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Technical Report

An Application Study of Quantum Computers to Optimization of Production Planning

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Abstract

Quantum computers are attracting great attention as they are expected to solve certain problems better than classical computers. Nippon Steel Corporation is considering applying quantum computers to optimize logistics and production planning, and to conduct quantum chemical calculations. This article introduces an optimization of logistics and production planning, as an example of problems that classical computers cannot solve. A simplified problem is derived and solved with a quantum annealing machine by D-wave and gate-based quantum computers by IBM. Today's quantum hardware involves constraints on the number of qubits and influence of noise, which limits the scale of the problem reached by quantum hardware by themselves. We adopted methods where quantum hardware was combined with classical computers and confirmed that optimal solutions are obtained.

1. Introduction

In recent years, quantum computers have been attracting attention as the next generation of high-speed computers. In classical digital computers, each bit normally has two states: 0 or 1. But quantum computers allow the superposition of states as taught by quantum mechanics. It may be possible to speed up calculations by calculating a large number of states in parallel and devising an algorithm that leaves the desired state at the end.[1] Quantum computers are expected to find use in many fields, such as combinatorial optimization problems, quantum chemical calculations, and machine learning. There are various methods for constructing qubits, such as superconductivity, ion traps, light, and cold atoms. Their development is being actively promoted around the world.

There are two main methods for quantum computers: the quantum gate-based method and the quantum annealing method. The quantum gate-based method performs calculations by combining quantum versions of the logical operations used in current classical computers and is versatile. However, qubits are easily affected by noise from outside the system. It is necessary to implement a mechanism to correct errors caused by noise. Including the number of qubits required for error correction, it has been pointed out that approximately 1 million qubits would be required for a practical quantum computer. However, the level currently in practical use is several hundred qubits. This has motivated researchers to explore the utility of quantum hardware without quantum error correction techniques, giving rise to the noisy intermediate-scale quantum (NISQ) era. On the other hand, the quantum annealing method is specialized to solve problems like combinatorial optimization problems. The objective function to be minimized can be described by an Ising model (a model that consists of lattice points that take two states and that considers only the interaction between adjacent lattice points). The annealing method (also called the simulated annealing method) is available as a search method for good solutions inspired by annealing in metallurgical engineering. The quantum annealing method is a quantum version of the annealing method.[2, 3] The quantum annealing method is less versatile than the quantum gate-based method but is superior to the quantum gate-based method in terms of the number of qubits available. For example, the Canadian company D-Wave Systems, Inc. has recently achieved an order of magnitude of more qubits (approximately more than 5 000 qubits) than

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the quantum gate-based method. For limited classes of problems, the quantum annealing method has the potential to solve larger problems. In addition, the pioneering efforts of D-Wave have prompted the development of technology that can solve Ising-style optimization problems at high speed with classical computers.[4–7)]

Nippon Steel Corporation is considering production planning and logistics optimization, and quantum chemical calculation as the fields where quantum computers can be used. Regarding the optimization of production planning and logistics, the steel industry is characterized by a breakdown-type manufacturing method in which a large number of products are made from several types of raw materials. Optimization of production planning, such as grouping and processing sequence determination in each process, is important.[8)] Additionally, since manufacturing involves a number of processes, from blast furnace to surface coating, it is also important to optimize logistics, including the transportation of intermediate products within the steelworks and the transportation of products from the steelworks to the customer. These optimization efforts involve the problem of a so-called combinatorial explosion in which as the number of objects to be optimized increases, the number of possible solutions increases dramatically and requires an enormous amount of calculation time. Through various efforts, optimization calculations for single process have almost reached a practical level when it comes to optimizing production plans within the steelworks.[8)] However, even the latest classical computers are often unable to provide production planning when multiple processes are involved. So, there are great expectations for quantum computers. This technical paper reports the results of attempts made to solve a two-process production planning optimization problem using both the quantum annealing method and the quantum gate-based method. The problem setting is described in Chapter 2, the results of the quantum annealing method are presented in Chapter 3, the results of the quantum gate-based method are presented in Chapter 4, and the summary is described in Chapter 5.

