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Dear SciPost Team

We are pleased to resubmit the attached manuscript entitled "*Finite-Volume self-consistent approach at ultra-low temperatures: Theory and application to 1D electron gas at the Si-SiO2 interface*" by Vahid Mosallanejad, Haiou Li, Gang Cao, Kuei-Lin Chiu, Wenjie Dou, Guo-ping Guo for reconsideration in SciPost.

We would like to thank the referees for their very helpful comments and suggestions. We modified the manuscript substantially in response to requested changes (as detailed on the next pages). In responses to request changes, we used the font color blue to highlight the referee's comments while our respond is typed in conventional dark color font. In addition, we have highlighted changes in the manuscript with the red-color font. We have taken weaknesses seriously and we have increased the level of clarity. Particularly, we drop accusation of Finite-Difference and Finite Element discretization scheme for solving the Schrödinger-Poisson system at sub-kelvin temperatures. We also polished the manuscript so that the content would be more appreciable. Specifically, we have added descriptions for Eq. (6) and Eq. (9), and a flowchart figure. In addition, we improved presentations of sections 2.7 and 2.8. In Fig. S2 (d), we had shown a typical course mesh of the Finite-Element only to show the style of mesh. In practice, we performed mesh convergence verification where we used a few meshing styles and range of sizes down to a min mesh size 0.5 nm. Triangles are not visible on such a fine mesh. So, we had decided to use the word "typical" in the old manuscript to justify Fig. S2 (d). With our new Supplemental Information, we have improved the mesh presentation in the section S4. We also have addressed few questions raised by referees in their "Report" section. Note that changes do not affect the theory presented in our work. We hope the article is now suitable for reconsideration in SciPost.

Thank you very much for your consideration.
Yours sincerely,

Vahid Mosallanejad, Kuei-Lin Chiu

Reviewer 2

Report 2 on 2022-8-6

In my opinion, the work is a good stepping stone towards the authors addressing interesting physics questions in quantum devices. In it's current form, however, I do not believe it fulfills the acceptance criteria of the journal. It could possible open a new avenue of research if the authors provided stronger evidence of the superiority of their method. At the same time, I think this work (after some polishing) could be polished in a more specialized journal focused on computational methods. A couple of questions for the authors to consider: Are all 6 valleys of Si included in the calculation?

We thank the positive comments from the referee. We believe that we have introduced a new possibility that can address a wide range of real applications, ranging from the DFT calculations to the non-equilibrium green's function approaches. Regarding to the questions raised by the referee, here we considered $v_v = 2$. In Si-SiO_2 interfaces parallel to the (001) plane, the six equivalent conduction band minima Δ_6, splits into Δ_4 (four-fold degeneracy) and (two-fold degeneracy) Δ_2 bands. At low temperatures, only the Δ_2 bands are occupied by electrons, since Δ_2 bands are lower in energy. Therefore, we only considered $v_v = 2$. We have added the following sentence to the section 3.1 to make this point clear:

"Note that in the scaled geometry, mesh sizes vary between 4 m and 0.75 m. Moreover, we set $v_s = 2$ (spin) and $v_v = 2$ which means only the lowest two-fold degenerate band Δ_2 is considered (the crystal orientation [001] is along the z-axis) [48]."

If not, is this due to strain in the system or something? If so, the effective masses presented in Table 1 should only apply to the z valleys. The heavy effective mass for the x and y valleys are in the x and y directions, respectively.

