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Article

Quanestimation.jl: An open-source Julia framework for quantum parameter estimation[☆]

Huai-Ming Yu^{a,b}, Jing Liu^{a,b,*}^a Center for Theoretical Physics and School of Physics and Optoelectronic Engineering, Hainan University, Haikou 570228, China^b School of Physics, Huazhong University of Science and Technology, Wuhan 430074, China

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ABSTRACT

As the main theoretical support of quantum metrology, quantum parameter estimation must follow the steps of quantum metrology towards the applied science and industry. Hence, optimal scheme design will soon be a crucial and core task for quantum parameter estimation. To efficiently accomplish this task, software packages aimed at computer-aided design are in high demand. In response to this need, we hereby introduce QuanEstimation.jl, an open-source Julia framework for scheme evaluation and design in quantum parameter estimation. It can be used either as an independent package or as the computational core of the recently developed hybrid-language (Python-Julia) package QuanEstimation [Phys. Rev. Res. 4 (4) (2022) 043057]. Utilizing this framework, the scheme evaluation and design in quantum parameter estimation can be readily performed, especially when quantum noises exist.

1. Introduction

Quantum technologies have encountered a fast-developing era in recent years, and are now being enthusiastically pursued by international technology companies and governments worldwide. Together with the artificial intelligence, quantum technologies have been treated as the major origins of the next-generation technologies, and even the next industrial revolution.

Quantum technologies are founded on the principles of quantum mechanics and use quantum systems or quantum features to achieve advantages that classical systems cannot realize. As a core aspect of quantum technologies, quantum metrology utilizes quantum systems to perform precise measurements of physical parameters, such as the strength and frequency of an electromagnetic field or a signal. Its value has been successfully proved by many remarkable examples, such as the optical clocks [1] and atomic magnetometers [2].

Quantum parameter estimation [3,4] is the major theoretical support of quantum metrology due to the statistical nature of quantum systems. After decades of development, many elegant mathematical tools and optimal schemes have been provided and studied for quantum parameter estimation in various measurement scenarios. In practice, quantum noises are inevitable in the process of quantum parameter estimation,

which usually affects the optimality of the optimal schemes given in noiseless scenarios, and different physical systems may face different dominant quantum noises. These facts indicate that the scheme design in the presence of noise usually needs to be performed case by case. Therefore, software for scheme design is a natural requirement in the industrialization process of quantum parameter estimation and quantum metrology.

Due to this requirement, in 2022 we announced an open-source hybrid-language (Python-Julia) package named QuanEstimation for scheme evaluation and design in quantum parameter estimation [5]. Python is the interface of the package due to its popularity in the scientific community, and the computational core is written in Julia since it provides superior numerical efficiency in the scheme design. In recent years, Julia [6] has become an emerging platform for computation packages in quantum information, and several very popular and useful packages have been developed based on it, including QuantumToolbox.jl [7], QuantumOptics.jl [8], QuantumInformation.jl [9], Yao.jl [10], and QuantumControl.jl [11]. The Julia part of QuanEstimation is actually an independent and complete package named QuanEstimation.jl. In the hybrid-language package, the evaluation of various mathematical tools can be directly executed in the Python part. However, the optimization tasks in the scheme design will be transferred to the Julia

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* Corresponding author.

E-mail address: jing.liu@hainanu.edu.cn (J. Liu).

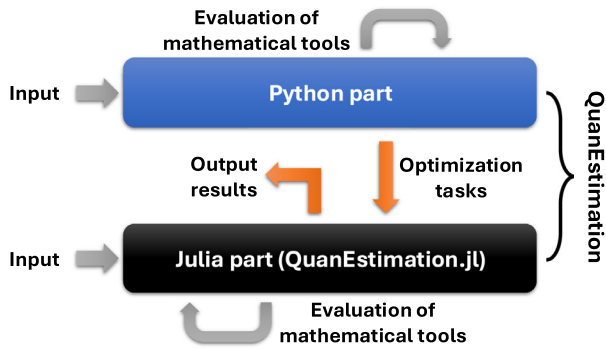


Fig. 1. Logical relation between the Python part and Julia part (QuanEstimation.jl) of QuanEstimation.

part, namely QuanEstimation.jl, and be executed, as illustrated in Fig. 1. Once the calculation is executed in QuanEstimation.jl, it will stay in this part until all results are obtained and output. In the meantime, as an independent and complete package, all the functions in the Python part also exist in QuanEstimation.jl. After the announcement of QuanEstimation, QuanEstimation.jl has been constantly updated and optimized structurally. Now it not only contains all the functions in the hybrid-language package, but also includes some new features like modules for specific physical systems.

In this paper, the architecture and package structure of QuanEstimation.jl will be thoroughly introduced. Furthermore, the methods to set up a scheme, including the general method and specific system modules, and the process of scheme design will be discussed, and corresponding demonstration codes will be presented. The usage of specific system modules will be illustrated with the Nitrogen-vacancy center magnetometers. In the end, we will also introduce the numerical error evaluation and control tools in the package, which can be used to check and ensure the validity of the designed scheme.