Quantum chemical calculations are not described in detail in this technical paper. Nevertheless, Nippon Steel has applied the first-principles calculation method to clarify the reaction functions in the iron manufacturing process and to design molecules. One example is the clarification of principles and rules that govern the macroscopic properties of products, such as the behavior of microscopic precipitates in steel and interactions between atoms[9, 10)]. Another is the separation and recovery of CO_2[11)]. We expect that quantum computers will improve the calculation accuracy, compared with the current classical computers. As a trial of quantum computer application to the electronic state calculation of iron-containing systems, we performed the energy calculation of the bcc and fcc structures of iron, which was difficult to perform with classical computers.[12)] Although only two qubits approximated the subject system, the method to reduce the effects of noise was also employed. We confirmed that the results of calculations by a real gate-based quantum computer agreed well with the results of calculations by a classical computer.

2. Overview of Two-Process Production Planning Optimization Problem

Production in the steel industry involves multiple processes. As shown in **Fig. 1**, the steel industry is characterized by a breakdown-type production structure in which semi-finished products are divided as they move to the downstream processes. For example, the unit throughput is about 300 tons in the upstream steelmaking process and about 10 tons in the downstream coating process. In the case of low-volume and high-mix, as practiced at Nippon Steel, one processing batch in an upstream process includes different semi-finished products and products that are divided in a downstream process. The grouping of semi-finished products and products between each process must be optimized. This optimization problem is solved under multiple constraints. For example, two products or semi-finished products with significantly different processing or specifications (chemical composition, width, thickness, etc.) cannot be grouped. The grouping of two products or semi-finished products that undergo similar processing is desirable from the viewpoints of quality, productivity, and production cost. However, too much grouping means the accumulation of a certain number of other products with similar processing. This may lead to inventory accumulation and delayed delivery. Optimizing the trade-off between grouping and delivery compliance is difficult, even within a single process. The problem becomes even more difficult when two or more processes are involved. New technologies such as quantum computers are needed in this sense.

We created an example of a production planning optimization

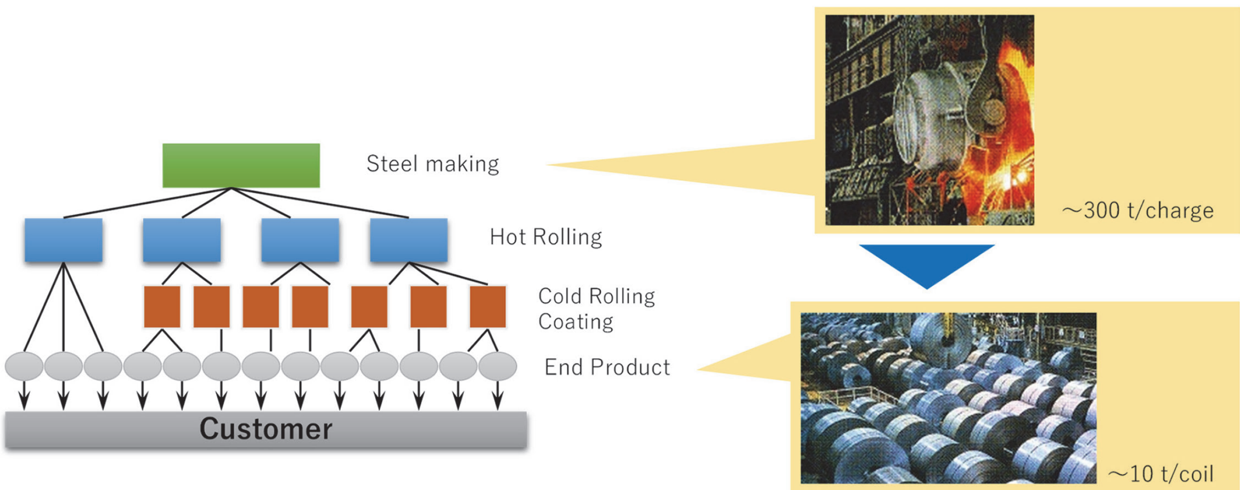

Fig. 1 Features of steel production structure: break down structure

Table 1 Available time slots (gray colored) in optimization of two-process production planning problem[13)]

k	1	2	3	4	5	...	N	$N+1$	...	$N+\Delta$
Process 1										
Process 2									…	

problem involving two processes and attempted to solve it using a quantum computer. The outline and assumptions are as follows. This example problem generally belongs to the job shop scheduling type of problem (**Table 1**).

