

Review

Problems on the Connection between Quantum and Classical Pictures (Commentary)

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量子力学的描像と古典的描像の共存における問題 (解説)

兵頭志明

Abstract

Computational observation of effective information of materials related to microscopic structures and macroscopic properties requires that the quantum mechanical picture be described systematically and consistently with classical physical pictures in advance. This problem is related to what is called the problem of measurement for a quantum mechanical system,

which has been a long-standing problem since the beginnings of quantum mechanics. Conclusion of this problem has not yet been established as common understandings. Brief explanations are presented here in relating matters in multiscale simulation of materials as well as a recently reported extrinsic method by which to avoid such problems.

Keywords

Multiscale simulation, Quantum mechanics, Classical physics, Problem of measurement for a quantum mechanical system, Density matrix representation, Properties of wavefunction

要 旨

材料における微視的な構造と巨視的な挙動とを関連付けて計算予測を行うためには、量子力学的な描像と古典物理学的な描像とが統一的に描かれる必要がある。この問題は、量子力学創成期より持ち越されてきたいわゆる「観測問題」と深く関

わる問題であり、未だ共通の認識が得られていない。材料のマルチスケールシミュレーションに関わる問題点と最近得られた形式的な回避策についての簡単な解説を行う。

キーワード

マルチスケールシミュレーション, 量子力学, 古典物理学, 量子系における観測問題, 密度行列の表現, 波動関数の性質

In order to realize the process of hierarchical material simulation combined with quantum mechanical scales, we have to consider the connection of quantum and classical subsystems within a region of interest. A quantum system is basically described by wavefunction and shows what is called "long-range correlation" originating from the coherent character of wavefunction.¹⁾ A classical system, on the other hand, can be described without information concerning the wavefunction and shows no coherency in the sense of the quantum theory. We must connect these two different types of subsystems consistently. It is well-known that the observation of a quantum mechanical system using a macroscopic device shows the problem of measurement for a quantum mechanical system, which is a long-standing problem in quantum theory.²⁾ This problem introduces several types of famous paradoxes in the fundamental theory of quantum mechanics.^{3, 4)} A typical paradox is shown in **Fig. 1**. Such paradoxes do not appear without any measurement by macroscopic apparatus. In other words, the interaction of a macroscopic apparatus and a quantum system give rise to such paradoxes. The same problem also appears in a quantum composite system having a macroscopically large scale.⁵⁾ The appearance of this serious and complicated problem originates from the connection of quantum and classical systems.

The fundamental characteristics of macroscopic systems are that the system has large degree of freedom and irreversibility. If we describe a system having a large degree of freedom by wavefunction, we can find many states constructed by wavefunctions with different phases. Each wavefunction is coherent in each state, but the magnitudes at arbitral spatial position are incoherently correlated. The locality of the spatial correlation is therefore obviously dependent on the degree of freedom for the objective system. If the spatial correlation is local in the description by wavefunctions, a classical description is expected to apply for this system. On the other hand, usually quantum systems can be described reversibly because there are definable contours of motions for constructing subsystems. This situation is equivalent to a classical system with a few amount

of degree of freedom. For example, the equation of motion is completely describable for a classical system constructed by a few point particles. Contrary of this situation, a system having an extremely large number of components cannot be described reversibly. The term long-range time-scale has meaning in a system of irreversibility, because that the correlation of motion on a short-range time-scale will be smeared out for motions in a system having a large degree of freedom. The