2. Architecture overview

2.1. Package architecture and structure

A typical scheme for quantum parameter estimation usually consists of four steps: state preparation, parameterization, quantum measurement, and classical parameter estimation [12–15]. The mission of scheme design for quantum parameter estimation in a specific scenario is to provide the optimal forms of these four steps (or some of them if the scenario requires certain fixed steps). Hence, the core philosophy of developing QuanEstimation.jl is the efficient realization of scheme design for quantum parameter estimation in a given scenario. This philosophy indicates that the architecture of QuanEstimation.jl must be centered around the scheme, as shown in Fig. 2(a). Therefore, defining a scheme is the first thing to do when using this package. Once the scheme is defined, the scheme evaluation, such as the calculations of various mathematical tools or metrological resources, and scheme design can be further performed. In the meantime, some utility tools like error evaluation/control and unit tests can also be executed. The error evaluation and control will be thoroughly discussed in Section 5. As a development tool, the unit tests would help the developers check the correctness and compatibility of the new codes. More details of it can be found in the documentation [16].

In QuanEstimation.jl, two methods can be used to define a scheme. The first and most common one is using the function `GeneralScheme()`, in which the basic elements of the scheme, such as the probe state, the parameterization process, and the measurement form, are manually input by the users. The system Hamiltonian, decay modes, and other systematic information are input when defining the parameterization process. The introduction and usage of this function will be thoroughly provided in Section 3. Currently, the parameteriza-

tion process can only be defined within the package. In the next version, we will include an interface to allow it, especially the dynamics process, to be defined via user-specific scripts that compact with other Julia ecosystems.

The second method to define a scheme is using the modules for specific quantum systems. These specific system modules are designed to improve the user experience and balance the efficiency and versatility of the package. In QuanEstimation.jl, each module is written as an independent package for the convenience of package development and management. The common parts used by all specific system modules are put into a base package named QuanEstimationBase.jl, as shown in Fig. 2(b). All modules of specific systems can call the functions in this base package to further perform the scheme evaluation and design. Furthermore, the functions only available in this physical system and algorithms that are particularly efficient for it are also written inside the module to improve the computing efficiency. More details and demonstration of the modules will be given in Section 3.2. All modules and QuanEstimationBase are made up of the entire package of QuanEstimation.jl.

2.2. Installation and calling

As a registered Julia package, QuanEstimation.jl can be easily installed in Julia via the package Pkg.jl. The specific codes for its installation in the Read-Eval-Print Loop (REPL) are as follows:

```
julia> using Pkg
julia> Pkg.add("QuanEstimation")
```

After the installation, it can be called in the REPL with the following codes:

```
julia> using QuanEstimation
```

All the subpackages and functions can be directly applied once the codes in above line are used. In the demonstration codes the functions are called specifically (for example using `QuanEstimation:SigmaX`) to the purpose of reminding the readers which functions are belong to the package.

3. Scheme setup

3.1. General scheme

A general scheme for quantum parameter estimation consists of four elements: probe state, parameterization process, measurement, and classical estimation strategy. These elements should be defined first when using QuanEstimation.jl. In the process of scheme design, these inputs, or some of them, work as the initial guesses of the optimizations. In QuanEstimation.jl, the scheme can be defined via the function `GeneralScheme()`, and all information in this function will be further used to construct a `struct` in Julia. The demonstration codes of its usage are as follows:

```
julia> using QuanEstimation:GeneralScheme,QubitDephasing,PlusState,SIC
julia> dynamics = QubitDephasing([0.5,0.5,0.5],"z",0.1,0.01:1)
julia> GeneralScheme(;probe=PlusState(), param=dynamics,
    measurement=SIC(2), x=nothing, p=nothing, dp=nothing)
```

In `GeneralScheme()`, the keyword arguments `probe=`, `param=`, and `measurement=` represent the input of the probe state, parameterization process, and measurement, respectively. In the case that a prior probability distribution exists, the regime of the arguments of the prior distribution, the distribution, and its derivatives should also be input via the keyword arguments `x`, `p`, and `dp`. The data types of the inputs are the same as those in the hybrid-language package, and more thorough demonstrations of them can be found in Ref. [5]. In the following, we will briefly introduce how to define these elements in QuanEstimation.jl.

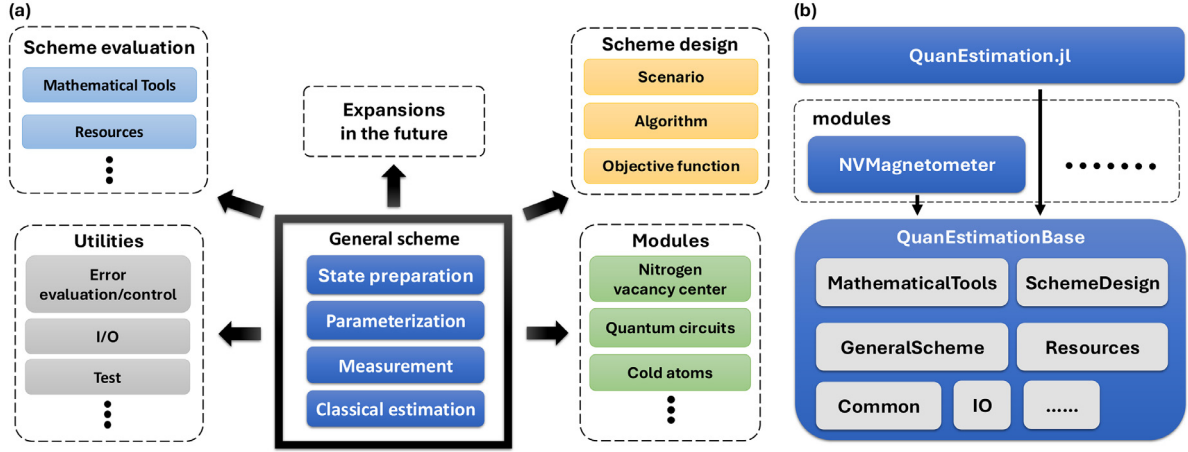


Fig. 2. (a) The architecture and (b) package structure of QuanEstimation.jl.