(1) N products are processed in the order of processes 1 and 2.
(2) The processing time is the same for all products and both processes. If the time is normalized by this processing time, the problem can be regarded as placing N products into the time slots prepared for each of the processes 1 and 2.
(3) Disregard the delivery time from process 1 to process 2.
(4) If a product is processed in process 1 at the time k, it can be processed in process 2 at the time k or after.
(5) Considering productivity, it is assumed that N products are processed continuously in both process 1 and process 2 without any rest time in between.
(6) Without any loss of generality, we may say that process 1 starts processing at time 1 (the first time slot). On the other hand, process 2 may start at a later time. Therefore, ($N+\Delta$) time slots are prepared. The size of the processing time difference Δ between the two processes is determined by the delivery date associated with each product.
(7) Delivery dates, attributes for process 1, and attributes for process 2 are defined for all products. An attribute refers to the type of chemical composition, shape, manufacturing conditions, etc., that indicate compatibility when sequentially processing the previous and subsequent products. When products with different attributes are processed successively, the cost of changing the attributes is added.
(8) The goal of this problem is to determine the optimal product processing order while considering the trade-off between manufacturing products with the same attributes together in each process and meeting delivery deadlines.

3. Solution Using Quantum Annealing Machine[13)]

We prepared two problems with the number of products $N=5$ and 8 and attempted to solve the problems by using a D-Wave quantum annealing machine (model: 2000Q™[14)]) equipped with superconducting qubits. In quantum annealing, similar to the annealing method using a classical computer, a bold search (corresponding to a high temperature) is performed in the initial stage of the search period. An optimal solution with the minimum energy (corresponding to a low temperature) is pursued in the later stage of the search period. At the current level of technology, it is not always possible to reach the optimal solution due to the large influence of noise from external systems. It is better to think of the annealing machine as a sampler that probabilistically generates various approximate solutions.[15)]

The D-Wave2000Q™ has approximately 2 000 physical qubits implemented in a chimera graph structure. The number of physical qubits that can be directly combined with one physical qubit is limited to 6. To solve optimization problems such as the one of the present study, where decision variables interact with almost all other decision variables, redundant physical qubits are required. The number of qubits required for M decision variables increases by the order of M^2.

To reduce the number of decision variables as much as possible, we decided to first find the optimal solution by fixing the processing time difference Δ between the two processes during the quantum annealing calculation and then search for the optimal solution while changing the processing time difference Δ in the outer loop.

For details, refer to Reference 13). When expressed in the quadratic unconstrained binary optimization (QUBO) format that can be minimized by a quantum annealing machine, the objective function becomes as follows:

$$E(\boldsymbol{x}) = \sum_{p=1}^{2} Cost_p(\boldsymbol{x}_p) + \rho \sum_{p=1}^{2} Penalty_p(\boldsymbol{x}_p) + \rho' \sum_{i=1}^{N} \sum_{s,s'=1}^{N} \Theta(s-(s'+\Delta))\, x_{1,i,s}\, x_{2,i,s'} \,. \tag{1}$$

The decision variable $x_{p,i,s}$ takes 1 if the product i ($i=1, 2, ..., N$) is processed s-th ($s=1, 2, ..., N$) in the process p ($p=1, 2$) and 0 otherwise. The first term is cost and includes the cost when attributes change and the cost when the delivery date is not exactly met. The second term represents the penalty in the processes 1 and 2. The third term indicates the inter-process penalty imposed when process 2 is performed before process 1.

In the case of the problems created this time, the $N=5$ problem can be solved by fixing the processing time difference Δ between the two processes. The D-Wave2000Q™ still cannot solve the $N=8$ problem. Therefore, as a method for reducing the number of variables further, we decided to solve the original problem by dividing it into smaller problems by applying the Lagrangian decomposition and coordination (LDC)[16, 17)]. Specifically, as shown in Eq. (2) below, the Lagrangian undetermined multiplier λ_i was introduced for the inequality constraint regarding the processing order between the processes. Then, the objective function was divided into two for processes 1 and 2, as shown in Eqs. (3a) and (3b), respectively.

