Generalized Lee-Suzuki Method for Constructing Effective Interactions: technicalities

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I. INTRODUCTION

II. THEORETICAL FRAMEWORK

We start with a brief review of the GLS method [1]. We want to obtain effective interaction R acting on model space P, in case when unperturbed hamiltonian H_0 is non-degenrate, i.e.,

$$PH_0P = \sum_{\alpha}^{d} \epsilon_\alpha P_\alpha \qquad \text{and} \qquad P = \sum_{\alpha}^{d} P_\alpha \tag{1}$$

where $P_\alpha P_\beta = \delta_{\alpha\beta} P_\alpha$ and d is the dimension of the model space. The unperturbed energies ϵ_α are generally different from each other.

One then defines a $\widehat{Q}$-box as

$$\widehat{Q}(\epsilon_\alpha) = PVP + PVQ\frac{1}{\epsilon_\alpha - QHQ}QVP \tag{2}$$

and the generalized (or multi-energy) $\widehat{Q}$-box as

$$\widehat{Q}_m(\epsilon_1\epsilon_2\ldots\epsilon_{m+1}) = (-1)^m PVQ\frac{1}{\epsilon_1 - QHQ}\frac{1}{\epsilon_2 - QHQ}\cdots\frac{1}{\epsilon_{m+1} - QHQ}QVP \tag{3}$$

The GLS effective interaction is then given by the following iteration sequence

$$R_n = \sum_\alpha (P - {Z_\alpha}^n)^{-1}\widehat{Q}_\alpha {P_\alpha}^{n-1} \tag{4}$$

where

$$\begin{aligned}
{Z_\alpha}^1 &= 0 \\
{Z_\alpha}^2 &= \sum_{\beta_1}\widehat{Q}_1(\epsilon_\alpha\epsilon_{\beta_1}){P_{\beta_1}}^0 \\
{Z_\alpha}^3 &= \sum_{\beta_1}\widehat{Q}_1(\epsilon_\alpha\epsilon_{\beta_1}){P_{\beta_1}}^1 + \sum_{\beta_1\beta_2}\widehat{Q}_2(\epsilon_\alpha\epsilon_{\beta_1}\epsilon_{\beta_2}){P_{\beta_1}}^0 R_2 {P_{\beta_2}}^1 \\
&\vdots \\
{Z_\alpha}^n &= \sum_{\beta_1}\widehat{Q}_1(\epsilon_\alpha\epsilon_{\beta_1}){P_{\beta_1}}^{n-2} + \sum_{m=2}^{n-1}\sum_{\beta_1\beta_1\ldots\beta_m}\widehat{Q}_m(\epsilon_\alpha\epsilon_{\beta_1}\epsilon_{\beta_2}\ldots\epsilon_{\beta_m}){P_{\beta_1}}^{n-m-1}\prod_{k=n-m+1}^{n-1} R_k {P_{\beta_{k-n+m+1}}}^{k-1}
\end{aligned} \tag{5}$$

To obtain R using iteration scheme defined by Eq. 4 one needs to choose explicit from for projection operators P_α^n. The simplest choice is to keep P_α^n fixed at its initial values, i.e.

$$P_\alpha^n = P_\alpha^0 = |\alpha\rangle\langle\alpha| \tag{6}$$

This choice of P_α^n defines the so called generalized Lee-Suzuki approach [1], or GLS. The other choice discussed in [1] is to define P_α^n in terms of model space wave functions obtained during iterations. Specifically, n-th approximation to the exact model space Schrödinger equation is

$$\left(\sum_\alpha \epsilon_\alpha P_\alpha^{n-1} + R_n\right) |\phi_\alpha^n\rangle = E_\alpha^n \, |\phi_\alpha^n\rangle \tag{7}$$

where E_α^n is the n-th aproximation to the true model space eigenvalue E_α. d Projection operators P_α^n can then be chosen as

$$P_\alpha^n = |\phi_\alpha^n\rangle\langle\tilde{\phi}_\alpha^n| \tag{8}$$

where $|\tilde{\phi}_\alpha^n\rangle$ is biorthogonal complements to $|\phi_\alpha^n\rangle$, such that $\langle\phi_\alpha^n|\,\tilde{\phi}_\beta^n\rangle = \delta_{\alpha\beta}$. This choice of projection opreators defines the generalized Lee-Suzuki method with self-consistent basis, or SCGLS. For the model calculations [1] it has been demonstrated that convergence of iterative scheme defined by Eq.4 is considerably better for SCGLS method than for GLS method.

