DTU Library

Development and Applications of Coupled- Cluster Methods for X-Ray Spectroscopy

Vidal, Marta Lopez

Publication date:
2020

Document Version
Publisher's PDF, also known as Version of record

Author Corrections

Page	Current Text	New Text
6	$\hat{f}_i = [...] = -\frac{1}{2}\sum_i^N \nabla_i^2 - \sum_A^N \frac{Z_A}{r_{iA}} + v^{\mathrm{HF}}(i)$	$\hat{f}_i = [...] = -\frac{1}{2}\nabla_i^2 - \sum_A^N \frac{Z_A}{r_{iA}} + v^{\mathrm{HF}}(i)$
15	[...] and inserting it into the similarity-transformed normal-ordered Hamiltonian $\bar{\mathcal{H}} = e^{-\hat{\mathcal{T}}}\hat{\mathcal{H}}e^{-\hat{\mathcal{T}}}$.	[...] and inserting it into the similarity-transformed normal-ordered Hamiltonian $\bar{\mathcal{H}}$.
22	$[\hat{\mathcal{H}}, \hat{\mathcal{R}}] \vert\Psi_i\rangle = \omega_f \hat{\mathcal{R}} \vert\Psi_i\rangle$	$[\bar{\mathcal{H}}, \hat{\mathcal{R}}] \vert\Phi_0\rangle = \omega_f \hat{\mathcal{R}} \vert\Phi_0\rangle$
28	$\gamma_q^p = \langle\Phi_0\vert \hat{\mathcal{L}} e^{\hat{\mathcal{T}}^\dagger} \hat{a}_p^\dagger \hat{a}_q e^{\hat{\mathcal{T}}^\dagger} \hat{\mathcal{R}} \vert\Phi_0\rangle_C$	$\gamma_q^p = \langle\Phi_0\vert \hat{\mathcal{L}} e^{-\hat{\mathcal{T}}} \hat{a}_p^\dagger \hat{a}_q e^{\hat{\mathcal{T}}} \hat{\mathcal{R}} \vert\Phi_0\rangle_C$
28	$(\gamma_{\mathcal{N}})_q^p = \langle\Phi_0\vert \hat{\mathcal{L}} e^{\hat{\mathcal{T}}^\dagger} \{\hat{a}_p^\dagger \hat{a}_q\} e^{\hat{\mathcal{T}}^\dagger} \hat{\mathcal{R}} \vert\Phi_0\rangle_C$	$(\gamma_{\mathcal{N}})_q^p = \langle\Phi_0\vert \hat{\mathcal{L}} e^{-\hat{\mathcal{T}}} \{\hat{a}_p^\dagger \hat{a}_q\} e^{\hat{\mathcal{T}}} \hat{\mathcal{R}} \vert\Phi_0\rangle_C$
28	$(\gamma_{\mathcal{N}})_i^a = t_i^a + r_0 l_i^a + r_0 t_{im}^{ae} l_e^m$ [...]	$(\gamma_{\mathcal{N}})_i^a = t_i^a + r_0 t_{im}^{ae} l_e^m$ [...]
38	In the Coulomb gauge,	In the Coulomb gauge, the coupling Hamiltonian contains then two terms; the dominant perturbative term describing one-photon absorption or emission of a particle of charge $-e$ and mass m is given in Gauss units by:
46	The CVS approximation [110] states that [...]	The CVS approximation states that [...]
223	reduced Planck constant $\hbar = 1.0546 \times 10^{-34}$ J	reduced Planck constant $\hbar = 1.0546 \times 10^{-34}$ J.s