. For $n \geq 2$, the two solutions are indistinguishable.

$$\frac{\omega_c}{2}(P^2 + X^2)\psi = \epsilon\psi, \quad (11)$$

with $\epsilon_n = (n + 1/2)\hbar\omega_c$, and to emphasize the role of the commutator which enters Eqs. (7) and (10). There are several discussions in the literature [14] to explain the disappearance of the phase term $1/2$ in the case of the Dirac spectrum, and we return to this point later. We notice from Eq. (10) that this disappearance comes simply from the commutator $[P, X] = -i$. In our case, the commutator which appears in Eq. (7), $[P, X^2] = -2iX$, modifies the quartic potential which becomes $X^4 + 2X$. This linear term is actually a small perturbation negligible when n is large. Taking into account this linear term, a numerical calculation of the eigenvalues of this modified quartic oscillator finally gives (Fig. 3)

$$\epsilon_n = \pm\alpha g(n)[(n + 1/2)f]^{2/3}, \quad (12)$$

where $g(0) \simeq 0.808$, $g(1) \simeq 0.994$. For $n \geq 2$, $g(n) \sim 1$ so that the WKB solution (9) of the quartic oscillator turns out to be extremely good. It is worth mentioning that since the two Dirac points $\boldsymbol{D}$ and $\boldsymbol{D}'$ have merged into a single point $\boldsymbol{D}_0$ for $t' = 2t$, the valley degeneracy has disappeared and the LLs degeneracy has recovered its usual value. Finally, one may question the domain of validity of our results when the condition $t' = 2t$ is not exactly fulfilled. We have checked that a crossover occurs from a Dirac-like $\sqrt{f}$ to a $f^{2/3}$ behavior when $nf \gtrsim [|t' - 2t|/t]^{3/2}$. In the region $t' > 2t$, this has to do with a crossover between a quadratic and a quartic oscillator [15].

We now comment on the relation between the phase factor γ entering the quantization of semiclassical orbits and a Berry phase. It has been established that [14]

$$\gamma = \frac{1}{2} - \frac{i}{2\pi}\oint_\Gamma \langle \boldsymbol{k}|\nabla_{\boldsymbol{k}}|\boldsymbol{k}\rangle \cdot d\boldsymbol{k},$$

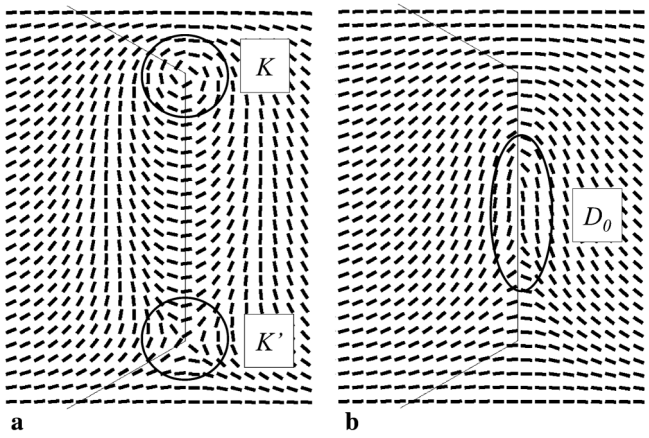

FIG. 4. Wave-vector dependence of the ratio $c_{\boldsymbol{k}}^B/c_{\boldsymbol{k}}^A$ for the eigenvectors (1). The figures represent a part of the Brillouin zone near the points $\boldsymbol{K}$ and $\boldsymbol{K}'$. (a) For $t' = t$, the Berry phase $\pm\pi$ on semiclassical orbits around the points $\boldsymbol{D} = K$, $\boldsymbol{D}' = \boldsymbol{K}'$ implies $\gamma = 0$. (b) For $t' = 2t$, the Berry phase on a contour around $\boldsymbol{D}_0$ vanishes, implying $\gamma = 1/2$.

where Γ is the contour of a semiclassical orbit. It is easily found from Eqs. (1) and (2) that, for the isotropic case $t' = t$, $\oint_\Gamma \langle \boldsymbol{k}|i\nabla_{\boldsymbol{k}}|\boldsymbol{k}\rangle \cdot d\boldsymbol{k} = \pm\pi$ around the points $\boldsymbol{D}$ and $\boldsymbol{D}'$ which can be seen as topological defects [see Fig. 4(a)], leading to $\gamma = 0$ as well known for graphene. For our case $t' = 2t$, these two topological defects $\boldsymbol{D}$ and $\boldsymbol{D}'$ merge into a single one $\boldsymbol{D}_0$ and *annihilate*. As may be seen on Fig. 4(b), we now obtain $\oint_\Gamma \langle \boldsymbol{k}|\nabla_{\boldsymbol{k}}|\boldsymbol{k}\rangle \cdot d\boldsymbol{k} = 0$, which explains why $\gamma = 1/2$.

Conclusion.—The field dependence of the LLs depends dramatically on the structure of the zero-field dispersion relation. In this Letter, we have presented an example with a unusual dispersion relation, which leads to a square-root energy dependence of the density of states and to a new field dependence $[(n + 1/2)B]^{2/3}$ of the LLs. More generally, we may consider a dispersion relation of the form $\epsilon = (p_x^\alpha + p_y^\beta)^\delta$. The area of the orbits of a given energy ϵ varies as $S(\epsilon) \propto \epsilon^{(\alpha+\beta)/\alpha\beta\delta}$, so that the Onsager quantization rule for energy levels leads to the general dependence of the Landau levels with the magnetic field

$$\epsilon_n(B) \sim [(n + \gamma)B]^{\alpha\beta\delta/(\alpha+\beta)}.$$

This dependence can also be obtained from a counting argument based on the energy dependence of the density of states which is easily found to vary as $\rho(\epsilon) \sim \partial S(\epsilon)/\partial\epsilon \sim \epsilon^{(\alpha+\beta)/\alpha\beta\delta-1}$ [16].

To conclude, we briefly comment on possible experimental realizations leading to such an electronic spectrum. An anisotropic version of the graphene structure with $t' \neq t$, called quinoid and discussed long ago by Pauling, could be induced by uniaxial stress or bending of a graphene sheet [17]. Moreover, it has been shown recently that a similar spectrum with Dirac cones could exist in an $2d$ organic conductor of the *ET* family [18]. The authors have considered the possibility of a transition driven by pressure between a "zero gap state" (with two Dirac cones) and a "narrow gap state." We note that, at the transition point, the two Dirac points merge into a single one with the same dispersion relation and the same physics considered in this Letter. We finally mention recent discussions on the feasibility of such a structure with cold atoms in an optical lattice created by laser beams [19,20]. Degenerate fermions in an optical lattice have recently been observed [21]. On the other hand, generating an effective magnetic field for neutral atoms is now routinely done by rotation of the atomic gas [22]. There is no technical objection to the realization of a rotating atomic Fermi gas in an optical lattice, for example, in a honeycomb lattice where the physics of Dirac Fermions could be investigated [23]. Then the condition $t' = 2t$ can be realized by tuning the laser intensities [19].

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