Random phase vector for calculating the trace of a large matrix

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We derive an estimate of the statistical error in calculating the trace of a large matrix by using random vectors, and show that the *random phase vector* gives the results with the smallest statistical error for a given basis set. This result supports use of random phase vectors in the calculation of density of states and linear response functions of large quantum systems.

In the fast algorithm called *order-N methods* for calculating the density of states (DOS) and linear response functions [1–17], the Monte Carlo calculation of the trace of large matrices by using the *random vector* often plays an important role. The central limit theorem guarantees the convergence of the result as the sample number K increases. Further experience shows another useful feature called the *self-averaging effect*: the fluctuation in some physical quantities such as the energy density and linear response functions decreases as the dimension N of the Hilbert space increases [9–11,13–17]. These two types of convergence make the random vector a very efficient numerical tool.

A special class of random vectors called the *random phase vector* [7–9] have been used in later papers [11–16] without examining its efficiency rigorously. In this article, we prove by following the scheme of Ref. [10] that the random phase vector is really the most efficient random vector in a wide class of random vectors. Then we illustrate the mechanism of the self-averaging with a simple model Hamiltonian.

A *(complex)* random vector is defined by

$$|\Phi\rangle \equiv \sum_{n=1}^{N} |n\rangle \xi_n, \tag{1}$$

where $\{|n\rangle\}$ is the basis set used in the computation and ξ_n are a set of complex random variables with the identical probability distribution satisfying the statistical relations

$$\langle\langle \xi_n \rangle\rangle = 0, \tag{2}$$

$$\langle\langle \xi_{n_1} \xi_{n_2} \rangle\rangle = 0, \tag{3}$$

$$\langle\langle \xi_{n_1}^* \xi_{n_2} \rangle\rangle = \delta_{n_1 n_2}, \tag{4}$$

where $\langle\langle \cdot \rangle\rangle$ stands for the statistical average. This class of random vectors defined in one orthonormal basis set have the coefficients ζ_l in another orthonormal basis set $|l\rangle$ (for example, the energy eigenstates $|E_l\rangle$ of the Hamiltonian H),

$$|\Phi\rangle = \sum_{l=1}^{N} |l\rangle \zeta_l \tag{5}$$

that satisfy the same statistical relations as Eqs. (2)–(4): Since the coefficients in the two basis sets are related by the unitary transformation

$$\zeta_l = \sum_{n=1}^{N} \langle l|n\rangle \xi_n, \tag{6}$$

$$\zeta_l^* = \sum_{n=1}^{N} \xi_n^* \langle n|l\rangle, \tag{7}$$

the statistical relations of ζ_n are derived as

$$\langle\langle \zeta_l \rangle\rangle = \sum_{n=1}^{N} \langle l|n\rangle \langle\langle \xi_n \rangle\rangle = 0, \tag{8}$$

$$\langle\langle \zeta_{l_1} \zeta_{l_2} \rangle\rangle = \sum_{l_1=1}^{N}\sum_{l_2=1}^{N} \langle l_1|n_1\rangle \langle l_2|n_2\rangle \langle\langle \xi_{n_1}\xi_{n_2} \rangle\rangle = 0, \tag{9}$$

$$\langle\langle \zeta_{l_1}^* \zeta_{l_2} \rangle\rangle = \sum_{l_1=1}^{N}\sum_{l_2=1}^{N} \langle n_1|l_1\rangle \langle l_2|n_2\rangle \langle\langle \xi_{n_1}^*\xi_{n_2} \rangle\rangle = \sum_{n=1}^{N} \langle l_2|n\rangle \langle n|l_1\rangle$$

$$= \langle l_2|l_1\rangle = \delta_{l_1 l_2}. \tag{10}$$

In view of the energy eigenstates, the random vector contains all eigenstates with equal probability and represents the system at a very high temperature. The *orthonormality* and *completeness* of random vectors

$$\langle\langle \langle\Phi|\Phi\rangle \rangle\rangle = N, \tag{11}$$

$$\langle\langle |\Phi\rangle\langle\Phi| \rangle\rangle = \mathbf{I}, \tag{12}$$

where $\mathbf{I}$ is the identity operator, are shown by using Eqs. (2)–(4).

