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Correction

Correction to: Canonical Quantum Observables for Molecular Systems Approximated by Ab Initio Molecular Dynamics

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Correction to: Ann. Henri Poincaré 19 (2018), 2727–2781 https://doi.org/10.1007/s00023-018-0699-x

On page 2744 in [1], it is stated that the nonlinear eigenvalue problem (3.8), i.e.

$$\left(V + \frac{1}{4M}\Psi\nabla\Psi^* \cdot \nabla\Psi\Psi^*\right)\Psi = \Psi\Lambda, \tag{0.1}$$

can be written as the nonlinear system of partial differential equations (3.13). That statement is not correct in general, which affects Theorem 3.2. In Theorems 3.6 and 3.7, an alternative to solving (0.1) exactly is used, namely to solve it approximately

$$\left(V + \frac{1}{4M}\Psi\nabla\Psi^* \cdot \nabla\Psi\Psi^*\right)\Psi = \Psi\Lambda + \mathcal{O}(M^{-2}),$$

with Λ diagonal, based on the following iteration. Let $\Psi[1] = [\psi_1\ \psi_2\ \ldots\ \psi_d]$ be the matrix of eigenvectors to V, with corresponding eigenvalues $\lambda_1, \ldots, \lambda_d$. The approximate eigenvectors $\Psi[2]$ are the normalized eigenvectors of

$$V + \frac{1}{4M}\Psi[1]\nabla\Psi^*[1] \cdot \nabla\Psi[1]\Psi^*[1]$$

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and $\Lambda[2]$ is the diagonal matrix with the corresponding eigenvalues. Since regular perturbation theory shows $\|\Psi[2]-\Psi[1]\|_{C^1(\mathbb{R}^{3N})}=\mathcal{O}(M^{-1})$, we obtain in (3.18) that $\bar{H}=\Psi^*[2]\#H\#\Psi[2]$ satisfies

$$\bar{H}(x,p)=\bar{H}_0(x,p)+r_0(x)$$

where the remainder $d\times d$ matrix $r_0(x)$ is small

$$\|r_0\|_{L^\infty(\mathbb{R}^N)}=\mathcal{O}(M^{-2}),$$

with the diagonal matrix

$$\bar{H}_0(x,p):=\frac{|p|^2}{2}\mathrm{I}+\Lambda[2](x).$$

Using Theorem 3.7, Theorem 3.2 is thus corrected as follows

Theorem 0.1. *Assume that $V\in[C^3(\mathbb{R}^N)]^{d^2}$, $\bar{A}_0$ and $\bar{B}_0$ are diagonal, the $d\times d$ matrix valued Hamiltonian H has distinct eigenvalues and that there is a constant C such that*

$$\begin{aligned}
\sum_{|\alpha|\leq 2}\|\partial_x^\alpha\psi_k\|_{L^\infty(\mathbb{R}^{3N})}&\leq C,\quad k=1,\dots,d,\\
\max_i\sum_{|\alpha|\leq 3}\|\partial_x^\alpha\partial_{x_i}\lambda_j\|_{L^\infty(\mathbb{R}^N)}&\leq C,\\
\sum_{|\alpha|\leq 3}\|\partial_z^\alpha\bar{A}_{jj}(0,\cdot)\|_{L^2(\mathbb{R}^{2N})}&\leq C,\\
\|e^{-\beta\bar{H}_0(z)}\|_{L^2(\mathbb{R}^{2N})}+\|\bar{B}_0(z)e^{-\beta\bar{H}_0(z)}\|_{L^2(\mathbb{R}^{2N})}&\leq C,
\end{aligned}$$

hold, then there is a constant c, depending on C, such that the canonical ensemble average satisfies

$$\begin{aligned}
&\Big|\frac{\mathrm{Tr}\left(\hat{A}_\tau\hat{\Psi}(\bar{B}_0e^{-\beta\bar{H}_0})\hat{}\,\hat{\Psi}^*\right)}{\mathrm{Tr}\left(\widehat{\hat{\Psi}e^{-\beta\bar{H}_0}}\hat{\Psi}^*\right)}-\sum_{j=1}^d\int_{\mathbb{R}^{2N}}\frac{\bar{A}_{jj}(0,z_\tau^j(z_0))\bar{B}_{jj}(z_0)e^{-\beta\bar{H}_{0jj}(z_0)}}{\sum_{k=1}^d\int_{\mathbb{R}^{2N}}e^{-\beta\bar{H}_{0kk}(z)}\,\mathrm{d}z}\,\mathrm{d}z_0\Big|\\
&\quad\leq cM^{-1},
\end{aligned}$$

where z_τ^j solves (3.22).

Reference

[1] Kammonen, A., Plecháč, P., Sandberg, M., Szepessy, A.: Canonical quantum observables for molecular systems approximated by ab initio molecular dynamics. Ann. Henri Poincaré **19**, 2727–2781 (2018)

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