Report of Referee B -- LY15778/Rivera

**The manuscript presents a variational approach to obtain the eigenspectrum of light-matter interaction models in the context of cavity QED. The approach aims at describing the ultrastrong coupling regime limit, in which the coupling strength is sufficiently intense to modify the vacuum properties of the light modes themselves.  With respect to ab-initio calculations based on density functional theory, the proposed approximated approach has the advantage of making it possible to investigate different interesting properties which are not accessible with exact methods. Remarkably, the proposed method allows one to obtain information on the real-space distribution of the cavity modes. The authors apply the method to an example that serves as a benchmark and that elucidates the origin of the saturation of the light-matter coupling strength in the ultrastrong coupling regime.  The proposed method can help to shed light on how fundamental phenomena as the Lamb shift or Casimir-Polder forces are modified in the USC regime. I believe the manuscript can be of interest to a broad audience, both at theoretical and experimental level.**

We thank the reviewer for their positive view of the manuscript.

**However, before recommending publication in PRL, some important issues should be addressed, and various improvement of the manuscript presentation should be implemented.  - The authors demonstrate the effectiveness of the variational method testing it on a simple unidimensional model, for different numbers of discrete levels of the bare matter system. The method predictions for the eigenenergies are in very good agreement with the results of numerical simulations. However, no information is shown about the accuracy of the predictions on any other physical quantity. As one of the main claim is that the proposed method allows one to obtain information about involved observables, I believe it is necessary to discuss whether the approximated eigenstates reproduce faithfully other physical properties. Moreover, as correlations are included only perturbatively, it would be interesting to show if the method can reproduce the amount of correlations or entanglement of the numerically-evaluated eigenstates.**

We thank the reviewer for this suggestion … mention something about Esq.

PA expectation value

**The results of the proposed method are compared with perturbation theory, but no information whatsoever is provided to clarify how the latter is applied. Some more detail should be included also regarding the numerical simulations, at least in the supplementary information.**

In the Supplementary Information, in the section “Derivation of results for one-dimensional cavity model in the main text”, we add a sub-section titled “Perturbative calculation of the energies” where we show the expressions used to perturbatively calculate the energies. Additionally, in the Supplementary Information, in the section titled “Derivation of results for one-dimensional cavity model in the main text” we have added information on how the numerical diagonalization is performed.

**Can the mode profiles shown in Fig2b be reproduced numerically?**

*Physical review letters* 112.1 (2014): 016401.

**- Some key references regarding implementations of USC systems are missing:  T. Niemczyk et al., Nature Physics 6, 772–776 (2010)  P. Forn-Díaz et al. Phys. Rev. Lett. 105, 237001 (2010)  D. Marković et al., Phys. Rev. Lett. 121, 040505 (2018)  - A recent work on the breakdown of gauge-invariance in the USC regime could be mentioned D. De Bernardis et al. Phys. Rev. A 98, 053819 (2018). A reference to introduce the Thomas-Reiche-Kuhn sum rule should be included after equation (11).**

We have included all of these references in the revised manuscript.We have also included a reference (where we discuss the TRK sum rule) to *Atom-Photon Interactions: Basic Processes and Applications,* by C. Cohen-Tannoudji *et al.*

**Right after equation (12) there might be a typo on $E^{(0)}$**

We thank the reviewer for pointing this out, the parentheses in the superscript have been removed.

**One of the main claims is that the method makes it possible to drop the dipole approximation. A detailed example goes probably beyond the reach of the present manuscript, but some further comment on this point could broaden its scope.**

We thank the referee for this point. We have included in the Supplementary Materials a new section entitled “Application of the variational theory to the free electron gas”. In it, we apply the equations derived in the main text and supplement to a gas of non-interacting electrons coupled to the electromagnetic field, and show that the result is the emergence of transverse and longitudinal plasma modes with the correct wavevector-dependent dispersion.

To come back to the reviewer’s comment, if the dipole approximation were taken to describe the electrons, which in our formalism, would amount to stating that the electron density is proportional to a delta-function), an incorrect equation would be obtained for the fields and the corresponding modes. Going further in the treatment of the electron gas by calculating correlations perturbatively, as we did in the main text for the Rabi-like model, one will find that the relevant matrix elements involve integrals over electronic and plasma plane waves, which again are non-dipolar in character.

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