The most important feature of random vectors is that the statistical average of $\langle\Phi|X|\Phi\rangle$ gives the trace of X as follows:

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$$\langle\langle\langle\Phi|X|\Phi\rangle\rangle\rangle = \sum_n X_{nn} + \sum_{n_1,n_2} \langle\langle \xi_{n_1}^* \xi_{n_2} - \delta_{n_1 n_2}\rangle\rangle X_{n_1,n_2} = \sum_n X_{nn}$$

$$= \mathrm{tr}[X]. \tag{13}$$

For numerical evaluation of Eq. (13) with K samples of random vectors, the second term of (13) gives the statistical fluctuation,

$$\delta X = \frac{1}{K}\sum_k \sum_{n_1,n_2} (\xi_{n_1}^{*(k)} \xi_{n_2}^{(k)} - \delta_{n_1 n_2}) X_{n_1 n_2}. \tag{14}$$

In the special case of the Hermitian matrix $X_{n_1 n_2} = X_{n_2 n_1}^*$, it is shown that δX becomes a real number by adding the expression (14) with the subscripts n_1 and n_2 exchanged. The order of the fluctuation for a general matrix X is estimated as

$$|\delta X|^2 = \frac{1}{K^2}\sum_{k,k'} \sum_{n_1 n_2 n_3 n_4} (\xi_{n_1}^{*(k)} \xi_{n_2}^{(k)} - \delta_{n_1 n_2}) X_{n_1 n_2} (\xi_{n_3}^{(k')} \xi_{n_4}^{*(k')}$$

$$- \delta_{n_3 n_4}) X_{n_3 n_4}^*$$

$$= \frac{1}{K^2}\sum_{k,k'} \sum_{n_1 n_2 n_3 n_4} \xi_{n_1}^{*(k)} \xi_{n_2}^{(k)} \xi_{n_3}^{(k')} \xi_{n_4}^{*(k')} X_{n_1 n_2} X_{n_3 n_4}^*$$

$$+ \frac{1}{K}\sum_k \sum_{n_1 n_2 n_3 n_4} \xi_{n_1}^{*(k)} \xi_{n_2}^{(k)} (-\delta_{n_3 n_4}) X_{n_1 n_2} X_{n_3 n_4}^*$$

$$+ \frac{1}{K}\sum_k \sum_{n_1 n_2 n_3 n_4} (-\delta_{n_1 n_2}) \xi_{n_3}^{(k)} \xi_{n_4}^{*(k)} X_{n_1 n_2} X_{n_3 n_4}^*$$

$$+ \sum_{n_1 n_2 n_3 n_4} \delta_{n_1 n_2} \delta_{n_3 n_4} X_{n_1 n_2} X_{n_3 n_4}^*. \tag{15}$$

By taking the statistical average of Eq. (15) and carefully evaluating $\langle\langle \xi_{n_1}^{*(k)} \xi_{n_2}^{(k)} \xi_{n_3}^{(k')} \xi_{n_4}^{*(k')}\rangle\rangle$ by using Eqs. (2)–(4), we obtain

$$|\delta X|^2 = \frac{1}{K}\left\{ (\langle\langle|\xi_n|^4\rangle\rangle - 1)\sum_n |X_{nn}|^2 + \sum_{n_1 \neq n_2} |X_{n_1 n_2}|^2 \right\}, \tag{16}$$

where the factor $(\langle\langle|\xi_n|^4\rangle\rangle - 1)$ is factored out because we assumed the identical probability distribution for all ξ_n. The factor $1/K$ ensures the behavior $|\delta X| \sim 1/\sqrt{K}$ expected from the central limit theorem. According to the inequality

$$\langle\langle|\xi_n|^4\rangle\rangle \geq (\langle\langle|\xi_n|^2\rangle\rangle)^2 = 1, \tag{17}$$

the fluctuation becomes the smallest for a given basis set if and only if $|\xi_n| = 1$ for each n and for each sample of random variables. One of such random vectors is called the *random phase vector* [7–9] and defined by