Table 1
Some integrated quantum states and operators in QuanEstimation.jl.

Function name	Probe state
PlusState()	$\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right)^T$
MinusState()	$\left(\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\right)^T$
BellState(1)	$\left(\frac{1}{\sqrt{2}}, 0, 0, \frac{1}{\sqrt{2}}\right)^T$
BellState(2)	$\left(\frac{1}{\sqrt{2}}, 0, 0, -\frac{1}{\sqrt{2}}\right)^T$
BellState(3)	$\left(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right)^T$
BellState(4)	$\left(0, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0\right)^T$
SigmaXO	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
SigmaYO	$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$
SigmaZO	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

In QuanEstimation.jl, the probe state is generally represented by a state vector or a density matrix. For a pure state, the data type of input probe state can either be a vector or a matrix and for a mixed state, it has to be a matrix. Several constantly used states are integrated into the package for convenience, as shown in Table 1, and more will be involved in the future. The basis of these states is the same as the input Hamiltonian. If $(1, 0)^T := |0\rangle$ and $(0, 1)^T := |1\rangle$, then the functions PlusState() and MinusState() are in fact the states $(|0\rangle + |1\rangle)/\sqrt{2}$ and $(|0\rangle - |1\rangle)/\sqrt{2}$. BellState(1) to BellState(4) are the states $(|00\rangle + |11\rangle)/\sqrt{2}$, $(|00\rangle - |11\rangle)/\sqrt{2}$, $(|01\rangle + |10\rangle)/\sqrt{2}$, and $(|01\rangle - |10\rangle)/\sqrt{2}$, respectively. Some Julia packages like QuantumToolbox.jl [7], QuantumOptics.jl [8], and QuantumInformation.jl [9] also contain many well-used quantum states, and the users can also call them for the generation of probe states.

The parameterization process plays a critical role in quantum parameter estimation. In general, this process is realized by quantum dynamics. In QuanEstimation.jl, the focus is primarily on the dynamics governed by the master equation in the Lindblad form:

$$\partial_t \rho = -i[H, \rho] + \sum_i \gamma_i \left(\Gamma_i \rho \Gamma_i^\dagger - \frac{1}{2} \{ \rho, \Gamma_i^\dagger \Gamma_i \} \right), \quad (1)$$

where ρ is the evolved density matrix, H is the total Hamiltonian, and Γ_i and γ_i are the i th decay operator and decay rate, respectively. γ_i could either be constant (a float number) or time-dependent (a vector). In the meantime, QuanEstimation.jl can also deal with the non-dynamical processes, such as the quantum channels described by Kraus operators, i.e.,

$\rho = \sum_i K_i \rho_0 K_i^\dagger$, where K_i is the i th Kraus operator satisfying $\sum_i K_i^\dagger K_i = \mathbb{I}$ with $\mathbb{I}$ the identity operator, and ρ_0 is the probe state.

In QuanEstimation.jl, the master equations can be defined via the function Lindblad(), and the quantum channels can be defined via the function Kraus(). The demonstration codes for calling these two functions are as follows:

```
julia> using QuanEstimation:Lindblad, SigmaX, SigmaY, SigmaZ, ZeroCTRL
julia> H0 = 0.5*SigmaX() + 0.5*SigmaZ()
julia> dH = [SigmaZ()]
julia> tspan = 0:0.01:1
julia> Hc = [SigmaY()]
julia> decay = [[SigmaX(), 0.01]]
julia> dynamics = Lindblad(H0, dH, tspan, Hc, decay; ctrl=ZeroCTRL(),
    dyn_method=:Ode)
```

```
julia> using QuanEstimation:Kraus
julia> E0 = [1 0; 0 sqrt(0.5)]
julia> E1 = [sqrt(0.5) 0; 0 0]
julia> K = [E0, E1]
julia> dK = [[0 0; 0 -0.5/sqrt(0.5)], [[0 0.5/sqrt(0.5); 0 0]]]
julia> channel = Kraus(K, dK)
```

In the function Lindblad(), the argument tspan is an array representing the time length for the evolution. In general, the argument H0 is a matrix or a vector of matrices representing the full Hamiltonian in the noncontrolled scheme or the free (noncontrolled) part of the Hamiltonian in the controlled scheme. It is a matrix when the Hamiltonian is time-independent and a vector with the length equivalent to that of tspan when it is time-dependent. The argument dH is a vector of matrices for time-independent Hamiltonians and a vector of vector of matrices for time-dependent Hamiltonians, which contains the derivatives of the Hamiltonian for the parameters to be estimated, same as that in the hybrid-language package [5].

Moreover, the Hamiltonian and its derivative can also be defined by functions. This can be done with the help of the function Hamiltonian(), which takes the functions H0(u), dH(u) and the values of u (a float number or a vector) as arguments. It is a multiparameter scenario when u is a vector. The output type of H0(u) should be a matrix, and that of dH should be a vector of matrices. In the case that the Hamiltonian is time-dependent, the functions should be in the form of H0(u, t) and dH(u, t). The demonstration codes for calling Lindblad() with the functions H0(u) and dH(u) are as follows:

```
julia> using QuanEstimation:SigmaX, SigmaZ, Hamiltonian, Lindblad
julia> H0(u) = (SigmaX()*cos(u) + SigmaZ()*sin(u))/2
julia> dH(u) = [(-SigmaX()*sin(u) + SigmaZ()*cos(u))/2]
julia> u = pi/4
julia> ham = Hamiltonian(H0, dH, u)
julia> decay = [[SigmaZ(), 0.01]]
julia> dynamics = Lindblad(ham, 0:0.01:1, decay)
```

The demonstration codes for the multiparameter scenario can be found in the documentation [16].

