Dear Editor, Dear Reviewers,

We would like to thank you for your time in reviewing our paper and providing valuable comments that led to possible improvements in the current version. We have carefully considered the comments and tried our best to address every one of them. We hope that the manuscript after careful revisions, will meet your high standards. We welcome further constructive comments if any. Below, we provide the point-by-point responses.

Sincerely,

R. Photopoulos and A. Boulet

1) *In the introduction, the authors point out that "non-perturbative methods express the problem with multidimensional integrals". It is not clear what is referred to here.*

Thank you for pointing this lack of precision. We complete the first paragraph of the I. INTRODUCTION by adding the following: "[...] can [...] in the Feynman's path integral formalism [...]". We also mention the Density Marix Renormalization Group (DMRG) method as a non-perturbative approach (refs. [7–10]) and add the following sentence for completness: "[...] or, alternatively, the problem can be tackled by optimizing a matrix product state tensor network using an iterative eigensolver such as the Lanczos algorithm [26, 27]".

Slightly below, they identify first-order perturbation theory with mean-field theory, which I find slightly confusing. Can BCS mean-field theory be considered as a first-order perturbation theory?

Thank you for pointing out this source of unclearness of our starting point. In this work we do not consider BMBPT (cf. for instance [17]). We add a comment to refer, from section II, the mean-field theory as Hartree-Fock approximation, that is to say the first-order in MBPT. We added the following in page 2: "In this work, we only consider the normal component, making the reference state $|\Phi_0\rangle$ the Hartree-Fock Slater determinant associated with $\hat{H}_0$."

2) *The main point of the authors is to show that, starting from Hamiltonian (4), one can reproduce the perturbation expansion order by order while satisfying the exact result $E_\infty/E_0 = \xi_0$. To do so, one has to introduce an unknown parameter, β, to second order; two parameters β_1 and β_2 to third order order, etc. The procedure followed to second order, Eq. (26), seems rather arbitrary. Could the authors justify it? Is it the only possible way to introduce the two parameters β_1 and β_2 and, if not, why choosing this one?*

Yes, this choice is quite arbitrary. The simplest choice we can think, in order to keep the β-independant ground state energy while keeping the proper limits, is a weighted arithmetic mean of the form: $r\Delta E(\beta_1) + (1 - r)\Delta E(\beta_2)$ with $0 < r < 1$. Making this choice led to the necessity to fix this r parameter on a fourth property that does not appear in our strategy at the third order in perturbation (we adjust the three paramaters $\{\beta_1, \beta_2, a_3\}$ on the three physical parameters $\{\gamma_2, \gamma_3, \xi_0\}$). Actually, it could be interesting to investigate further such parameterization but in the present article, and

for the sake of simplicity, we arbitrary choose the arithmetic mean ($r = 1/2$). We added, bellow eq. (26) the following sentences: "We note that this choice is arbitrary in the sense that any weighted arithmetic mean of the form $\Delta E(\beta) \to r\Delta E(\beta_1) + (1-r)\Delta E(\beta_2)$ can be used, where $0 < r < 1$ is a parameter to adjust. For simplicity and because the strategy developed in this work implies to adjust only three parameters at the third order in perturbation on the low- and high-scale limits, we chose the arithmetic mean $r = 1/2$."

3) *I do not understand the meaning of the sentence "which is again independent of β_1 and β_2" following Eq.(26).*

Since, as showed in the unnumbered equation right after Eq. (17c), $\Delta E(\beta)$ is β-independent, then $\Delta E(\beta_1) + \Delta E(\beta_2)$ is independent of β_1 and β_2. We remove the the sentence "which is again independent of β_1 and β_2" following Eq.(26) to avoid repetition in the text.

4) *It is shown how to reproduce the perturbation expansion order by order. I understand, although it is not said explicitly, that this is equivalent to avoiding double counting of correlations. A short discussion would be welcome.*

Thank you for pointing out the lake of discussion about this aspect. We add the following section in page 6:

III.B.4 Avoiding the double counting of correlations

We can observe that our method does not overcount the many-body correlations. This is due to the fact that we impose the low-scale expansion up to a given order in perturbation. Thus, even if many-body correlations are included in an effective Hamiltonian and potentially taken into account within the MBPT framework, the adjustment of the β-parameters in order to reproduce the low-scale expansion (2) in the limit $\lambda \ll 1$ avoid this eventual double-counting. To be more precise, if we reduce our strategy to the RSPT, that is to say setting $\beta = 1$, and keeping an effective Hamiltonian similar to (4), the low-scale expansion (2) cannot be recovered in the limit $\lambda \ll 1$. Therefore, our strategy consists in mimic the infinite series (2) with effective parameters $\{\widetilde{\gamma}_n\}$ for which the first parameters match the physical parameters $\{\gamma_n\}$ up to the order m that is considered to truncate the MBPT calculation, i.e. $\widetilde{\gamma}_1 = \gamma_1, \ldots, \widetilde{\gamma}_m = \gamma_m$, and $\widetilde{\gamma}_n \neq \gamma_n$ for $n > m$.