When SiO_2 grows parallel to the (001) plane, crystallographic symmetry breaks on the direction perpendicular to the interface. Even without extra strain, Δ_6, splits into Δ_4 (four-fold degeneracy) and (two-fold degeneracy) Δ_2 bands. In our schematic Fig1. (a), the Si's (001) plane is assumed to be at the x-y surface. For Δ_2 bands, the effective mass perpendicular to interface has a lager value, approximately $0.91m_0$, often refer to heavy longitudinal mass, i.e., $m_l=m_z$. On this situation, effective masses along the interface are isotropic and have a smaller value approximately $0.19m_0$, often refer to lighter transverse mass, $m_t=m_x=m_y$. please see Figs. 2 (a) and (b) in [*Nano Lett. 2008, 8, 5, 1335–1340*] or fig. 4 (e) in [*Journal of Applied Physics 108, 093716 2010*] where in the categorization on the latter reference, our device can be regarded as an example of one-dimensional electric confinement/two degree of freedom (1D EC/2DOF) surface inversion MOSFET. In fact, we further spatially confined the motion of electrons in the y direction by taking 150 nm width in the y-axis. The restriction on y-axis will not further alter the band property of Si, since 150 nm is much larger than the Bohr excitation radius of silicon (which is approximately 5 nm).

In Fig. 6, the results for FV-TF and FV-SC are quite different. For example, differs by ~ 40 meV. Can the authors provide an explanation for this large difference? Why is Thomas Fermi not working well in this situation?

The solution of Poisson's equation with Thomas-Fermi approximation provides us the $\phi(y,z)$ [and the band bending, $-\phi + \chi$]. ϕ is affected largely by two factors: 1) boundary condition and 2) charge densities. In our example, the positive boundary potential, $V_g>0$, pulls the conduction bands downward (such that a negative well introduced beneath the SiO_2)

whereas the negative electron density pushes the conduction band upward locally (just beneath the top gate against the SiO_2 barrier). Similarly, a hole density (if it was included) will pushes the conduction band downward. It is believed that the TF approximation for the electron density (n^{TF}) overestimates the correct self-consistent Schrödinger-Poisson (SP) electron density (n^{SP}) [presented in Eq. (6)]. Considering such an overestimation, the amount of upward shift sourced from n^{TF} is larger than that of n^{SP}. Hence, the bottom of well using TF approximation is higher (less negative) than that of self-consistent SP approach. Overestimation in n^{TF} is also evident in some other works for example see the Figure 9 in Ref [14].

Requested changes

1) If the authors wish to maintain their claim that their approach is superior to FDM and FEM, a much more complete comparison of the two methods needs to be undertaken. In my opinion, this strong claim should be dropped unless much stronger evidence can be provided of the inadequacy of the FEM and/or FDM methods.

Since 2015, We have solved couple of 2D/3D Schrödinger-Poisson's self-consistent problems in heterostructures using Finite-Volume and Finite-Difference discretization schemes. For instance, we have computed confined energies for a 3D lateral quantum dot in the GaAs/AlGaAs heterostructure using Finite-Element software and predictor-corrector method. The quantum dot formed by negatively biased stadium-shape lateral gates. Country to what X. Gao has reported in [*Journal of Applied Physics 114(16), 164302 (2013)*], on achieving the self-consistent convergency at 200mK, we have observed it is very challenging to achieve self-consistent convergence at temperatures below 4.2K (difficulties with both the achievement of convergence and the speed). However, we realized that smooth transition of material properties is helpful, to achieve the self-consistent convergency at 1K. In another attempt, we used Finite-Difference for a 2D problem which was a split gate over GaAs/AlGaAs heterostructure. We observed that the convergence fluctuates after certain iterations, similar to what observed in Ref [16]. In that 2D problem, using a mesh size as small as 0.5 nm did not help us to achieve self-consistent convergence. **Greg Snider** explained a convergence issue with respect to low temperature **in the manual** for his openly accessible 1d-Schrödinger-Poisson solver, with the following statement. "**A final word on the bane of all numerical analysis: convergence. This program's convergence characteristics are very good, with the exception of simulations involving dopant ionization at temperatures below 50K**".

Nevertheless, we drop the accusation of FEM and FDM in the new manuscript but only mentioned of the existing challenges. For example, we have modified the first sentence in the abstract as:

"Achieving self-consistent convergence for conventional effective-mass approaches at ultralow temperatures (below 4.2 *K*) is a challenging task, which mostly lies in the discontinuities in material properties (e.g., effective-mass, electron affinity, dielectric constant)."

