A comment on: "Universal control of superexchange in linear triple quantum dots with an empty mediator"

Marko J. Rančić

TotalEnergies, 8, Boulevard Thomas Gobert, Nano-INNOV – Bât. 861,– 91120 Palaiseau – France

In a recent preprint [1], G. X. Chan, P. Huang, and X. Wang claim that triple-quantum dot superexchange in a (1,0,1) charge configuration exhibits a change of sign (going from positive to negative) as a function of middle dot detuning. Furthermore, their claim is that charge sweet-spots exist for specific values of the inter-dot detuning. Their analysis is based on the Hubbard model and something to what they refer to as the "full Configuration-Interaction" method. All of this findings were already reported by M. J. Rančić and G. Burkard in Ref. [2] (2017) based on the Hubbard model. No reference to this manuscript was made in Ref. [1]. I have asked the authors to urgently modify the pre-print and position their work with respect to the previously conducted study - which they rejected to do at the current moment, quoting that pp. "it is not their style to modify preprints before they were accepted". This alongside with a very similar style of some figures lead me to the conclusion that they are deliberately misleading the scientific community and trying to adopt other peoples work and ideas as their own.

I. INTRODUCTION

The triple quantum dot loaded with two electrons exhibits a plethora of rich physics. This system has been especially appealing for experimental studies in the area of semiconductor spin quantum information processing.

II. M. J. RANČIĆ AND G. BURKARD PHYS. REV. B 96, 201304 (2017)

In Ref. [2] starting from the Hubbard model without inter-dot Coulomb penalization

\[ H = \sum_{i\sigma} (\epsilon_i + E_{i\sigma}) n_{i\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \sum_{(ij) \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma}, \]

and applying the powerful Schrieffer-Wolff transformation the following expression is derived for the superexchange interaction in the (1,0,1) charge configuration

\[ J_{SE} = 4t^4U \frac{U (12\delta^2 + \epsilon^2) - \delta (8\delta^2 + 6\epsilon^2)}{(\epsilon^2 - 4\delta^2)^2 (U - 2\delta) (U^2 - \epsilon^2)}. \]

III. G. XU. CHAN, P. HUANG, AND X. WANG ARXIV:2203.15521 (2022)

In much similarity to Ref. [2] the authors base their study on the Hubbard model and the Schrieffer-Wolff transformation in the same (1,0,1) charge configuration. The sole difference is that they chose the inter-dot Coulomb penalization to be non-zero, leading to the fact that (1,0,0) and (0,1,1) charge states are raised higher in energy as compared to (2,0,0), (0,2,0) and (0,0,2). This would correspond to adding the following term in Eq. [1] \( \sum_{(ij)} V_{ij} n_i n_j \). However, \( U \gg V \) and neglecting \( V \) in favor of \( U \) simplifies calculations significantly.

The authors of Ref. [1] focus on a particular energy ordering in the part of the study (Section IIB) \( E_{101} < E_{110:011} < E_{200:002} \), with all other states being treated as higher in energy. Such a process is described by \( J_{SE}^0 \) in Tab. [1]. By going through the calculations in Eqs. (3a-4c) I obtained a result \( J_{SE} \), up to a numerical difference (factor of $\sqrt{2}$ the origin of which I cannot determine) and a factor of 2 next to $\epsilon$ because different definitions were used.

In Fig. [1] a comparison between Fig. 3 of Ref. [2] (subfigure (a)) and Fig. 8 (f) of Ref. [1] is displayed (marked as subfigure (b)). The green area in subfigure (a) corresponds to that of subfigure (b) however is different with respect to subfigure (b) due to the presence of the (0,2,0) state. This is a consequence of the finite

\[ \delta_0 = \frac{1}{2} \left( 1 + \frac{1 - \epsilon^2}{q^{1/3}} + q^{1/3} \right); \epsilon_0 = \pm \frac{2\sqrt{(3 - 2\delta)^2 \delta^2}}{\sqrt{6}\delta - 1}, \]

where, \( q = 1 - \epsilon^2 + \sqrt{(\epsilon^2(\epsilon^2 - 1))^2} \) all given in units of Coulomb repulsion U. this points are not simultaneously "sweet spots" - superexchange changes signs in them.

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*marko.rancic@totalenergies.com
Table I. Six possible superexchange paths involving spin-conserving tunneling with corresponding expressions \( J_{\text{SE}} = \sum_i J_{\text{SE}}^i \).

The parameters for which the sign of \( J_{\text{SE}} \) is valid are the Coulomb repulsion \( U = 1 \) meV, the detuning between the outer dots \( \epsilon = -1.34U \), the detuning between the middle dot and the average of the outer dots \(-0.2U < \delta < 0.3U\).

Figure 1. Superexchange as a function of \( \epsilon \) and \( \delta \). (a) Results of Ref. [2] and (b) results of [1], figure rotated and legend rearranged so that the resemblance with subfigure (a) is obvious. Area to which authors of Ref. [1] focus is marked with a green box in subfigure (a).

In my opinion, some scientific value might exist in the full Configuration-Interaction numerical calculations of superexchange which the authors claim to have done. However, no level of detail is provided about details of such calculations.

Finally, the authors claim to predict the existence of "sweet spots" in Fig. 8 (d) and (h). Predictions of sweet spots has been the main goal of Ref. [2]. They have been analytically found and are marked \( J_1 - J_4 \) in Fig. [1].

Let me conclude that in my opinion some scientific value might exist in Ref. [1] in the full Configuration-Interaction numerical calculations of superexchange which the authors claim to have done. However, no level of detail is provided about details of such calculations.

To sum up, Ref. [1] copies all findings of Ref. [2] without referencing to it. The authors have rejected to immediately modify their pre-print and position their work with respect to a previous study which has been accepted in a prestigious peer-reviewed journal in 2017. In my opinion some scientific value might exist in the full Configuration-Interaction calculations the authors claim to have done but no detail about them is provided. Such work would clearly have been differentiated from Ref. [3] if it was to have any value what-so-ever.

[1] G. X. Chan, P. Huang, and X. Wang, Universal control of superexchange in linear triple quantum dots with an empty mediator. arXiv preprint arXiv:2203.15521 (2022)
[2] M. J. Rančić and G. Burkard, Ultracoherent operation of spin qubits with superexchange coupling, Phys. Rev. B 96, 201304 (2017).

[3] K. Deng and E. Barnes, Interplay of exchange and superexchange in triple quantum dots, Phys. Rev. B 102, 035427 (2020).