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Manthe correctly states that the derivation in his Ref. 2 includes the description of natural single-particle states as a special case.\(^1\) The difference with the derivation in my paper is that, whereas I derive the equations of motion directly from relations that define single-particle states that give an optimal wave function,\(^2\) the derivation in Ref. 1 uses a variational principle to insure that the wave function will be optimal. The single-particle states in the two derivations are linear combinations of each other, and give the same wave function. The method using the variational principle yields the stronger statement that the wave function is optimal for any number of single-particle states and not only in the limit of an infinite number. In my paper I have to note that the variational principle and my derivation give the same equations of motion in order to get this stronger statement.\(^2\)

Since neither Manthe's choice nor mine of the single-particle states shows a clear computational advantage over the other, the question becomes how these single-particle states might be chosen as to give the fastest simulation. This may not be an easy question to answer as changes in the single-particle states as well as the coefficients may determine the computational effort.

Finally, I would like to clarify a minor point concerning the uniqueness of the natural single-particle states. If one tries to approximate a given wave function \(\Psi\) using \(N\) natural single-particle states for a certain coordinate, then these natural single-particle states do not depend on \(N\). This is obvious, as the defining equation for these states does not depend on \(N\), but only on \(\Psi\) [see Eqs. (9) and (10) of Ref. 2]. However, in order to integrate the equations of motion exactly, one would need \(\Psi\), whereas one only has an approximation. Hence, the natural single-particle states in a simulation are only approximate and therefore dependent on \(N\).

I would like to thank Dr. Manthe for making me rethink about the MCTDH approximation and deepening my understanding of it.