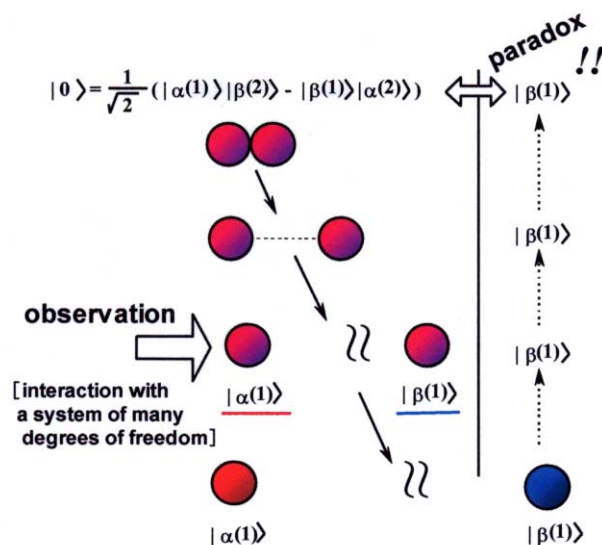


Fig. 1 Schematic view of a typical paradox in the problem of measurement for quantum mechanical systems. This is Bohm's version of the Einstein-Podolsky-Rosen Paradox. The entire system is constructed by two subsystems, 1 and 2. Each subsystem has two eigenstates, α and β . The initial state of this system was set as the full contact condition. The wave function for this initial state $|0\rangle$ is a familiar form in quantum mechanics, as shown at the top of the figure. If the result of an observation, applied at several times after the beginning of separation into two subsystems, was that subsystem 1 was in the α state, we can know automatically that subsystem 2 is in the β state. Observation by macroscopic apparatus corresponds to this microscopic system interacting with a system of large degree of freedom. A possible explanation for this result is that subsystem 1 has been in the α state and subsystem 2 has been in the β state since the time at the beginning of separation. This means that subsystem 2 has already been defined as being in the β state since the beginning of separation without any interaction with external systems. However, this is inconsistent with the initial condition, and therefore concludes a paradox.

memories of contours of motion disappear after smearing, and the system cannot return to exact past states reversibly. A statistic treatment should be applied to such a system for analysis. Although this is also true for a quantum system having a large degree of freedom, conventional quantum theory does not include irreversibility. Irreversibility is an essential characteristic of a macroscopically large system. Interaction between a classical macroscopic system having a large degree of freedom and a quantum system having a small degree of freedom should be described by different theories for what are essentially different physical situations. Such complexities exist in problems concerning the interaction of a macroscopic apparatus and a quantum system, and also in a quantum composite system having a macroscopically large scale.

Recently, it was reported that classically definable characteristics of a macroscopic quantum mechanical subsystem can be safely (without any paradox) reproduced by averaging the states on a corresponding subsystem over the generalized density matrix or the statistical operator.⁵⁾ The quantum mechanical coherency is removed by this averaging process. In other words, the averaging in a density matrix representation can reproduce a classically definable decoherent state. The condition to satisfy decoherency is such that the subsystem contains a statistically large degree of freedom. Although the density matrix representation is familiar in quantum chemistry,⁶⁾ less consideration has been given in relation to the description of quantum mechanical composite systems.

When the total wavefunction, $|\psi_T\rangle$, of a focused system is expanded in a linear combination of given basis functions, $\{|\chi_i\rangle\}$;

$$|\Psi_T\rangle = \sum_i A_{T,i} |\chi_i\rangle, \dots \dots \dots (1)$$

the density matrix, $\hat{\rho}_T$, can be expressed as

$$\begin{aligned} \hat{\rho}_T &= |\Psi_T\rangle\langle\Psi_T| \\ &= \sum_i \sum_j A_{T,i} A_{T,j} |\chi_i\rangle\langle\chi_j|, \dots \dots \dots (2) \end{aligned}$$

Using this expression, Eq.(2), the expectation value of any kind of observable, \hat{O} , can be obtained as

$$\begin{aligned} \langle\hat{O}\rangle &= \text{Tr}^{(T)}\{\rho_T \hat{O}\} \\ &= \sum_k |A_{T,k}|^2 \langle\chi_k | (\hat{\rho}_T \hat{O}) | \chi_k\rangle \\ &= \sum_k |A_{T,k}|^2 A_{T,k} \sum_j A_{T,j} \langle\chi_j | \hat{O} | \chi_k\rangle \dots \dots \dots (3) \end{aligned}$$

Here $\text{Tr}^{(T)}\{X\}$ is the trace operation, which means the summation over diagonal elements of the given observable X in matrix form. This operation averages out the quantum mechanical uncertainty parts in the full expression of the system, i.e., the parts describing the quantum mechanical correlations. If we can take the basis functions, which is diagonalizing the state of the total system, the coefficients in Eqs.(1)-(3), $\{A_i\}$, can be replaced by unity. These are familiar expressions in the fundamental quantum mechanics.⁷⁾ Machida chose a composite system consisting of N subsystems having arbitrary spin to investigate a generalized Einstein-Podolsky-Rosen (EPR) problem,³⁾ and Machida and Miyoshi considered the results of the measurement of various components of spin in the k th subsystem at an arbitrary time after that at an initial state.⁵⁾ If the total wavefunction is expressed by a linear combination of the products of wavefunctions of each subsystem, $s, |\mu, i_s\rangle$;

$$|\psi_T\rangle = \sum_{i_1, i_2, \dots, i_N} C(i_1, i_2, \dots, i_N) |\mu, i_1\rangle |\mu, i_2\rangle \dots |\mu, i_N\rangle, \dots (4)$$

instead of Eq.(1), the density matrix of this entire system is

$$\begin{aligned} \hat{\rho}_T &= |\Psi_T\rangle\langle\Psi_T| \\ &= \sum_{i_1, i_2, \dots, i_N} \sum_{j_1, j_2, \dots, j_N} C(i_1, i_2, \dots, i_N) C^*(j_1, j_2, \dots, j_N) |\mu, i_1\rangle\langle\mu, j_1| \\ &\quad \otimes |\mu, i_2\rangle\langle\mu, j_2| \otimes \dots \otimes |\mu, i_N\rangle\langle\mu, j_N| \dots \dots \dots (5) \end{aligned}$$

