

## ERRATA

### Erratum: Adiabatic density-functional perturbation theory [Phys. Rev. A 52, 1096 (1995)]

Xavier Gonze

[S1050-2947(96)03411-7]

PACS number(s): 31.15.Ew, 02.70.-c, 71.10.+x, 99.10.+g

Some equations appearing in this paper need to be corrected. I thank R. W. Nunes for pointing out the errors or inaccuracies (i)–(iii) to me.

(i) In Eq. (18), the projector operators should not be affected by the inversion operation:

$$G_{\perp\alpha} = P_{\perp\alpha} [(\epsilon_{\alpha} - H)^{(0)}]^{-1} P_{\perp\alpha}.$$

(ii) In Eq. (51), the second  $\delta$  function should have the argument  $m - j - k - l$ , like the other  $\delta$  functions appearing in this equation.

(iii) A few terms that appear when the perturbation affects the explicit form of the Hartree and exchange-correlation energy are missing in Eqs. (125)–(127):  $(T+v)^{(1)}$  should be replaced systematically by  $(T+v+v_{\text{Hxc},0})^{(1)}$  in these equations.

(iv) One term is missing in Eq. (55), that should read

$$P_c(H^{(0)} - \epsilon_{\alpha}^{(0)})P_c|\Phi_{\alpha}^{(i)}\rangle = -\sum_{j=1}^i P_c H^{(j)}|\Phi_{\alpha}^{(i-j)}\rangle + \sum_{\beta=1}^N \sum_{j=1}^{i-1} \Lambda_{\alpha\beta}^{(j)} P_c|\Phi_{\beta}^{(i-j)}\rangle.$$

As a consequence, Eq. (139) should also be changed:

$$P_c(H^{(0)} - \epsilon_{\alpha}^{(0)})P_c|\Phi_{\alpha}^{(2)}\rangle = -P_c(H^{(2)}|\Phi_{\alpha}^{(0)}\rangle + H^{(1)}|\Phi_{\alpha}^{(1)}\rangle) + \sum_{\beta=1}^N \Lambda_{\alpha\beta}^{(1)} P_c|\Phi_{\beta}^{(1)}\rangle.$$

(v) The summation on  $\beta$  should start from 1 and not 0 in Eqs. (45) and (54).

(vi) The first two papers in Ref. [20] should be M. Buongiorno Nardelli, S. Baroni, and P. Giannozzi, Phys. Rev. Lett. **69**, 1069 (1992); S. de Gironcoli and S. Baroni, *ibid.* **69**, 1959 (1992). Reference [22] should be S. de Gironcoli, S. Baroni, and R. Resta, Phys. Rev. Lett. **62**, 2853 (1989).

Finally, I want to mention that the time-reversal symmetry was used in order to get Eqs. (125), (126), (128), and (129), while Eqs. (127) and (130) are valid even if the time-reversal symmetry is broken.