5) *At the top of page 4, "an energy operator $\hat{\omega}|\Psi_0\rangle$" should be replaced by "an energy operator $\hat{\omega}$".*

Thank you for pointing out this misprint. We modified "an energy operator $\hat{\omega}|\Psi_0\rangle$" to "an energy operator $\hat{\omega}$".

6) *The various examples considered in the manuscript are quite convincing except the 1D Hubbard model. In the case $U/t > 0$, it seems that the second-order perturbation theory results are better than the $l = 0$ and $l = 1$ results.*

It is accidental and because of the fact that the range to display the results as a function of U/t is restricted. Actually, the second-order perturbation theory results is valid only for $U/t \ll 1$ and diverge in the limit $U/t \to \infty$ due to the polynomial form of the energy. This effect is visible on the figure displayed as a function of $(U/t)^{-1}$ where we observe a large deviation (even more, a divergence) of the second-order perturbation theory results compared to exact calculation for $(U/t)^{-1} < 0.1$. To make clear this aspect, we plot the fig. 4(c) in a wider range: $0 < U/t < 15$.

Moreover I do not understand what the model with $l = 2$ and $l = 3$, mentioned in the caption of Fig. 4, refer to.

Thank you for pointing out this misprint. The mention to $l = 2$ and $l = 3$ have been removed from the caption of Fig. 4. We also removed the mention to $l = 3$ in other captions.

7) *The authors discuss only the calculation of the ground state energy. In many-body systems, correlation functions are also of prime interest. Is the method proposed in the manuscript restricted to thermodynamic quantities or would it be possible to also compute one- and two-particle Green functions?*

Yes, it is possible to access to the one- and two- particle Green functions. By definition, using standard approaches, the many-body Green function is obtained by the expectation value of time ordered field operators (of the unperturbed/non-interacting system) according to the ground state given by Eq. (13b); schematically : $G = -(i/\hbar)\langle\Psi_0|T[\cdots]|\Psi_0\rangle$. In our approach, we can obtain the many-body Green function by the replacement of $|\Psi_0\rangle$ by $|\Psi_0(\beta)\rangle$ given by Eq. (17b).

Additional minor changes:

- Misprint in eq. (39) have been corrected: minus sign added for the first term of the right hand side.

- We added refs. [29, 30] on MBPT and [24] on Monte Carlo algorithm in the I. INTRODUCTION.
- We added refs. [66–76] (realistic models), [77–80] (linear response theory) and [39,81] (link DFT/EFT) in the section VII. CONCLUSION: DISCUSSION AND OUTLOOK.
- We added the term "strongly" and replaced the term "interactions" by the term "Hamiltonians" to the title of the part III: "Extension of the MBPT with strongly correlated effective Hamiltonians".
- We modified the title of section VII: "CONCLUSION AND DISCUSSION" → "CONCLUSION: DISCUSSION AND OUTLOOK".
- Minor language improvements:
  - page 1:
    "Another approach, the Density Functional Theory, is a third class of methods to solve quantum many-body problems [...]"
    →
    "Another approach, namely the Density Functional Theory, is a third class of methods used to solve quantum many-body problems [...]"
  - page 6:
    "Here, the strategy consists of adding an additional parameter [...]"
    →
    "Here, the strategy consists of including an additional parameter [...]"
  - page 6:
    "With the new method proposed "
    →
    "Considering the new method proposed "
  - page 8:
    "The Hamiltonian, with at most two-body interaction, [...]"
    →
    "The many-body Hamiltonian expressed in the second quantization formalism, with at most two-body interaction, [...]"

- page 8:
  "This definition of the energy allows for [...]"
  →
  "This definition of the reduced GS energy allows for [...]"
- page 13:
  "[...] our extended MBPT is valid for various system, [...]"
  →
  "[...] our extended MBPT is valid for various correlated system, [...]"
- page 13:
  "[...] to apply the method in such a formalism."
  →
  "[...] to apply our method in such a formalism."