To the best of our knowledge, there are no publication focus on comparing convergence properties of the existing methods at low and ultra-low temperatures. Therefore, existing problems are not well documented. We will hopefully cover the convergence behavior of

the three discretization schemes comprehensively in the future. We have mentioned it in the conclusion remarks by saying:

"The current work lacks a direct comparison between FV-SP with Finite-Difference SP (FD-SP) and Finite-Element SP (FE-SP). In the future, we aim to compare the convergence performance of FV-SP with FD-SP and FE-SP for realistic structures."

Furthermore, we inspect our Finite-Element Thomas-Fermi (FE-TF) model once again and practice multiple mesh configurations from 1.4 nm to an extreme 0.5 nm mesh sizes. Using a uniform triangular mesh with the minimum mesh size 0.5 nm, we were able to achieve convergence at 65 K. The convergence problem of FE-TF model did not resolve entirely using smaller mesh sizes (e.g., with a minimum mesh size as small as 0.25 nm). Nevertheless, we kept over observations on the convergence problem of FE-TF on the Supplementary Information S4 to keep the consistency while we have improved the presentation of S4.

2) Directly after Eq. (9), the authors say, "It is important to note that analytical integration has been employed to derive the line-integral terms in the second line of the above relation, and that will improve the achievable accuracy of Finite-Volume method as compared to FDM." It is not true that 2nd line only comes from direct analytical integration. In fact, a finite difference approximation is being made. Consider for example just the first term in the integrand in Eq. (9). It should read

$$\int_{z_s}^{z_n}\int_{y_w}^{y_e}\partial_y(\Gamma_y(y,z)\partial_y\phi(y,z))\,dydz = \int_{z_s}^{z_n}\left[\Gamma_y(y_e,z)\partial_y\phi(y_e,z)-\Gamma_y(y_w,z)\partial_y\phi(y_w,z)\right]dz$$
$$\approx \left[\Gamma_y(y_e,z_p)\partial_y\phi(y_e,z_p)-\Gamma_y(y_w,z_p)\partial_y\phi(y_w,z_p)\right]\Delta z.$$

You have to assume that the integrand doesn't change along z for the integral to be exact instead of approximate. It's fine to use this approximation of course, but it should be noted that it is an approximation.

Your statement is correct. We have improved the presentation of Eq. (9) and added a proper explanation to justify this approximation as the followings:

"In the above approximation, the analytical integration has been used to derive the line-integral terms. In the next step, we have assumed that new integrands (flux) do not change along integration paths. Equivalently, the average flux is assumed to be identical to the value of the flux computed at the center of the face [20]. It is important to note that, partial use of analytical integrations will improve the achievable accuracy of Finite-Volume method."

Note that we said "**partial**" in the last sentence of above explanation.

3) In Fig. 9, the authors compare what they call population factors ($\mathcal{F}_{-1/2}(\frac{\mu-eE_i}{k_BT})$) at different temperatures. This makes little since since the occupation of subband i is proportional to. $(k_BT)^{1/2}\mathcal{F}_{-1/2}(\frac{\mu-eE_i}{k_BT})$. Including the $(k_BT)^{1/2}$ factors makes the comparison between temperatures more sensible.