$$E_{\mathrm{LDC}}(\boldsymbol{x}) = Cost(\boldsymbol{x}) + \rho \sum_{p=1}^{2} Penalty_p(\boldsymbol{x}_p) + \sum_{i=1}^{N} \lambda_i (t_{1,i} - t_{2,i}) \,. \tag{2}$$

$$E_1(\boldsymbol{x}_1) = Cost_1(\boldsymbol{x}_1) + \rho\, Penalty_1(\boldsymbol{x}_1) + \sum_{i=1}^{N} \lambda_i t_{1,i} \,, \tag{3a}$$

$$E_2(\boldsymbol{x}_2) = Cost_2(\boldsymbol{x}_2) + \rho\, Penalty_2(\boldsymbol{x}_2) - \sum_{i=1}^{N} \lambda_i t_{2,i} \,. \tag{3b}$$

In the original QUBO model, the number of variables required for the number of products N was $2N^2$ (with the assumption that Δ was fixed). The problem division reduces the number of required variables to N^2. In this study, the number of processes is 2. More generally, when the number of processes is N_p, the number of required variables is reduced from $N_p \times N^2$ to N^2.

Figure 2 illustrates the processing algorithm when the problem was divided by LDC into two for processes 1 and 2. The quantum annealing machine is responsible only for solving the problem divided into two for processes 1 and 2 (the thick-bordered step in Fig. 2). The other steps are handled by a classical computer in a hybrid manner. The algorithm is one commonly used in LDC, but we added a twist that takes advantage of the characteristics of quantum annealing in order to calculate a feasible solution. When obtaining a feasible solution with normal LDC, a search is performed using a heuristic method while focusing on Lagrangian undetermined multipliers that correspond to constraint equations that violate the constraints. Current quantum annealing machines are samplers that probabilistically generate various approximate solutions. In this study, we took advantage of this immature nature of quantum annealing machines. That is, we adopted a method of searching for a better feasible solution by attempting to combine solution candidates that lower the objective function within each process. These solution candidates were selected from among 1 000 candidates produced for each of processes 1 and 2.

The above method was applied to the N=5 and N=8 problems. The results are shown in **Tables 2** and **3**, respectively (average values of 5 repeated experiments). For N=5, the results obtained by solving without using LDC and with using D-Wave2000Q™ alone are also shown for comparison. In this problem, there is a trade-off between delivery time and attribute change. The balance of weights with respect to these costs is changed in three ways (w_g=4, 10, 100; the larger the w_g is, the higher the cost of changing the attributes). The error in Tables 2 and 3 is the relative error with respect to the determined optimal energy value (solved using a classical computer). LDC reached the optimal solution under all conditions, including not only N=5 but also N=8, which cannot be solved by the D-Wave2000Q™ alone. Even with the D-Wave2000Q™ alone, the optimal solution was reached in all trials except for w_g=4. Tables 2 and 3 also show the calculation time results. t_{LDC} is the total computation time taken by LDC. t_{cloud} is the cloud calculation time, including communication time with the cloud and the time related to the D-Wave2000Q™ including quantum annealing. t_{unemb} is the time required for unembedding*1. As shown in Fig. 2, LDC has a loop structure involving the updating of the Lagrangian undetermined multipliers and uses the D-Wave2000Q™ many times, resulting in long calculation times.

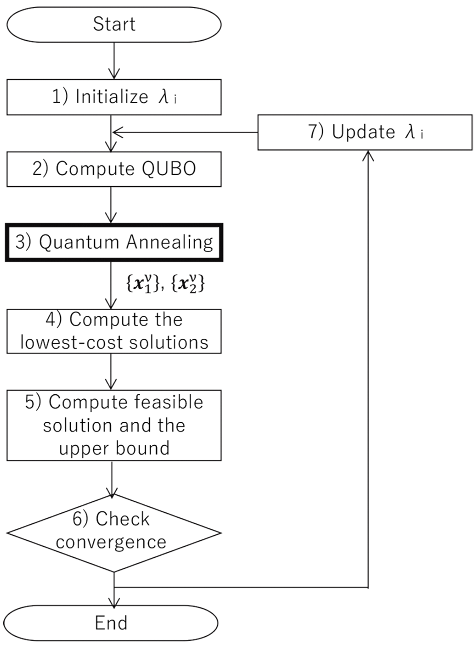

Fig. 2 Algorithm based on Lagrangian decomposition and coordination (The bold frame represents the part calculated by quantum annealing.)

