U(n) Dyadic Tamm-Dancoff Equation based on a Matrix-Valued Generator Coordinate

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The Tamm-Dancoff (TD) method is a standard procedure of solving the Schrödinger equation of fermion many-body systems. It, however, meets a serious difficulty when an instability occurs in the symmetery adapted ground state of the independent particle approximation (IPA) and the stable IPA ground state becomes of broken symmetry. If one uses the stable but broken symmetry IPA ground state as the starting approximation, approximate TD wave functions also become of broken symmetery. However, if we start from a symmetery adapted but unstable wave function, the convergence of the TD expansion becomes bad. To eliminate such a dilemma, in [1] we have provided a symmetry projected $U(n)$ TD equation suitable for descrption of a strong collective correlation

$$\sum_{\rho'}\sum_{(b_1j_1)<\cdots<(b_{\rho'}j_{\rho'})}\mathcal{D}^{\rho}{}_{a_1i_1\cdots a_\rho i_\rho}\mathcal{D}^{\rho'*}{}_{b_1j_1\cdots b_{\rho'}j_{\rho'}}\Big\{H^I_{KK}(p^*,p)-E^I_\omega S^I_{KK}(p^*,p)\Big\}\mathcal{C}^I_{K\omega,b_1j_1\cdots b_{\rho'}j_{\rho'}}=0, \qquad (1)$$

$$\left.\begin{aligned} H^I_{KK}(g,g)&=\langle\phi_m|U^\dagger(g)H|\Phi^I_{KK}(g)\rangle=\int D^{I*}_{KK}(s)H(g,sg)ds=H^I_{KK}(p^*,p)|\Phi_{00}(g)|^2,\\ S^I_{KK}(g,g)&=\langle\phi_m|U^\dagger(g)|\Phi^I_{KK}(g)\rangle=\int D^{I*}_{KK}(s)S(g,sg)ds=S^I_{KK}(p^*,p)|\Phi_{00}(g)|^2,\end{aligned}\right\} \qquad (2)$$

where the ρth-order covariant differential operator $\mathcal{D}^\rho_{a_1i_1\cdots a_\rho i_\rho}$ is defined as

$$\mathcal{D}^\rho_{a_1i_1\cdots a_\rho i_\rho}\equiv\mathcal{A}(e_{a_1i_1}\cdots e_{a_\rho i_\rho})+\mathcal{A}(e_{a_2i_2}\cdots e_{a_\rho i_\rho}\frac{\partial}{\partial p^\dagger_{a_1i_1}})+\cdots+\mathcal{A}(\frac{\partial}{\partial p^\dagger_{a_1i_1}}\cdots\frac{\partial}{\partial p^\dagger_{a_\rho i_\rho}}). \qquad (3)$$

The coset variable p' in the g' frame is related to the coset variable p in the g frame as

$$p'=p+q(1+e^*q)^{-1},\quad q\equiv(\bar{w}^\dagger\tilde{C})^{-1}\overset{\circ}{p}(Cw)^{-1},\quad e\equiv-p^{\mathrm{T}}(1+p^*p^{\mathrm{T}})^{-1}, \qquad (4)$$

whose transformation rule causes the non-Euclidian properties of the coset variables because the coset variables (the geminals) are quantities defined on the non-commutative $U(n)$ group, which belong to the Grassmann manifold $U(n)/(U(m)\times U(n-m))$. Equation (4) makes a cricial role to deduct group theoretically a new dyadic TD equation which is expressed in a higher order differential equation with respect to the geminal particle-hole coset variables p_{ia} [2,3], as is seen in the above formula (3).

We expand the state $|IK\omega\rangle$ as,

$$|IK\omega\rangle=\sum_\rho\sum_{(b_1j_1)<\cdots<(b_\rho j_\rho)}\Gamma^I_{K\omega,b_1j_1\cdots b_\rho j_\rho}|\Phi^\rho_{b_1j_1\cdots b_\rho j_\rho}(\breve{g})\rangle, \qquad (5)$$

which is just the dyadic TD expansion of the eigenstate of the Hamiltonian H. The $|\Phi^\rho_{b_1j_1\cdots b_\rho j_\rho}(\breve{g})\rangle$ is the TD basis with ρ particle-hole pairs in a physical fermion space. We make an approximation to the projected $U(n)$ TD expansion of (5) up to the first order and determine simultaneously both the expansion coefficients and the coset variable p in Eq. (1).

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References

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