Comment on "On the Original Proof by Reductio Ad Absurdum of the Hohenberg–Kohn Theorem for Many-Electron Coulomb Systems"

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ABSTRACT: We argue with Kryachko's criticism [Int J Quantum Chem 2005, 103, 818] of the original proof of the second Hohenberg-Kohn theorem. The Kato cusp condition can be used to refute a "to-be-refuted" statement as an alternative to the original proof by Hohenberg and Kohn applicable for Coulombic systems. Since alternative ways to prove falseness of the "to-be-refuted" statement in a reduction ad absurdum proof do not exclude each other, Kryachko's criticism is not justified.

Key words: Hohenberg-Kohn theorems; reductio ad absurdum; Kato cusp condition; Coulombic systems

In the recent article [1], the original proof of the first Hohenberg–Kohn theorem [2] was criticized "the usual reductio ad absurdum proof of the Hohenberg–Kohn theorem is unsatisfactory." Inspecting the paper shows, however, that the considerations presented do not justify such a bold conclusion. The author notes that, as the consequence of the Kato cusp condition [3], the external potential can be uniquely reconstructed from the information contained in the electron density for a Coulomb system (see also the relevant paper by March [4]). However, this observation cannot be used to question the validity of the original reductio ad absurdum (RAA) proof. In an RAA proof, the validity of a false statement is analyzed aiming at refuting it. In some cases, a given statement can be refuted in different ways. In our view, the author's analysis of the Kato cusp condition, if used as a part of an alternative

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TABLE I

Outlines of the two considered reductio ad absurdum proofs of the theorem $\sim p \Rightarrow \sim q$, where p denotes the statement $v_1(\mathbf{r}) - v_2(\mathbf{r})$ = const and q denotes the statement $\rho_0^1 = \rho_0^2$.*

	Hohenberg–Kohn	Alternative
A. Statement to be refuted ($\sim t$)	$\sim t \equiv \sim p \wedge q$	$\sim t \equiv \sim p \wedge q$
B. Demonstration that $\sim t$ is false	Variational principle leading to $E_0^{(1)} + E_0^{(2)} < E_0^{(1)} + E_0^{(2)}$	As a consequence of the Kato cusp condition, the statement $q \Rightarrow p$ is true [1, 3, 4]
	Ref. [2]	But $q \Rightarrow p$ and t are equivalent statements
C. Conclusion	t is true	t is true

* Both proofs concern nondegenerate states.

RAA proof of the first Hohenberg–Kohn theorem, provides such an example.

For the sake of brevity, we use the symbolic notation for the Hohenberg–Kohn theorem: $\sim p \Rightarrow \sim q$, where p denotes the statement ($v_1(\mathbf{r}) - v_2(\mathbf{r})$ = const) and q denotes another statement ($\rho_0^1 = \rho_0^2$). The negation of the Hohenberg–Kohn theorem reads $\sim p \wedge q$, where $\wedge$ denotes logical AND. The statement that the Kato cusp condition:

$$\left.\frac{\partial \rho(\vec{r})}{\partial \vec{r}}\right|_{r=0} = -\frac{2Z}{a_0}\left.\rho(\vec{r})\right|_{r=0}, \qquad a_0 = \frac{\hbar^2}{me^2} \tag{1}$$

allows one to reconstruct uniquely the external potential from the electron density in the Coulomb systems can be written as $q \Rightarrow p$ in this convention. The author's criticism of the original proof is based on the observation that since the statement $\sim p \wedge q$ violates the Kato cusp condition, its use in the original Hohenberg–Kohn proof is not justified.

Table I shows that the Kato cusp condition can be used as a key element in another RAA proof, which parallels the original one. The logical outline of two proofs (details of steps **B** are given in the original papers by Hohenberg and Kohn [2] and Kryachko [1]) makes it evident that the Kato cusp condition can be used to demonstrate that the negation of the Hohenberg–Kohn theorem is false. The nature of an RAA proof is such that any consideration demonstrating falseness of the to-be-refuted assumption ($\sim p \wedge q$ in this case) is sufficient. The proofs given by Hohenberg and Kohn and the alternative one, which uses the contradiction demonstrated by Kryachko in step **B,** are different but lead to the same conclusion that the statement $\sim p \wedge q$ is false. In the Hohenberg–Kohn case, the consequence of a false assumption is shown to be false, whereas in the Kryachko's case the falseness of the to-be-refuted assumption is demonstrated directly. It should be noted, however, that neither proof is universal. Each holds only for a well-defined type of potentials. The author's proof concerns Coulomb potentials. In the Hohenberg–Kohn case, the group of considered potentials comprise those for which the inequality, written in the notation of Ref. [1], $\langle \Psi_0^{(1)} | H_2^N | \Psi_0^{(1)} \rangle > \langle \Psi_0^{(2)} | H_2^N | \Psi_0^{(2)} \rangle$ holds.

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