This study was conducted around 2020, using the state-of-the-art model at that time, the D-Wave2000Q™. Since then, a new model called the Advantage™ has been released by D-Wave[18]. It has approximately 5 000 qubits. Each physical qubit can directly connect to up to 15 other physical qubits. However, for problems like the one addressed in this study, where the number of decision variables scales quadratically with the number of products N, reducing the problem size by dividing the problem into smaller ones for each process is still important.

4. Problem Solving Using Gate-Based Quantum Computer[19)]

To demonstrate the effectiveness of quantum computers using a current noisy intermediate-scale quantum (NISQ) computer, it is necessary to make the size (depth) of quantum circuits as short as possible in order to complete the calculation while maintaining the quantumness. A variational quantum algorithm (VQA)[20)] is proposed as a means to address this issue. As shown in **Fig. 3**, a quantum circuit is expressed by a parameter. Using energy minimization as the objective function, the parameter is optimized in a hybrid quantum-classical loop to form a desired quantum state. The VQA can be used not only for combinatorial optimization problems such as the one in this study, but also for a variety of applications, including quantum chemical calculation and machine learning.

We compared four different VQAs using an IBM superconducting quantum computer for the example problem of optimizing a production plan over two processes described in Chapter 2. The four

*1 Embedding is the process of mapping a QUBO-style problem to the chimera structure, including the redundant physical qubits required due to the large number of interactions between variables. Unembedding is the inverse operation of embedding, where the results of quantum annealing are converted into the original QUBO format.

Table 2 Average relative error and computation times in five-product problem[13)]

	w_g = 4				w_g = 10				w_g = 100			
	Error	t_{cloud}	t_{unemb}	t_{LDC}	Error	t_{cloud}	t_{unemb}	t_{LDC}	Error	t_{cloud}	t_{unemb}	t_{LDC}
Hybrid LDC	0.0	17.05	4.38	25.45	0.0	18.32	4.17	26.45	0.0	16.89	4.17	25.07
D-Wave 2000Q	0.07	1.74	0.49	–	0.0	2.32	0.49	–	0.0	2.24	0.49	–

Table 3 Average relative error and computation times in eight-product problem[13)]

	w_g = 4				w_g = 10				w_g = 100			
	Error	t_{cloud}	t_{unemb}	t_{LDC}	Error	t_{cloud}	t_{unemb}	t_{LDC}	Error	t_{cloud}	t_{unemb}	t_{LDC}
Hybrid LDC	0.0	25.60	13.71	50.90	0.0	47.67	27.07	97.65	0.0	24.79	13.97	50.23
D-Wave 2000Q	–	–	–	–	–	–	–	–	–	–	–	–

methods are a quantum approximate optimization algorithm (QAOA)[21], a variational quantum eigensolver (VQE)[22], a variational quantum imaginary time evolution (VarQITE)[23], and a filtering variational quantum eigensolver (F-VQE)[24].

The QAOA is based on quantum adiabatic calculations like quantum annealing. It solves the energy expression (Hamiltonian) of a multi-process planning optimization problem by reflecting it in a quantum circuit. Still, the circuit tends to become deeper compared to the VQE. The VQE is a simple method of executing the VQA mentioned above, but the Hamiltonian is not considered in the parameters representing the quantum circuit. The search for the optimal combination is left to a classical computer that performs the parameter search. Based on the VQE, the VarQITE updates the parameters according to an imaginary time evolution scheme in which the state is evolved in imaginary time according to the Schrödinger equation to obtain the ground state. By operating a filter to reduce the high-energy state components and increase the ground state components, the F-VQE aims to quickly and stably converge the state which is determined by applying a quantum circuit to the state.

A two-process production planning optimization problem was created with the number of products $N=20$. Even if the time difference is fixed, about $2\times20^2=800$ variables are required. However, due to the limited number of qubits in current hardware and their noise levels, it is not feasible to handle this problem directly using quantum computation. As a result, a classical computer was employed in advance to solve this $N=20$ problem. After finding the optimal solution using the classical computer, we further investigated

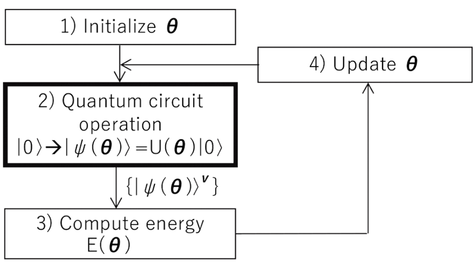

Fig. 3 Overview of variational quantum algorithm (The bold frame represents the part calculated by a quantum computer.)

whether it was possible to determine correct answers for certain variables through optimization techniques without prior knowledge of these correct answers.