Table 2

Currently available control functions in QuanEstimation.jl. In the expressions T is the end time of the array $\mathbf{tspan}$, and $\lfloor \cdot \rfloor$ denotes the floor function.

Functions	Arguments	Control shape
ZeroCTRL()	$\backslash$	0
LinearCTRL(k, c_0)	$k: k, c_0: c_0$	$kt + c_0$
SineCTRL(A, ω, ϕ)	$A: A, \omega: \omega, \phi: \phi$	$A \sin(\omega t + \phi)$
SawCTRL(k, n)	$k: k, n: n$	$2k \left(\frac{nt}{T} - \lfloor 0.5 + \frac{nt}{T} \rfloor \right)$
TriangleCTRL(k, n)	$k: k, n: n$	$2 \left 2k \left(\frac{nt}{T} - \lfloor 0.5 + \frac{nt}{T} \rfloor \right) \right - 1$
GaussianCTRL(A, μ, σ)	$A: A, \mu: \mu, \sigma: \sigma$	$A e^{-(t-\mu)^2/(2\sigma)}$
GaussianEdgeCTRL(A, σ)	$A: A, \sigma: \sigma$	$A - A e^{-t^2/\sigma} - A e^{-(t-T)^2/\sigma}$

The argument `decay` is a vector containing the information of both decay operators and decay rates, and its input rule is `decay = [[Gamma1, gamma1], [Gamma2, gamma2], ...]`, where `Gamma1` (`Gamma2`) and `gamma1` (`gamma2`) represent the first (second) decay operator and decay rate, respectively. So do others, if there are any. Here the decay rate `gamma1` (`gamma2`) can either be a float number (representing a fixed decay rate) or a vector (representing a time-dependent decay rate), and when it is a vector, its length should be identical with `tspan`. The argument `Hc` is a vector of matrices representing the control Hamiltonians. Its default value is `nothing`, which represents the noncontrolled scheme. The argument `ctrl` is a vector of vectors containing the control amplitudes for the control Hamiltonians given in the argument `Hc`. Its default value `ZeroCTRL()` represents the zero control amplitudes for all control Hamiltonians. Some frequently used control amplitudes are integrated into the package for convenience, as given in Table 2, and more will be added in the future.

In `Lindblad()`, the master equation is solved via the package `DifferentialEquations.jl` [17] by default, and the corresponding setting is `dyn_method=:Ode` (or `\texttt{dyn\_method=:ode}`). Alternatively, it can also be solved via the matrix exponential method by using `dyn_method=:Expm` (or `\texttt{dyn\_method=:expm}`), which is suitable for small to medium-sized systems.

In the function `Kraus()`, K and dK are vector of matrices and vector of vector of matrices representing the Kraus operators and corresponding derivatives on the parameters to be estimated. Similar to the function `Lindblad()`, here the Kraus operators and their derivatives can also be defined as functions $K(u)$ and $dK(u)$, of which the output types are also vector of matrices and vector of vector of matrices. In this case, the function `Kraus()` is called via the following format:

```
julia> using QuanEstimation:Kraus
julia> u = pi/4
julia> K(u) = [[1 0; 0 sqrt(1-u)], [0 sqrt(u); 0 0]]
julia> dK(u) = [[[0 0; 0 -0.5/sqrt(1-u)], [[0 0.5/sqrt(u); 0 0]]]
julia> channel = Kraus(K, dK, u)
```

More demonstration codes of this case can be found in the documentation [16].

Regarding the measurement, the data type of the input measurement is a vector of matrices with each entry an element of a set of positive operator-valued measure (POVM). If no specific measurement is input, the rank-one symmetric informationally complete POVM (SIC-POVM) will be used as the default choice, which can also be manually invoked via the function `SIC()`.

After the scheme setup is finished, the metrological quantities can be readily evaluated. All the metrological quantities given in the hybrid-language package [5] are available in `QuanEstimation.jl`, such as the Quantum Cramér-Rao bounds [3,4] and various types of quantum Fisher

information matrix (QFIM) [14], Holevo Cramér-Rao bound (HCRB) [18–21], and Nagaoka-Hayashi bound (NHB) [21–23]. Demonstration codes for their calculations in `QuanEstimation.jl` is as follows:

```
julia> using QuanEstimation:Lindblad,ZeroCTRL,GeneralScheme,PlusState
julia> using QuanEstimation:Hamiltonian,SIC,SigmaX,SigmaY,SigmaZ
julia> using QuanEstimation:QFIM,CFIM,HCRB,NHB
julia> using LinearAlgebra:I
julia> H0(u) = (SigmaX()*cos(u)+SigmaZ()*sin(u))/2
julia> dH(u) = [(-SigmaX()*sin(u)+SigmaZ()*cos(u))/2]
julia> ham = Hamiltonian(H0, dH, pi/4)
julia> dynamics = Lindblad(ham, 0:0.01:1, [SigmaY()], [[SigmaZ(), 0.01]])
julia> scheme = GeneralScheme(; probe=PlusState(), param=dynamics,
measurement=SIC(2))
julia> QFIM(scheme; LDtype=:SLD)
julia> CFIM(scheme)
julia> HCRB(scheme; W=I(1))
julia> NHB(scheme; W=I(1))
```