We thank the referee for this suggestion. We have incorporated the factor $(k_BT)^{1/2}$ in the new manuscript in two figures. Firstly, newly named Fig. 10 (a) and (b) [previously was named Fig. 9 (a) and (b)]. Secondly, newly named Fig. 13 (b) [previously was named Fig 12 (b)]. We kept the plots of the factor $log(\mathcal{F}_{-1/2}(e_i))$ intact to offer readers the values of this factor in newly named Figs. 10 (c) and (d). In addition, we have modified the descriptions related to the Fig 10 in the manuscript as:

"As a part of the n(x, y)'s characterization, we plotted the $(k_B T)^{1/2}(\mathcal{F}_{-1/2}(e_i))$ in Figs. 10 (a) and (b) to convey the contribution of each quantum state in the total electron density at three different temperatures. We plotted this factor for the first thirty states at T = 80 K and T = 4.2 K in Fig. 10(a), while the same factor is plotted at T = 4.2 K and T = 50 mK in Fig. 10(b). We also plot the corresponding $log(\mathcal{F}_{-1/2}(e_i))$ in Fig. 10(c) and Fig. 10(d), respectively. As shown by filled circles in Fig. 10(c), it is not quite distinguishable which states are filled and which states are empty at 80 K. This is why the predictor-corrector method needs more states (n_Q > 40) to converge as compared to the case at lower temperatures. Based on Fig. 10(d), it is tempting to use only n_Q = 8 at T = 50 mK, since the $\mathcal{F}_{-1/2}(e_9)$ is extremely small. While a setup with n_Q = 8 did not converge, the same setup with n_Q = 10 is converged regardless of the value of μ_e. This shows the importance of the factor $(k_B T)^{1/2}$. The FV-SP method with n_Q = 10 also delivered a same set of subband energy and the same profile of electron density as the FV-SP method with n_Q = 40 did. Thus, the numerical sensitivity to the choice of n_Q is reduced at lower temperatures. In general, choosing appropriate n_Q depends on the geometrical and material properties as well as the top gate voltage. Proper selection of n_Q may require a trial test. An initial convergence test can be performed with an overstimulated guess for n_Q. After the convergence has been achieved, the values of $(k_B T)^{1/2}(\mathcal{F}_{-1/2}(e_i))$ can be inspected to estimate which states are significantly contribute to the electron density and which are unnecessary."

We have also modified the description related to Fig.13(b) as:

Furthermore, evolution of the factor $(k_B T)^{1/2}(\mathcal{F}_{-1/2}(e_i))$ due to the increase of the top gate voltage are plotted in Fig. 13(b).

4) When making figures where comparisons are being done, it's a good idea to use the same scale on the color bars. For example, Fig. 6 (a) and (b) are results for the same problem using the FV-TF and FV-SC methods. Comparing these results is difficult since different color scales are used. Same with Fig. 8 (a) and (b).
We thank the referee for this suggestion, and we have corrected the color range as requested.

5) Minor comment: the typical word is bound states not bounding states.
Thanks for commenting on this problem. Accordingly, all "bounding" replaced by "bound".

6) At several places, the authors mention the smallness of quantities in SI units. The solution to this is to use units more natural to the problem. For example, using nm instead of meters.
With the ***Scaling*** section, we wanted to emphasis that it is a good idea to map nm scale into the meter scale. To increase the clarity, we have modified the explanations for the self-consistent electron density on Eq. (6) in terms of units "length^{-1}" and "length^{-2}" and not necessary by unit "m^{-1}" and "m^{-2}". We have also changed m^{-1} to "length^{-1}" on the explanation of one-dimensional electron density, n_{1D}, in Eq. (33). In the results section, the real geometry is shown in nm scale while we have presented the self-consistent and Thomas-fermi electron densities in the unit m^{-3}, the n_{1D} in the unit m^{-1} and wavefunctions in the unit m^{-1} to emphasis that we indeed have employed the scaling length $L_{sc} = 10^{-9}$. We did not express electron

densities as conventional (e.g., cm^{-3}), since the current work is a theoretical study and it does not focused on experimental data. To emphasis on this point even more, we have added to following sentences to sections 3.1 and 3.2:
"Note that in the scaled geometry, mesh sizes vary between 4 m and 0.75 m."

"Note that, the $n(x, y)$ is expressed with the unit m^{-3} since we factored out the nanometer scale on the scaling processes (see subsection 2.4)."