Second referee

We have defined the light-matter interaction using the formalism described in :

S. Ismail-Beigi, E.K. Chang and S. Louie

expressed in the velocity gauge and accounting for nonlocal potentials.

One can show that using a gauge transformation, the Hamiltonian is transformed into the effective Hamiltonian (Eq.(6)). Note that this gauge transformation is valid to all orders in the vector potential A(t).

At this point, the interaction Hamiltonian has to be treated with great care, when expanding the wavefunction onto Bloch states. We have followed the procedure used by

E. I. Blount, F. Seitz, and D. Turnbull, Solid State Phys. 13, 305 (1962)

and

J. E. Sipe and A. I. Shkrebtii, Phys. Rev. B 61, 5337 (2000).

It amounts to split the operator r into the interband (r\_e) and intraband (r\_i) parts. The only contributions to the final expression Eq. (8) are quantities defined in terms of r\_e and r\_i, that can be computed for Bloch states.

Section II.B has been slightly rewritten and reorganized.

The equivalence between the length and velocity (or transverse) gauges has been checked by Sipe and co-authors in the case of SHG for local potentials (see PRB 43 8990 (1991)). This demontration can be further extended to the case of nonlocal potentials, even when using the cut-function used in Section III.

Concerning the suggestion of the referee to compare with the PAW approach, as performed in PRB 63, 125108 (2001), we agree that this would give very interesting insights in the case of SHG. However, our framework used for the surface cannot be presently extended to PAW.