In the function `QFIM()`, the keyword argument `LDtype=:SLD` means that the calculated QFIM is based on the symmetric logarithmic derivative (SLD), same as that in the hybrid-language package. Details of calling other types of QFIM can be found in Ref. [5]. In the functions `HCRB()` and `NHB()`, the argument `W` represents the weight matrix, and its definition can also be found in Ref. [5]. In the case that a prior distribution exists, Bayesian types of QFIM or other tools like the Van Trees bound (VTB) [24], and its quantum version (QVTB), also known as Tsang-Wiseman-Caves bound [25], should be used for the evaluation of precision limit. Here we present the demonstration codes for the calculations of VTB and QVTB:

```
julia> using QuanEstimation:Lindblad,GeneralScheme,Hamiltonian
julia> using QuanEstimation:SigmaX,SigmaZ,PlusState,SIC,VTB,QVTB
julia> xspan = range(0, pi; length=200)
julia> mu = pi/2
julia> p = xspan .|> xspan->exp(-(xspan-mu)^2/2)
julia> dp = xspan .|> xspan->-xspan-mu)*exp(-(xspan-mu)^2/2)
julia> H0(x) = (SigmaX()*cos(x)+SigmaZ()*sin(x))/2
julia> dH(x) = [(-SigmaX()*sin(x)+SigmaZ()*cos(x))/2]
julia> ham = Hamiltonian(H0, dH, pi/4)
julia> dynamics = Lindblad(ham, 0:0.01:1, [SigmaZ(), 0.01])
julia> scheme = GeneralScheme(; probe=PlusState(), param=dynamics,
measurement=SIC(2), x=xspan, p=p, dp=dp)
julia> VTB(scheme)
julia> QVTB(scheme)
```

The outputs of all these functions are vectors representing the time evolutions of the metrological quantities.

The advantage of using `GeneralScheme()` is the flexible choice of physical systems. In principle, any quantum system can be implemented in `QuanEstimation.jl` to evaluate the metrological quantities or perform scheme design, regardless of the computing efficiency. However, many physicists mainly focus on certain specific physical systems. The convenience of scheme setup and computing efficiency of scheme design for these systems are critical to them, which may not be fully satisfying with the function `GeneralScheme()`. For the sake of improving the efficiency of scheme setup and scheme design for certain specific systems, the modules are developed in `QuanEstimation.jl`, which is a significant feature that did not appear in the last version of the hybrid-language package [5], and will be thoroughly introduced in the next section.

3.2. Modules for specific systems

Many quantum systems have present significant advantages in various scenarios of quantum parameter estimation, such as the Nitrogen-vacancy centers [26], cold atoms [13,27], trapped ions [28], optomechanical systems [29,30], and quantum circuits [28,31,32]. For these specific quantum systems, the Hamiltonian structures and the parameters to be estimated are usually fixed. Hence, for the researchers fo-

cusing on a specific quantum system, especially those not experienced in Julia or even coding, a module that integrates the Hamiltonian and other information of this system would make QuanEstimation.jl more user-friendly. In the meantime, a module for a specific physical system would also make it easier to adjust the codes according to the features of this system and implement the algorithms that are particularly efficient for the scheme design in this system. The computing efficiency of the scheme design would then be improved.

All specific system modules will be structurally written as independent packages for the convenience of development and maintenance. However, they can be directly called when using QuanEstimation is applied. Currently, most modules are still under construction and will be available in both the hybrid-language package and Julia package in a short time. In this paper we take the Nitrogen-vacancy center magnetometer as an example of the modules and demonstrate its usage. Some other packages like qsensoropt [33,34] can also be used to design magnetometer with Nitrogen-vacancy center. The Hamiltonian of the Nitrogen-vacancy center is [35–38].

$$H_0/\hbar = D S_3^2 + g_S \vec{B} \cdot \vec{S} + g_I \vec{B} \cdot \vec{I} + \vec{S}^T \mathcal{A} \vec{I}, \quad (2)$$

where $S_i = s_i \otimes \mathbb{I}$ and $I_i = \mathbb{I} \otimes \sigma_i$ ($i = 1, 2, 3$) are the electron and nuclear (^{15}N) operators. s_1 , s_2 and s_3 are spin-1 operators with the expressions

$$s_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad (3)$$

$$s_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad (4)$$

$$s_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \quad (5)$$

The vectors $\vec{S} = (S_1, S_2, S_3)^T$, $\vec{I} = (I_1, I_2, I_3)^T$, and $\mathcal{A}$ is the hyperfine tensor, and in this case $\mathcal{A} = \text{diag}(A_1, A_1, A_2)$ with A_1 and A_2 the axial and transverse magnetic hyperfine coupling coefficients. The hyperfine coupling between the magnetic field and the electron is approximated to be isotropic. $g_S = g_e \mu_B / \hbar$ and $g_I = g_n \mu_n / \hbar$ with g_e (g_n) the g factor of the electron (nuclear), μ_B (μ_n) the Bohr (nuclear) magneton, and $\hbar$ the Planck's constant. $\vec{B}$ is the external magnetic field that needs to be estimated. In this system, the control Hamiltonian can be expressed by

$$H_c/\hbar = \sum_{i=1}^3 \Omega_i(t) S_i, \quad (6)$$

where $\Omega_i(t)$ is a time-varying Rabi frequency. Due to the fact that the electron suffers from the noise of dephasing in practice, the dynamics of the Nitrogen-vacancy center is then described by

$$\partial_t \rho = -i[H_0 + H_c, \rho] + \frac{\gamma}{2}(S_3 \rho S_3 - S_3^2 \rho - \rho S_3^2), \quad (7)$$

where γ is the dephasing rate, which is usually inversely proportional to the dephasing time T_2^* .