First, we compared the four VQA methods mentioned above through an experiment set to optimize five variables. We found that the F-VQE converged quickly and had a high probability of sampling the optimal solution. Next, using this F-VQE, we investigated scaling by increasing the problem size (by increasing the number of variables for which the correct answer was unknown). **Figure 4** shows the changes in energy and probability of sampling the correct answer with respect to the number of parameter updates for each problem size. In all cases, the energy approaches the minimum value corresponding to the optimal solution. The probability of sampling the correct answer is 80% when the problem size is ten variables, 70% when the problem size is 12 variables, 60% when the problem size is 16 variables, and 25% when the problem size is 23 variables. Considering the current classical computer power, 23 variables are still small, and the sampling probability of 25% is not that high. But even with noise and errors in the hardware, it is possible to find the optimal solution from a search space as large as 2^{23}. It turned out that the solution can be found with a sampling probability of a significant order.

5. Summary

Among the many complex production and logistics planning optimization issues that exist within Nippon Steel, we focused on a production planning optimization problem that spans multiple processes as a problem that is expected to make a breakthrough through the use of quantum computers. We attempted to solve the problem by using a quantum annealing machine and a gate-based quantum computer. Both types of machines currently have issues such as limitations on the number of qubits that can be used effectively and noise effects. Therefore, as hybrid methods with classical computers, the Lagrangian decomposition coordination method was used for the former, and the VQA was used for the latter. As a result, we confirmed that the optimal solution could be reached in either case. The development of quantum computers is being actively pursued both domestically and internationally. We hope that future advances in hardware will make it possible to solve larger-scale problems and that this technology will be applied to optimization problems that

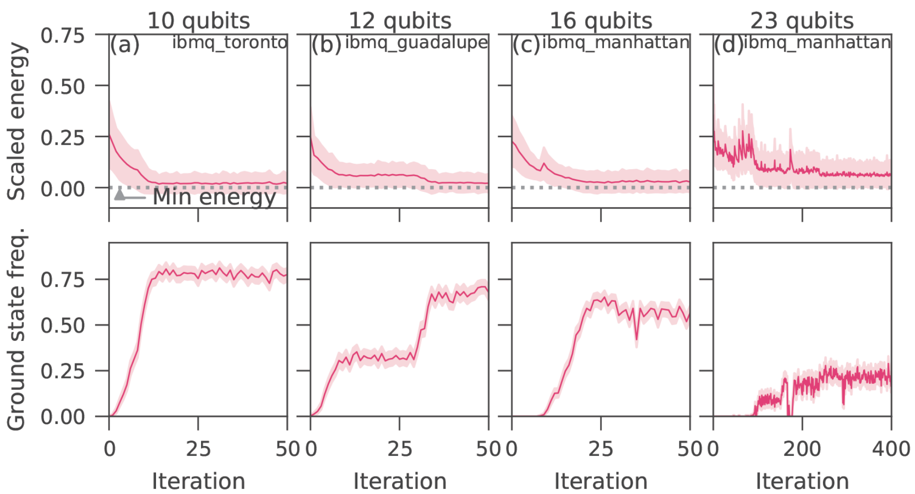

Fig. 4 Energy rescaled with the maximum energy eigenvalue (top panels) and ground state frequency (bottom panels) for each number of qubits freed[19]. Error bands are the standard deviation and 95% confidence interval for the top and bottom panels, respectively.

cannot be achieved with classical computers.

* Parts of this manuscript were modified, and created in accordance with the Creative Commons Attribution 4.0 International License[*2] from the article titled "A case study of variational quantum algorithms for a job shop scheduling problem" by D. Amaro, M. Rosenkranz, N. Fitzpatrick, K. Hirano, and M. Fiorentini and published in EPJ Quantum Technology 9, 5 (2022).

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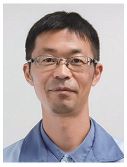

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