Facco Bonetti *et al.* Reply: In the following we address the arguments of Niquet, Fuchs, and Gonze (NFG) [1] in their logical order.

(1) We nowhere claim that the Krieger-Li-Iafrate results for v_c^{MP2} prove anything. They just illustrate the origin of the divergence of v_c^{MP2} most clearly.

(2) Turning to the full optimized potential method solution, NFG concede that our analytical example unambigously proves the existence of the mechanism, which is responsible for the divergence. However, NFG argue that this example is oversimplified as it does not allow a cancellation between the two components of Q_c, the orbital-derivative term Q_c^a and the eigenvalue-derivative term Q_c^b. In order to address this point let us first consider E_c^{MP2} for a spin-saturated 2-level system with one occupied level F and one unoccupied level U. One finds

$$Q_c^a = \phi_F^\dagger \phi_U \frac{[(UF\|UU) - (FF\|FU)](UU\|FF)}{2(\epsilon_F - \epsilon_U)^2} + \text{c.c.},$$

$$Q_c^b = (|\phi_U|^2 - |\phi_F|^2)\frac{|(FF\|UU)|^2}{2(\epsilon_F - \epsilon_U)^2},$$

with $(FU\|FF)$ being defined by Eq. (1) of [2]. It is obvious that asymptotically Q_c^a and Q_c^b do not cancel. The same effect is present for any finite Hilbert space.

(3) One might still hope that the resummation of unoccupied states inherent in E_c^{MP2} leads to the desired cancellation. To investigate this issue the complete Q_c is decomposed into three terms, $Q_c = Q_c^{DD} + Q_c^{DC} + Q_c^{CC}$, reflecting the discrete (D) or continuum (C) nature of the two particle-hole excitations involved. Q_c^{DD} is plotted in Figs. 1(a) and 1(b) for He. Figure 1(a) demonstrates (i) the convergence of Q_c^{DD} for given r with increasing number n of shells included, and (ii) the oscillatory behavior of Q_c^{DD}, consistent with $\int_0^\infty dr Q_c^{DD} = 0$. Figure 1(b) exhibits the completely different asymptotic behavior of Q_x, $Q_c^{DD,a}$ and $Q_c^{DD,b}$. Consequently, for any system with a discrete spectrum Q_c/Q_x and thus v_c^{MP2} diverges.

(4) Finally, the role of the continuum states has to be examined. This is most easily done by putting the atom in a sphere of radius R [requiring hard wall boundary conditions for the radial orbital, $\overline{\varphi}_{\epsilon l}(R) = 0$] and then taking the limit $R \to \infty$. The standard normalization of continuum states, $\overline{\varphi}_{\epsilon l}(r \to \infty) \sim \cos[kr - \pi(l+1)/2 - \eta_l]$ [$\epsilon = k^2/(2m)$], corresponds to $\int_0^R dr \overline{\varphi}_{\epsilon l}^2 = R/2$. One finds

$$Q_{c,-}^{DC,b} = \int_0^\infty d\epsilon \left(\frac{2m}{\epsilon}\right)^{1/2} \sum_{nl} \frac{[\varphi_{nl}^2 - 2\varphi_{10}^2]R_{n\epsilon,l}^2}{(2\epsilon_{10} - \epsilon_{nl} - \epsilon)^2},$$

$$Q_{c,+}^{DC,b} = \frac{2}{R}\int_0^\infty d\epsilon \left(\frac{2m}{\epsilon}\right)^{1/2} \sum_{nl} \frac{\overline{\varphi}_{\epsilon l}(r)^2 R_{n\epsilon,l}^2}{(2\epsilon_{10} - \epsilon_{nl} - \epsilon)^2},$$

$$R_{n\epsilon,l} = \int_0^R dr dr' \frac{r_<^l}{r_>^{l+1}} \frac{\varphi_{10}(r)\varphi_{nl}(r)\varphi_{10}(r')\overline{\varphi}_{\epsilon l}(r')}{(2l+1)^{1/2}},$$

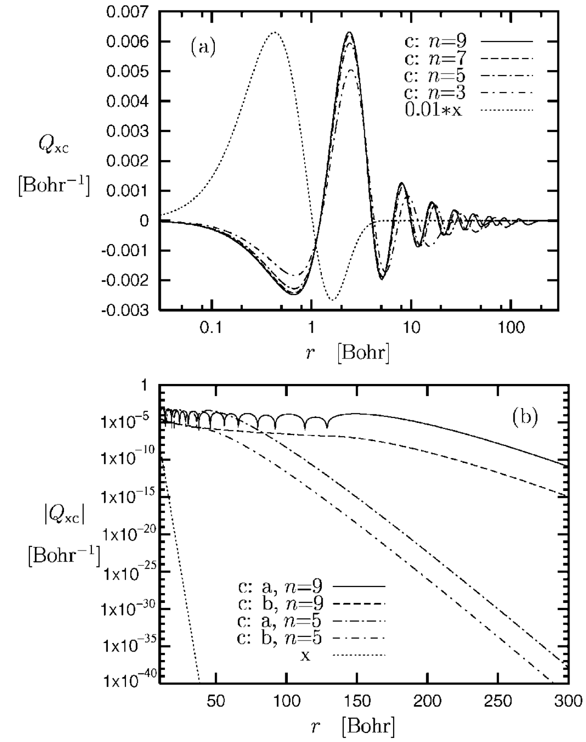

FIG. 1. Q_{xc} for He (the nodes of $Q_c^{DD,a}$ are suppressed).

where $Q_c^{DC,b} = Q_{c,-}^{DC,b} + Q_{c,+}^{DC,b}$ has been split according to negative and positive ϵ_{nl} in $\partial E_c^{MP2}/\partial \epsilon_{nl}$. $Q_{c,+}^{DC,b}$ vanishes for $R \to \infty$, so that $\int_0^\infty dr \lim_{R\to\infty} Q_c^{DC,b} \neq 0$ (while $\lim_{R\to\infty}\int_0^R dr Q_c^{DC,b} = 0$). The infinitesimal local contribution of $Q_{c,+}^{DC,b}$ is not visible in Fig. 1 of [2]. The same is true for $Q_{c,+}^{CC,b}$ and related terms in Q_c^a.

(5) Concerning the asymptotic behavior of Ψ_1 and Φ_0, one can verify that both functions show the same exponential decay, but a different power law behavior. Thus Ψ_1/Φ_0 and v_c^{MP2} diverge as a power of r.

In summary, there can be no doubt that the results of [2] are basically correct. The onset of the divergence of v_c^{MP2} is even visible in the basis set representation shown in Figs. 2 and 3 of [3], in spite of the fact that use of a basis set ultimately truncates the divergent behavior.

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