$$|\Phi_{random\ phase}\rangle \equiv \sum_{n=1}^N |n\rangle e^{i\theta_n}, \tag{18}$$

where θ_n are a set of independent uniform random variables defined in $[-\pi, \pi]$. Obviously, the random variables $\xi_n = e^{i\theta_n}$ satisfy the statistical relations (2)–(4). Further, each sample

of random phase vectors is automatically normalized without statistical fluctuation,

$$\langle\Phi_{random\ phase}|\Phi_{random\ phase}\rangle = \sum_{n',n} e^{i(\theta_n - \theta_n')}\langle n'|n\rangle = \sum_{n=1}^N 1 = N. \tag{19}$$

This result is consistent with the observation in Ref. [10] that normalized random vectors give less statistical errors than unnormalized random vectors. It is important to note that the definition of the random phase vector $|\xi_n| = 1$ depends on the choice of the basis set. For example, let us examine a unitary transformation of the coefficients $\xi_i = e^{i\theta_i}(i = 1, 2)$ of a random phase vector,

$$\zeta_1 = \frac{1}{\sqrt{2}}\xi_1 + \frac{1}{\sqrt{2}}\xi_2, \tag{20}$$

$$\zeta_2 = \frac{1}{\sqrt{2}}\xi_1 - \frac{1}{\sqrt{2}}\xi_2. \tag{21}$$

The transformed coefficients ζ_n, of course, satisfy the relation (2)–(4), but $|\zeta_n| = 1 \pm \cos(\theta_1 - \theta_2) \neq 1$. Therefore the random phase vector in the original basis set is not a random phase vector in the new basis set. For the random phase vector in a given basis set, the fluctuation (16) reduces to a simple form [8],

$$|\delta X|^2 = \frac{1}{K}\sum_{n_1 \neq n_2} |X_{n_1 n_2}|^2, \tag{22}$$

which becomes zero for diagonal matrices as expected. Note that the fluctuation (22) depends on the choice of the basis set and that it is very important for reducing the fluctuation to choose a basis set that makes off-diagonal matrix elements as small as possible. For a Hermitian matrix X, in theory, we can choose a basis set that diagonalizes X and removes the fluctuation completely.

As a complex random vector (1), a real random vector can be defined by using real random variables with the identical probability distribution satisfying the statistical relations

$$\langle\langle\xi_n\rangle\rangle = 0, \tag{23}$$

$$\langle\langle\xi_{n_1}\xi_{n_2}\rangle\rangle = \delta_{n_1 n_2}. \tag{24}$$

Unlike a complex random vector, a real random vector in one basis set is not necessarily mapped by the unitary formation (6) to a real random vector in another basis set. However, if we stick to the original basis set, Eqs. (11)–(15) are also valid for real random vectors. Before evaluating $|\delta X|^2$ for real random vectors, let us assume for simplicity that X is a *symmetric* matrix. This does not limit the generality of our argument because any matrix X can be decomposed into the sum of the symmetric and antisymmetric parts,

$$X = \tfrac{1}{2}(X + X^t) + \tfrac{1}{2}(X - X^t) = S + A, \tag{25}$$

where X^t represents the transpose of X, and $\mathrm{tr}[X] = \mathrm{tr}[S]$ since $\mathrm{tr}[A] = 0$. Therefore if X is not symmetric then we may cal-

culate the trace of the symmetric part S. By taking the statistical average of Eq. (15) and carefully evaluating $\langle\langle \xi_{n_1}^{(k)} \xi_{n_2}^{(k)} \xi_{n_3}^{(k')} \xi_{n_4}^{(k')} \rangle\rangle$ by using Eqs. (23) and (24), we obtain

$$|\delta X|^2 = \frac{1}{K}\left\{ (\langle\langle |\xi_n|^4 \rangle\rangle - 1) \sum_n |X_{nn}|^2 + 2 \sum_{n_1 \neq n_2} |X_{n_1 n_2}|^2 \right\}. \tag{26}$$

As in the case of complex random vectors, the real random vector with the minimum fluctuation is the random vector with $\xi_n = \pm 1$, (the *random sign vector*). The random sign vector may be regarded as a random phase vector with the binary phase $\theta_n = 0, \pi$ and satisfies the normalization (19) without fluctuation. For the random sign vector in a given basis set, the fluctuation (26) reduces to a simple form

$$|\delta X|^2 = \frac{2}{K} \sum_{n_1 \neq n_2} |X_{n_1 n_2}|^2, \tag{27}$$

which is twice as large as that of the random phase vector (22). Therefore use of the random phase vector rather than the random sign vector is recommended except in special cases where the evaluation of matrix elements is substantially accelerated by using real numbers instead of complex numbers.