The multi-energy $\widehat{Q}$-box can be conveniently expressed as a linear combination of the standard $\widehat{Q}$-boxes according to [1]

$$\widehat{Q}_m(\epsilon_1\epsilon_2\ldots\epsilon_{m+1}) = \sum_{k=1}^{m+1} C_k(\epsilon_1\epsilon_2\ldots\epsilon_{m+1})\,\widehat{Q}(\epsilon_k) \tag{9}$$

where

$$C_k(\epsilon_1\epsilon_2\ldots\epsilon_{m+1}) = \prod_{\substack{i=1\\ i\neq k}}^{m+1} \frac{1}{\epsilon_k - \epsilon_i} \tag{10}$$

If all $m+1$ energy arguments of $\widehat{Q}_m$ are degenerate, i.e. $e_1 = e_2 = \cdots = \epsilon_{m+1}$, expression for the multi-energy $\widehat{Q}$-box coincides with expression for the degenerate model space $\widehat{Q}$-box, i.e.

$$\widehat{Q}_m(\epsilon_1\epsilon_1\ldots\epsilon_1) = \frac{1}{m!}\frac{d^m\widehat{Q}(\epsilon)}{d\epsilon^m}\bigg|_{\epsilon=\epsilon_1} \tag{11}$$

A. Computation of Multi-Energy $\widehat{Q}$-box

To calculate $\widehat{Q}_m(\epsilon_1\epsilon_2\ldots\epsilon_{m+1})$ when $m > 1$, one should modify expression given by Eq. 9 to account for possible degeneracies in energy arguments $(\epsilon_1\epsilon_2\ldots\epsilon_{m+1})$. When energy arguments of $\widehat{Q}_m(\epsilon_1\epsilon_2\ldots\epsilon_{m+1})$ are not all different, some of the $C_k(\epsilon_1\epsilon_2\ldots\epsilon_{m+1})$ coefficients

given by Eq. 10 are individually divergent, but the resulting value of multi-energy $\widehat{Q}$-box is still finite.

To cast Eq. 9 into numerically tractable form, we start with introducing short-hand notation for arguments of multi-energy $\widehat{Q}$-box

$$(\epsilon_1 \epsilon_2 \ldots \epsilon_{m+1}) = [\,\epsilon\,]_{m+1} \tag{12}$$

Without loss of generality we assume that all d unperturbed model space energies ϵ_α are non-degenerate. When $m+1 > d$, set of energy arguments $[\,\epsilon\,]_{m+1}$ will contain degeneracies.

Further, we introduce concept of position subset S_α within set of positions of multi-energy $\widehat{Q}$-box arguments $[\,\epsilon\,]_{m+1}$. Position subset S_α is defined as containing positions of s_α energy arguments, with values of each argument equal to ϵ_α, i.e.

$$[\,\epsilon\,]_{m+1} \supset [\,\epsilon_1\,]_{s_1} \oplus [\,\epsilon_2\,]_{s_2} \oplus \cdots \oplus [\,\epsilon_d\,]_{s_d} \tag{13}$$

where

$$\sum_{\alpha}^{d} s_\alpha = m+1 \quad \text{and} \quad s_\alpha \in [0, m+1] \tag{14}$$

Assuming that $\epsilon_k = \epsilon_\alpha$ (or equivalently, that position of k-th energy argument belongs to S_α), Eq. 10 can be factorized as

$$C_k([\,e\,]_{m+1}) = C_k([\,\epsilon_\alpha\,]_{s_\alpha}) \times \prod_{\substack{i=1 \\ i \notin S_\alpha}}^{m+1} \frac{1}{\epsilon_k - \epsilon_i} \tag{15}$$

Coefficient $C_k([\,\epsilon_\alpha\,]_{s_\alpha})$ in the above equation is divergent when $s_\alpha > 1$, while the product factor is always finite. Sum of Eq. 9 will then contain partial sum of s_α individually divergent contributions of the form

$$\sum_{k \in S_\alpha} C_k([\,\epsilon\,]_{m+1})\, \widehat{Q}(\epsilon_k) = \sum_{k \in S_\alpha} C_k([\,\epsilon_\alpha\,]_{s_\alpha}) \times \prod_{\substack{i=1 \\ i \notin S_\alpha}}^{m+1} \frac{1}{\epsilon_k - \epsilon_i} \times \widehat{Q}(\epsilon_k) \tag{16}$$

Making use of Eq. 11 and recalling that for $\forall k \in S_\alpha$, $\epsilon_k = \epsilon_\alpha$, sum of Eq. 16 can be written as a finite expression

$$\prod_{\substack{i=1 \\ i \notin S_\alpha}}^{m+1} \frac{1}{\epsilon_\alpha - \epsilon_i} \times \sum_{k \in S_\alpha} C_k([\,\epsilon_\alpha\,]_{s_\alpha})\, \widehat{Q}(\epsilon_\alpha) = \prod_{\substack{i=1 \\ i \notin S_\alpha}}^{m+1} \frac{1}{\epsilon_\alpha - \epsilon_i} \times \widehat{Q}_{s_\alpha - 1}(\epsilon_\alpha) \tag{17}$$

Summing up contributions from all position subsets S_α, for multi-energy $\widehat{Q}$-box one finally obtains

$$\widehat{Q}_m([\,\epsilon\,]_{m+1}) = \sum_{\alpha}^{d} \mathrm{sgn}(s_\alpha) \prod_{\substack{i=1 \\ i\notin S_\alpha}}^{m+1} \frac{1}{\epsilon_\alpha - \epsilon_i}\, \widehat{Q}_{s_\alpha - 1}(\epsilon_\alpha) \tag{18}$$

Expression of Eq. 18 is finite and can be used in numerical calculations.

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[1] K. Suzuki, R. Okamoto, P. J. Ellis, and T. T. .S. Kuo, Nucl. Phys. **A567**, 576-590, (1994)