Here, the abbreviation, ${}_p x_q$, introduced by Motoyoshi et al.,⁸⁾ denotes a set of $x_p, x_{p+1}, \dots, x_{q-1}, x_q$, where p and q are integers. The states $|\mu, i_k\rangle$ are given by the simultaneous eigenstates of the eigenvalue equations for the spin states in k th subsystem and μ denotes spatial components of the spin, (x, y, z) . The symbol \otimes indicates the matrix product (all of the combinations of elements in each matrix should be counted individually in this operation). Taking the partial trace of $\hat{\rho}_T$ over the k th subsystem gives

$$\begin{aligned}
& \text{Tr}^{(T)}\{\hat{\rho}_T(\mu)\} \\
&= \hat{\rho}_{1,2,\dots,k-1,k+1,\dots,N}(\mu) \\
&= \sum_{\mathbf{i}_N} \sum_{\mathbf{j}_N \neq \mathbf{k}_N} C(\mathbf{i}_N) C^*(\mathbf{j}_N) |\mu, \mathbf{i}_1\rangle \langle \mu, \mathbf{j}_1| \\
&\quad \otimes |\mu, \mathbf{i}_2\rangle \langle \mu, \mathbf{j}_2| \otimes \dots \otimes |\mu, \mathbf{i}_{k-1}\rangle \langle \mu, \mathbf{j}_{k-1}| \\
&\quad \otimes |\mu, \mathbf{i}_{k+1}\rangle \langle \mu, \mathbf{j}_{k+1}| \otimes \dots \otimes |\mu, \mathbf{i}_N\rangle \langle \mu, \mathbf{j}_N|. \quad (6)
\end{aligned}$$

Adopting this operation over all subsystems except for the k th subsystem,

$$\begin{aligned}
& \hat{\rho}_k(\mu) = \text{Tr}^{(1,2,\dots,k-1,k+1,\dots,N)}\{\hat{\rho}_T(\mu)\} \\
&= \sum_{\mathbf{i}_N} \sum_{\mathbf{j}_k} C(\mathbf{i}_N) C^*(\mathbf{j}_k) |\mu, \mathbf{i}_k\rangle \langle \mu, \mathbf{j}_k| \\
&\quad \dots \dots \dots (7)
\end{aligned}$$

is obtained as the density matrix of the k th subsystem. Here, $\hat{\rho}_k(\mu)$ is expressed explicitly by the basis functions of the k th subsystem only, and the influences of the other subsystems are implicitly expressed in the coefficients, $C(\mathbf{i}_N) C^*(\mathbf{j}_k)$. There are no remaining coherent terms like cross terms of k th and k' th ($k' \neq k$) basis functions. The result of Eq.(7) does not claim that the quantum mechanical pure state of the k th subsystem represents the entire system in the measurement process. The state in the last step in Fig. 1, for example, should be considered as one of the possible results after the measurement, and the states in all the steps should be understood in the expression of mixed states. This means that the paradox, like EPR type paradox, is avoidable in the measurement of a quantum mechanical subsystem, which is interacting with its environment in a composite entire system. Therefore, averaging the states on environment subsystems over the density matrix representation can be considered to reproduce safely (without any paradox) corresponding classically definable characteristics (the results of measurement) of an entire system. Equation (7) is still a general and conceptual formula, and can not be applied to the explicit calculation in the present form. It is necessary that future investigations should be continuously progressed. However, the results

introduced by Eq. (7) are valuable for the process of hierarchical material simulation combining with quantum mechanical scales.

When we divide a system into an objective microscopic subsystem and an environmental subsystem, the same procedure in the problem of a quantum composite system can be applied. Although explicit formulation for averaged states of a divided subsystem over a density matrix representation has not yet been derived, it can be correctly expected that the subsystem with averaged states is safely reproducible by means of classical expressions. Therefore, it is expected that the structure on a subsystem can also be defined by a classical description, which is suitable for noticed phenomena and is independent of quantum mechanical descriptions. The electronic structure is transformed into the electron distribution describable by the density matrix. Once the electrostatic and/or the electrodynamic properties on the corresponding subsystem are defined within the mesoscopic environment structure, the electrostatic potential reproduced by these properties can be added to the Hamiltonian of the focused microscopic subsystem. The long-range property of electrostatic potential requires the effects of environmental mesoscopic structure to be explicitly considered. The process of hierarchical material simulation with quantum mechanical scales can therefore be implemented using averaged properties over a density matrix representation on a meso-scale structural calculation.