In QuanEstimation.jl, this module can be used to define the scheme by calling the function NVMagnetometerScheme(). The coefficients of the Hamiltonian in the module are taken as those given in Refs. [35,36]. After the scheme is defined, the scheme evaluation and

design can be further applied. The demonstration codes for calling this module and evaluating the value of QFI are as follows:

```
julia> using QuanEstimation:NVMagnetometerScheme,QFIM
julia> scheme = NVMagnetometerScheme()
NVMagnetometerScheme
├── StatePreparation => DensityMatrix
│   ├── ndim = (6,)
│   └── ψ0 = [0.7071067811865475, 0.0, 0.0,
│           0.0, 0.7071067811865475, 0.0]
├── Parameterization => LindbladDynamics
│   ├── tspan = 0.0:0.01:2.0
│   ├── Hamiltonian => NVCenterHamiltonian
│   │   ├── D = 18032.741831605414
│   │   ├── gS = 176.1176841602438
│   │   ├── gI = 0.027143360527015815
│   │   ├── A1 = 22.933626371205488
│   │   ├── A2 = 19.038051480754145
│   │   └── B = [0.5, 0.5, 0.5]
│   ├── Controls
│   │   ├── Hc = [S1, S2, S3]
│   │   └── ctrl = nothing
│   └── decays
│       ├── decay_opt => [S3]
│       └── γ = 6.283185307179586
└── Measurement
    ├── M = nothing
    └── F = QFIM(scheme)
```

The progress of other modules, such as the Mach-Zehnder interferometer, cold atoms, trapped ions, optomechanical systems, and quantum circuits, will be constantly updated in the documentation [16].

4. Scheme design

Scheme design is the major mission of QuanEstimation.jl, and also the key reason why Julia is used to write the computational core of the hybrid-language package [5]. In QuanEstimation.jl, the process of scheme design consists of three steps, including initialization, optimization, and output, as shown in Fig. 3. Three elements are required in the first step. Apart from defining the scheme, the optimization scenario must be specified, and the objective function and optimization algorithm should be chosen.

As discussed in the previous section, the scheme can be defined via the general approach or specific system modules. Specifying the optimization scenario means the user needs to clarify which part of the scheme needs to be optimized. Currently, the package includes probe state optimization, control optimization, measurement optimization, and comprehensive optimization, same as those in the hybrid-language package. Detailed introduction of them can be found in Ref. [5]. The probe state, control, measurement, and comprehensive optimization can be specified via the functions StateOpt(), ControlOpt(), MeasurementOpt(), and CompOpt(). In the case of measurement optimization, QuanEstimation.jl now provides three types of scenarios, including rank-one projective measurements, linear combinations, and rotations of a set of input measurements. The desired optimization strategy can be selected by setting mtype=:Projection, mtype=:LC, or mtype=:Rotation, respectively. Regarding the comprehensive optimization, four types of joint optimization, including the probe state and measurement (realized by setting type=:SM), probe state and control (type=:SC), control and measurement (type=:CM), and all three variables together (type=:SCM), can be executed.

After specifying the optimization scenario, the objective function and algorithm for optimization should be chosen. This part can be neglected if the user has no preference on the objective function and algorithm since all scenarios have default choices. Most metrological tools can be taken as the objective function. QuanEstimation.jl includes both gradient-based algorithms, such as the gradient ascent pulse engineering algorithm and its advanced version based on automatic differentiation, and gradient-free algorithms such as particle swarm optimization and differential evolution. Details of the available algorithms and objective functions in each scenario can be found in Ref. [5].

The information created in the step of initialization is stored as a struct in QuanEstimation.jl, which not only contains the information of the scheme but also the supplementary information that can assist the

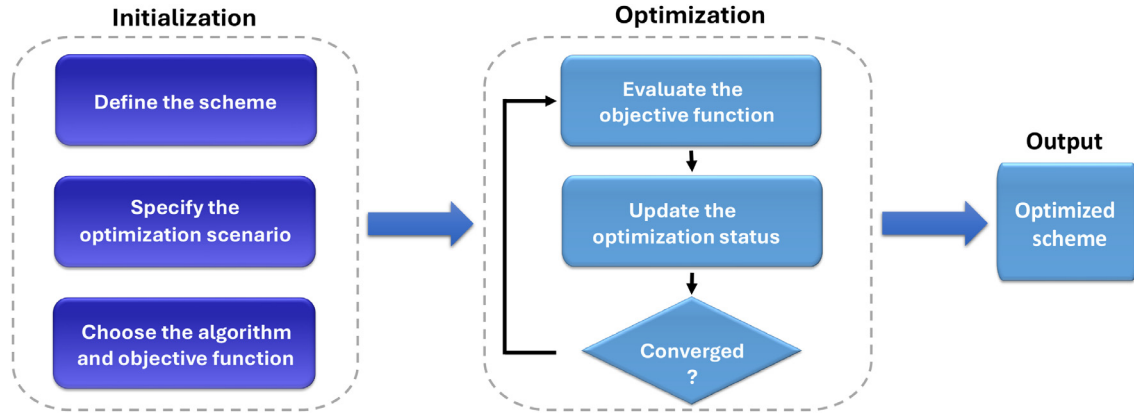


Fig. 3. The process of scheme design in QuanEstimation.jl, which includes three steps: (1) initialization, (2) optimization, and (3) output.

precision analysis of the optimized scheme, such as the number of iterations used during the optimization process and the convergence criteria of optimization.

