The referee’s comments are in **bold**, our reply is in unbolded black, and additions to the manuscript are in unbolded blue.

Report of Referee A -- LY15778/Rivera

**Authors attempt to formulate variational approach to quantum electrodynamics. It is condemned to failure from the early beginnings, because at each order of the perturbation theory the parameters like mass or charge need to be renormalized. It will make sense, however, to consider variational approach to study few level atoms interacting with few photon modes. It would resemble the idea of dressed states by Cohen-Tannoudji, see for example his textbook "Photon and Atoms, Introduction to Quantum Electrodynamics".  If Authors see any advantages of their variational method over dressed states approach, they should consider any specific example and obtain new results, that can be experimentally verified. Otherwise, their work does not satisfy PRL criteria of impact and innovation.**

We thank the reviewer for their important question. Our method is specifically useful in regimes of light-matter coupling in which the dressed state approach does not accurately describe the physics.

To summarize what we will argue in depth below, the dressed state approach does not accurately describe light-matter coupling when the rotating wave approximation (RWA) is invalid. The lack of validity of the RWA is critical to recent experiments that have demonstrated the “ultrastrong coupling regime” of quantum electrodynamics (QED), both in superconducting qubit systems and systems in which an ensemble of emitters is collectively coupled to light. See for example Refs. 3-18 of the manuscript, as well as *Nature Physics* 6.10 (2010): 772. These references are also well-summarized in this very recent review: *Nature Reviews Physics* 1.1 (2019): 19.

Beyond extremely simplified models such as the two-level single mode Rabi model, and the Hopfield model, the only methods to study such ultrastrongly coupled QED systems are numerical diagonalization approaches in which one numerically expresses the full light-matter Hamiltonian and diagonalizes it. This approach however is unscalable in that the dimension of the Hilbert space becomes prohibitive if: more than one atom or electron is in the system, or many cavity modes are taken into account. In typical ultrastrongly coupled QED systems, non-resonant contributions from multiple cavity modes become important, and many virtual photons occupy these modes. **The main advantage of our approach over dressed states is that it can describe ground and excited-state energies and observables in ultrastrongly coupled systems. The main advantage of our approach over numerical diagonalization is that it can handle situations with many modes in a scalable way, while also flexible to describe systems with electron-electron interactions.**

At the same time, our approach, as we have shown in the manuscript, leads to results in very good agreement with numerical diagonalization in precisely this ultrastrong coupling regime. Moreover, as we showed in the manuscript, we applied this approach to a multi-level, multi-mode version of the Rabi model, which qualitatively very-well describes experimental ultra-strongly coupled QED systems. **We made explicit experimentally verifiable predictions about the energy spectrum of the system**, as well as about the electromagnetic field fluctuations as they are modified by light-matter coupling, which in principle can be measured through techniques such as those in *Science* 322.5906 (2008): 1357-1360 or *Science* (2015): aac9788.

Another important advantage that our approach has over the dressed state approach, which is more methodological, and thus secondary, is that the dressed state approach, being analytical in nature, only can be profitably used on a QED Hamiltonian describing two atomic levels coupled to a single light-mode. It also indeed can be used on three-level systems although the expressions become considerably more cumbersome. This is excellent for the vast number of systems where a strong laser field populating a single mode is present, and resonant effects dominate the physics. In these regimes, the dressed state approach is certainly one of the best approaches. However, in ultrastrongly coupled QED systems, it is known that multi-mode effects can play an important role as well as multi-level effects, and off-resonant effects, as well as effects when no strong driving field is present (see for example *Nature Physics* 6.10 (2010): 772). Our approach, as exemplified by the results in our manuscript, which pertain to a four-level system coupled to fifty cavity modes, captures all of these effects.

In what follows, we elaborate on some additional important differences in the physics described by the dressed state approach versus our approach are:

1. While a dressed-state approach to describing coupling between an atom and a cavity *in the absence of a driving field* predicts no change in the ground state in the coupled light-matter system, our approach does correctly predict a change in the ground state, due to two mechanisms. The first is the change in the frequencies of the modes of the electromagnetic field, as a result of light-matter coupling (see Equation (12)) of the main text.

The second mechanism is the energy shift of the ground state due to virtual emission and re-absorption of cavity photons. This position-dependent energy shift of the ground state leads to Casimir-Polder forces, which are known to be beyond the rotating-wave approximation. Importantly however, while the typical treatment of Casimir-Polder forces relies on perturbation theory, our theory predicts accurate results for energy shifts and forces in the non-perturbative regime. In particular we find the new result that the Casimir-Polder force in the non-perturbative regime can be understood as virtual emission and re-absorption of photonic quasiparticles whose electromagnetic field fluctuations are very different from those of the bare cavity (see Figure 2b). We briefly note that in the context of dressed states, the dressed states can be used to perturbatively calculate Bloch-Siegert shifts, which are corrections beyond the RWA. However, this approach implicitly assumes that the RWA presents a weak correction to the states and dynamics, which is not the case in ultrastrongly coupled QED systems.

Therefore, if one does spectral measurements on the system in order to measure the excitation energies, one will find that our approach correctly captures the excitation energies, while the dressed state approach does not. Alternatively, if one measures the vacuum forces on emitters in the cavity, one will find a large deviation from the conventional Casimir-Polder theory. Both of these measurements are clear experimental pathways to verify our predictions.

In order to communicate these points to the reader, we have now added a discussion of the dressed state approach in the main text. In particular, we have added a new paragraph in the final paragraph of the first page:

The variational method developed in this manuscript is particularly suited for dealing with QED systems in the ultrastrong coupling regime, in which the rotating-wave approximation no longer holds. Thus, methods based on the Jaynes-Cummings model such as dressed state approaches [42] are no longer accurate in this regime. Moreover, our approach is particularly suited to scalably dealing with systems with many emitter levels, as well as many cavity modes which may have large virtual photon occupation numbers.

[42] Cohen-Tannoudji, C., Dupont-Roc, J., and Grynberg, G. Atom-Photon Interactions. (1992.)