Let us illustrate the efficiency of various types of random vectors in the case of the Hamiltonian operator for a particle moving in the one-dimensional space under the influence of the local potential $V(x)$,

$$H = \frac{p_x^2}{2m} + V(x). \tag{28}$$

Discretizing the one-dimensional space of size $L = N\Delta x$ into N meshes $x_i = i\Delta x (i = 1, \ldots, N)$ by the finite difference method gives the Hamiltonian matrix, which is tridiagonal,

$$H_{ij} = \frac{\hbar}{2m(\Delta x)^2}(\delta_{i,j+1} - 2\delta_{i,j} + \delta_{i,j-1}) + \delta_{i,j}V(x_i). \tag{29}$$

The fluctuation $|\delta H|^2$ for random phase vectors, complex random Gaussian vectors, random sign vectors, and real Gaussian vectors is respectively estimated as 2, 6, 4, and 12 in the unit of $(\hbar/2m(\Delta x)^2)^2 N$ by using Eqs. (16) and (26), and the fact that $\langle\langle |\xi_n|^4 \rangle\rangle = 1, 2, 1$, and 3, respectively. The fluctuation of the random phase vector is six times less than that of the real Gaussian random vector, which means that the random phase vector requires six times less samplings for a given accuracy.

In contrast to the random vector dependence of the fluctuation, it is rather difficult to discuss the self-averaging effect in a general way because the effect depends on the choice of the basis set and also on the physical nature of the matrix X such as whether the quantity is intensive or extensive. Therefore let us first examine the self-averaging effect of the energy density in the above example. The fluctuation for the random phase vector becomes

$$\delta H/L \sim \left(\frac{\hbar}{2m(\Delta x)^3} \right) \frac{\sqrt{2}}{\sqrt{KN}}, \tag{30}$$

as $N \to \infty$, indicating the self-averaging behavior, $1/\sqrt{N}$. It is interesting that the local potential $V(x)$ does not contribute to the fluctuation at all in the calculation with the real space basis set. When the spectral density such as the DOS and linear response function, the dimension N of the matrix in the above estimation should be replaced by N_{eff}, the number of resonances within the spectral resolution $\Delta\omega$, e.g., $N_{eff} = \rho(\omega)\Delta\omega$ for the DOS. Therefore to reach the same accuracy we need more random vectors for higher energy resolution or lower temperature. See Ref. [10] for a more sophisticated analysis. To understand the general tendency of the self-averaging, let us assume that typical matrix elements of X have values of $O(1)$. Then the fluctuation $|\delta X|^2$ in Eqs. (16) and (26) becomes $O(N)$ for sparse or banded matrices and $O(N^2)$ for dense matrices. Since the average value, $\text{tr}[X]$, becomes $O(N)$, the relative fluctuation $\delta X/\text{tr}[X]$ becomes $O(1/\sqrt{N})$ for sparse or banded matrices and $O(1)$ for dense matrices. This means that the self-averaging is effective for sparse or banded matrices but not for dense matrices.

In summary, we have proved that the random phase vector is the most efficient choice among the random vectors with the identical probability distribution satisfying Eqs. (2)–(4). The fluctuation for the random phase vector is expressed as the sum of the square norm of the off-diagonal elements. We show also that the *smallness* and *sparseness* of the off-diagonal elements are crucial for the self-averaging effect. Accordingly our recommended recipe for efficient calculation is to choose a basis set that makes the off-diagonal elements small and sparse (or banded) as much as possible, and then use the random phase vector.

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