On a macroscopic scale that is sufficiently large compared to the characteristic spatial frequency of the inhomogeneity, the inhomogeneous structure is painted over the slowly varying structure (see Fig. 2). A focused material can be considered as being nearly homogeneous on such a scale. However, the microscopic condition on the scale of a small molecule is still in the inhomogeneous environment. A part of the material is influenced by the structural inhomogeneity varying with the characteristic spatial frequency. The restriction condition should be defined by the macroscopic boundary condition of the noticed material. The electronic state on a microscopic scale, on the other hand, should be defined within the inhomogeneous environment. Therefore, the restriction condition and the

electronic state should be defined individually on each suitable scale, and the information on each scale should be transformed between each of them. In order to realistically perform such a process, we should define the process for describing the systems of different spatial frequencies simultaneously. Such a process of definition has already been realized by the multi-grid technique in numerical calculations for many kinds of differential equations with finite-size grids.⁹⁾ Another possible process for simultaneously describing systems of different spatial frequencies has been proposed as the “wavelet” method.¹⁰⁾ Although the numerical calculation technique is already guided by the multi-grid and/or the wavelet schemes, a serious problem still remains with the cooperation of macroscopic and microscopic definitions. This problem usually appears in connecting quantum and classical subsystems, as was discussed above. It was seen that the process of hierarchical material simulation combined with quantum mechanical scales can be implemented using averaged properties over a density matrix representation on a meso-scale

structural calculation.

The problem of measurement for a quantum mechanical system discussed here is a well-known long-standing problem in quantum theory. Most chemists and physicists in the material science field, however, have paid little attention to this problem. A part of the reason of this state seems to be that this problem has been a rather philosophical problem without any practical meaning for long time. Main reason, however, can be guessed as that the quantum mechanical description gives sufficiently accurate predictions that are practical for several types of problem in material science. The consideration of such a complicated serious philosophical problem seems impractical. For quantum mechanical systems, the theory has given accurate results for many types of phenomena and no bankruptcy of the theory has been found. With the advance of material science in new areas of research, typically nanoscience and nano-technology, hierarchical concepts for the basis of theoretical treatment have gained interest. When considering a quantum mechanical material system using a hierarchical concept, the

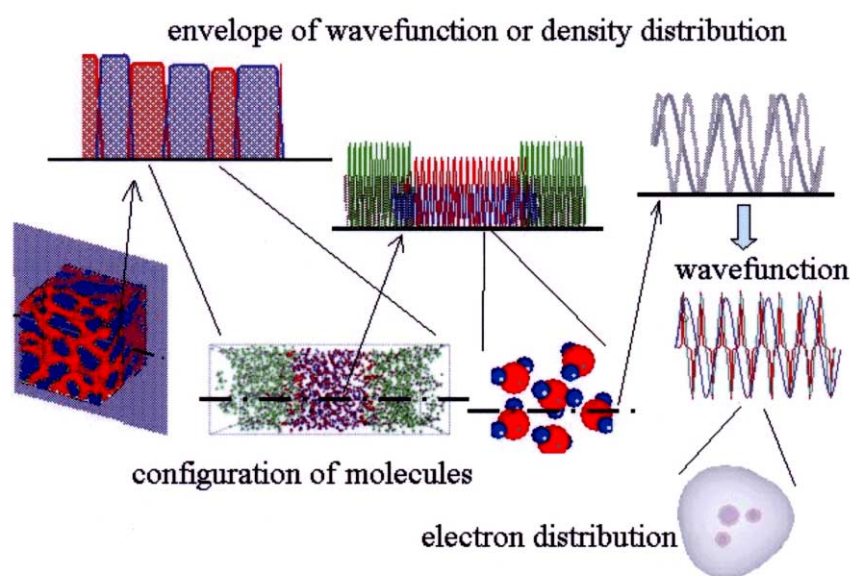


Fig. 2 Various scales of spatial frequencies of inhomogeneity. The frequency patterns in wavefunction are very complicated because a large number of states having different phases exist in each scale of the structures. Therefore, for simplicity, the frequency patterns are instead illustrated in the envelope of the wavefunctions. The same patterns can be seen in the density distribution. The explicit structure, shown here, is obtained from a polyelectrolyte-water nano-composite system reported in another article in the present issue.^{a)}

a) Yamamoto, S. : R&D Rev. of Toyota CRDL, **38**-1 (2003), 10

problem of measurement for a quantum mechanical system must be addressed. This problem seems indispensable in new fields of science. Although a consensus on the quantum measurement problem has not yet been well established, it can be possible to avoid some paradoxical problems from hierarchical investigations.

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