Once the initialization is finished, the scheme is then ready to be optimized. In the step of optimization, the scheme data are updated by the selected optimization algorithm, and the objective function is evaluated, as shown in Fig. 3. This process continues until the convergence conditions are met. After the value of the objective function is converged, the optimized scheme is then output. The data will be saved into files (HDF5 format with extension name.dat) via the JLD2 package and printed on the screen.

Here we provide the demonstration codes for the scenario of control optimization:

```
julia> using QuanEstimation:NVMagnetometerScheme
julia> using QuanEstimation:ControlOpt,optimize!,autoGRAPE
julia> scheme = NVMagnetometerScheme()
julia> opt = ControlOpt()
julia> optimize!(scheme, opt; algorithm=autoGRAPE(), savefile=true)
```

More examples and demonstrations of other scenarios can be found in the documentation [16].

Adaptive measurement is another well-used scenario in quantum parameter estimation [15,39–45], in which a vector of tunable parameters is used to enhance the measurement precision. Similar to the hybrid-language package, QuanEstimation.jl can also realize the adaptive measurements. To do it, the function `AdaptiveStrategy()` should be used first before defining the scheme to claim the regime of the parameters to be estimated, the prior distribution, and its derivatives to the parameters. The process of scheme setup is the same as other scenarios, which can be realized by `GeneralScheme()` or certain specific system modules. Then the function `adapt!()` is called to perform the adaptive measurement. The demonstration codes for the adaptive measurement are as follows:

```
julia> using QuanEstimation:GeneralScheme,Hamiltonian,Lindblad
julia> using QuanEstimation:PlusState,SIC,SigmaX,SigmaZ
julia> using QuanEstimation:AdaptiveStrategy,adapt!
julia> xspan = range(0, pi; length=200)
julia> mu = pi/2
julia> p = xspan .|> xspan->exp(-(xspan-mu)^2/2)
julia> dp = xspan .|> xspan->exp(-(xspan-mu)^2/2)
julia> strat = AdaptiveStrategy(; x=xspan, p=p, dp=dp)
julia> H0(x) = (SigmaX()*cos(x)+SigmaZ()*sin(x))/2
julia> dH(x) = [(-SigmaX()*sin(x)+SigmaZ()*cos(x))/2]
julia> ham = Hamiltonian(H0, dH, pi/4)
julia> dynamics = Lindblad(ham, 0:0.01:1, [[SigmaZ(), 0.01]])
julia> scheme = GeneralScheme(; probe=PlusState(), param=dynamics,
    measurement=SIC(2), strat=strat)
julia> adapt!(scheme; method="FOP", savefile=false, max_episode=1000)
```

More details on the usage of adaptive measurement are given in Ref. [5] and the documentation [16]. The online and offline adaptive phase estimations in the Mach-Zehnder interferometer are integrated into the

module of Mach-Zehnder interferometer, and will be thoroughly introduced in another paper.

5. Numerical error evaluation and control

To evaluate the numerical precision of the output scheme or the calculated mathematical tools, the computational errors should be evaluated, and sometimes even controlled. QuanEstimation.jl provides two functions `error_evaluation()` and `error_control()` to help the users perform the error evaluation and control. The error evaluation uses the given precision of the input data to evaluate the error scaling of the output, and the error control uses the given error of the output to provide a suggested precision scaling of the input data. The demonstration codes for their usage are given as follows:

```
julia> using QuanEstimation:NVMagnetometerScheme
julia> using QuanEstimation:error_evaluation,error_control
julia> scheme = NVMagnetometerScheme()
julia> error_evaluation(scheme; input_error_scaling=1e-8,
    objective="QFIM", SLD_eps=1e-8)
julia> error_control(scheme; output_error_scaling=1e-6,
    objective="QFIM", SLD_eps=1e-8)
```

In QuanEstimation.jl, the total error of the output, such as the QFIM, is evaluated via the error propagation relation

$$\delta f = \sqrt{\sum_i \left(\frac{\partial f}{\partial x_i} \right)^2 \delta^2 x_i}, \quad (8)$$

where $f = f(x_1, x_2, \dots)$ is the output with x_i the i th input parameter. δf and δx_i represent the errors of f and x_i , respectively. The specific processes of error evaluation and control in the package are illustrated in Fig. 4.

The function `error_evaluation()` provides the evaluated error of the output at the final evolution time according to the given precision of the input data. In the evaluation process, the precision of the input data is assumed to be the same, which can be set via the key argument `input_error_scaling` in the function. In practice, if not all the input data can be set to the same precision, the input precision used for error evaluation can be taken as the worst one among them. In the case that the dynamics is calculated by the method `Expn` (`dyn_method=:Expn`), the gradients in Eq. (8) are all evaluated via automatic differentiation through chain rules, as shown in Fig. 4. When the dynamics is solved by `Ode` (`dyn_method=:Ode`), the errors of the evolved state and its derivatives are roughly evaluated as the summation of the input precision scaling and the time step to the fourth power, which is due to the fact that the global error of Tsitouras 5/4 Runge-Kutta method can be roughly expressed by $\mathcal{O}(h^4)$ [46] with h the time step. In the case of adaptive timestepping, the largest time step is used to evaluate the global error. Next, the evolved state and its derivatives are taken as the new input and the error of output is further evalu-

