Erratum: Valley-based field-effect transistors in graphene [Phys. Rev. B 86, 165411 (2012)]

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A mistake occurs in Eq. (4) for the estimate of α_{vo} in the FET channel, and should be corrected as follows. In the calculation of the valley splitting energy δE we have missed contributions from the third-order perturbation theory, for example,

$$\sum_{n,m}{}' \frac{\langle 0|e\varepsilon_y y|n\rangle\langle n|Dy^4|m\rangle\langle m|H_{vo}(\text{due to the quadratic potential})|0\rangle}{(-n\hbar w_0)(n-m)\hbar w_0}\text{etc.}$$

In comparison to the original (second-order perturbation-theoretical) expression given for δE, these additional contributions have the same dependence in ε_y, D, k_x, and Δ, as the second-order expression. More importantly, it is found that the overall third-order contributions cancel exactly with the second-order expression, yielding a vanishing δE to the first-order relativistic correction.

As shown below, δE becomes finite in the presence of a gap variation in the y direction, for example, $\Delta(y) = \Delta + \Delta'(y)$, where $\Delta'(y)$ describes the variation. $\Delta'(y)$ may be a piecewise constant, for example, $\Delta'(y) = 0$ in the channel, and $\Delta'(y) = \Delta'_0$ outside the channel. (See the discussion at the end for a feasible realization of a gap varying structure.) In the following calculation we model $\Delta'(y)$ with a quadratic function, for example, $\Delta'(y) = \delta y^2$, where $\delta \ll m^* w_0^2$ (i.e., weak gap variation).

First, on account of the gap variation in this case, the Schrödinger equation in (3) is modified as follows:

$$\left(H^{(0)} + H'_{vo} + H_0^{(1)}\right)\phi_{n\tau} = E_{n\tau}\phi_{n\tau}, \quad H^{(0)} = \frac{\vec{p}^2}{2m^*} + [V(y) + \Delta'(y)], \quad H'_{vo} = H_{vo} - \tau\frac{\hbar}{4m^*\Delta}[\nabla\Delta'(y)\times\vec{p}]\cdot\hat{z}. \tag{3'}$$

$H_0^{(1)}$ here denotes the valley-independent relativistic correction, and is irrelevant for the present discussion. Notice in the above equation the modification of the valley-orbit interaction, for example, $H_{vo} \to H'_{vo}$, in the presence of $\Delta'(y)$. Moreover, in order to facilitate the calculation, we shift the y coordinate, for example, $y \to y + y'_\varepsilon[y'_\varepsilon \equiv e\varepsilon_y/(m^* w_0^2 + 2\delta)]$, and write in $H^{(0)}$,

$$V(y) + \Delta'(y) \approx \frac{m^* w_0^2 y^2}{2} - Dy^4 + 4Dy'_\varepsilon y^3 + \delta y^2,$$

where we have ignored the terms which are $O(y'^2_\varepsilon)$.

δE is given by the following first-order perturbation-theoretical expression due to H'_{vo},

$$\delta E = -\frac{\tau\hbar^2}{4m^*\Delta}k_x\left\langle\phi_{0\tau}^{(0)}\right|\{\partial_y[V(y) - \Delta'(y)]\}\left|\phi_{0\tau}^{(0)}\right\rangle, \quad E_{n\tau}^{(0)}\phi_{n\tau}^{(0)} = H^{(0)}\phi_{n\tau}^{(0)}.$$

To the first order in δ this yields the following results:

$$\delta E \approx -\tau\frac{6e\hbar^3}{m^{*4}\Delta_0 w_0^5}D\delta\varepsilon_y k_x, \quad \alpha_{vo} = \frac{6e\hbar^3}{m^{*4}\Delta_0 w_0^5}D\delta\varepsilon_y. \tag{4'}$$

Except for the δ dependence introduced here by the gap variation, the expressions in Eq. (4′) exhibit exactly the same functional dependence in D, ε_y, Δ, and k_x as the previous ones in Eq. (4).

We estimate α_{vo} with the same parameters (e.g., D, $\hbar w_0/\Delta$, ε_y) used earlier, and take $\delta = 0.2\beta\Delta$. This gives $\alpha_{vo} \sim 5.4 \times 10^{-12}$ eV m, which is of the same order of magnitude as the previous estimate.

Finally, we note that the condition of gap variation in the present discussion can be realized, in principle, by at least two methods, as follows. (I) In the case of monolayer graphene grown on h-BN, one can make a trough in the BN substrate, and place the graphene layer upon the substrate. While the (strip) region of graphene on top of the trough is free-standing and gapless, the graphene-substrate interaction generates a gap in graphene next to the trough. This structure provides not only a gap variation but also a gap-caused quantum confinement for electrons in the strip, resulting in a quantum wire. (II) In the case of bilayer graphene, a gap can be generated by applying a dc bias across the two layers,[1] and a variation in the dc bias produces a varied band gap in graphene.[2]

[1] E. McCann, Phys. Rev. B **74**, 161403 (2006); E. McCann and V. I. Fal'ko, Phys. Rev. Lett. **96**, 086805 (2006); E. V. Castro, K. S. Novoselov, S. V. Morozov, N. M. R. Peres, J. Lopes dos Santos, J. Nilsson, F. Guinea, A. K. Geim, and A. H. Castro Neto, *ibid.* **99**, 216802 (2007).

[2] It can be shown theoretically that the valley-based FET proposed here can also be realized in dc-biased bilayer graphene with Bernal stacking.