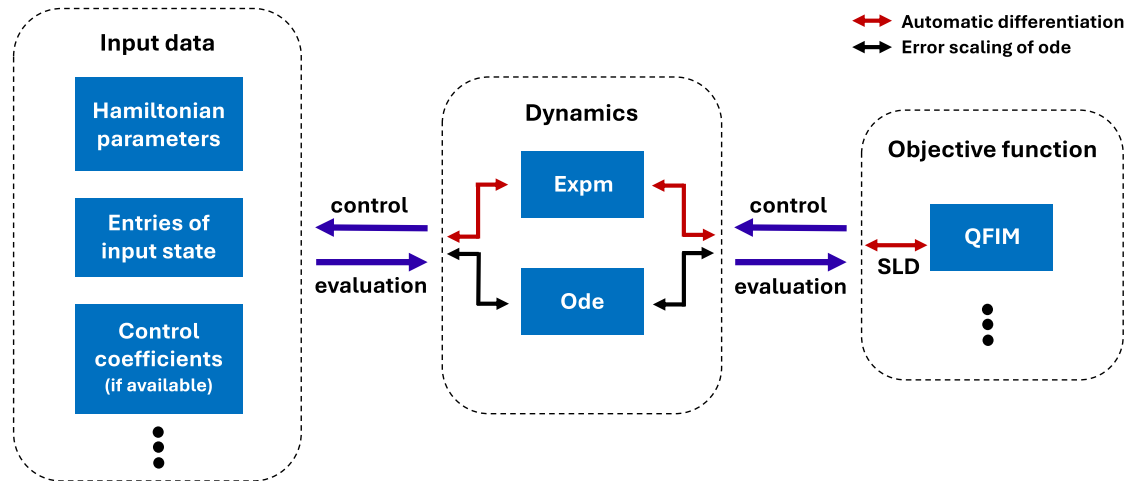


Fig. 4. Processes of computational error evaluation and control in QuanEstimation.jl.

ated via the error propagation relation, in which the gradients are also evaluated by automatic differentiation.

In the case that the output is the QFIM, the machine epsilon (set by the keyword argument `SLD_eps`) in the calculation of SLD would also contribute to the final error. Here the machine epsilon means that if an eigenvalue of the density matrix is less than the given value, it will be truncated to zero in the calculation of SLD [5]. A proper setting of `SLD_eps` would help to improve the calculation stability of the QFIM. When the function `error_evaluation()` is executed, the difference between the QFIMs before and after the truncation is applied will be shown on the screen (denoted by δF). If this value is too large, the value of `SLD_eps` should be reset.

The function `error_control()` provides a suggested precision scaling of the input data based on the required error scaling of the output, which is set by the argument `output_error_scaling`. We still assume the precision of all input data is the same in this function. In practice, the users can take this suggested precision as the worst precision requirement for all input data. As long as the precision of all inputs is higher than the suggested scaling, the error of output would meet the user's requirement. In the case that `Expm` is applied, the suggested input precision scaling is fully evaluated via Eq. (8). When `Ode` is applied, the required error of the evolved state is also evaluated by automatic differentiation, and then the suggested input precision is calculated as the difference between the error of the evolved state and the (largest) time step to the fourth power.

6. Future developments and extensions

Alongside enhancing the general computational efficiency of QuanEstimation.jl, our development roadmap prioritizes the development of modules for specific quantum systems or scenarios, including but not limited to the abstract models like the $SU(2)$ and $SU(1,1)$ interferometers, various toy models in quantum optics, quantum networks, and specific physical systems like quantum circuits, trapped ions, and cold atoms. Each module would be constructed as an independent sub-package. Concurrently, integration of more cutting-edge methodologies in quantum information and condensed-matter physics, and even those in computing science is also an important content for the development in the future.

Recent advancements in quantum experimental technologies have enabled the automation of numerous experimental processes. In the meantime, the strategic vision driving the development of QuanEstimation and QuanEstimation.jl centers on the automatic realization of scheme design in quantum parameter estimation. Building upon this

vision, another key development direction is the seamless integration of intelligent scheme design with experimental execution. This adaptive framework will enable dynamic scheme optimization through real-time environmental feedback, with redesigned configurations being autonomously deployed to maintain optimal estimation performance under varying conditions.

7. Summary

The development of QuanEstimation.jl aims at efficient scheme evaluation and design for quantum parameter estimation. This package can work as the computational core of its hybrid-language counterpart or as an independent package. The usage of QuanEstimation.jl is based on the construction of schemes. Once a scheme is constructed, all the metrological quantities discussed in Ref. [5] can be evaluated and the optimal schemes can be provided according to the user's requirements. To balance the versatility and efficiency, we introduce modules in the package for specific physical systems and demonstrate its usage with the Nitrogen-vacancy center magnetometer. The package version of QuanEstimation.jl with respect to the contents of this paper is v0.2. The source codes can be found in GitHub [47] and the documentation is available in the link in Ref. [16].

Declaration of competing interest

The authors declare that they have no conflicts of interest in this work.

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Author profile

Jing Liu (BRID: 06559.00.90699) is a professor at Center for Theoretical Physics and School of Physics and Optoelectronic Engineering, Hainan University. He obtained his bachelor's degree in 2010 at Hangzhou Dianzi University and PhD in 2015 at Zhejiang University. From 2015 to 2017, he was a postdoctoral fellow at the Chinese University of Hong Kong. From 2018 to 2024, he worked in Huazhong University of Science and Technology as an associate professor. His main research interests focus on the topics in quantum metrology, quantum control, quantum information theory, and foundations of quantum mechanics, especially the design of high-precision measurement schemes using the features of quantum mechanics.