# Supplementary Materials for

## Noise-Resilient Quantum Metrology with Quantum Computing

Xiangyu Wang, Chenrong Liu, Xue Lin, Yu Tian, Yishan Li, Xinfang Nie, Yufang Feng,
Yuxuan Zheng, Ying Dong, Xinqing Wang, and Dawei Lu

\*\*Corresponding authors:\*\*
Ying Dong, yingdong@cjlu.edu.cn;
Xinqing Wang, wxqnano@cjlu.edu.cn;
Dawei Lu, ludw@sustech.edu.cn

10

1

#### 11 This PDF file includes:

- Supplementary Materials
- Figs. S1 to S7
- References

15

# 16 Contents

17 1	SUPPLEMENTARY SECTION 1: THEORETICAL MODEL	3
18	1.1 Fidelity	3
19	1.2 Quantum Fisher Information	6
20	1.3 Noise model	8
	SUPPLEMENTARY SECTION 2: RANDOM NOISE IN THE EXPERIMENT	8
23 3	SUPPLEMENTARY SECTION 3: LOSS FUNCTION	11
24 4	SUPPLEMENTARY SECTION 4: PQC MODEL	12

#### 25 1 SUPPLEMENTARY SECTION 1: THEORETICAL MODEL

<sup>26</sup> The initial state  $|\psi_0\rangle$  is evolved into  $|\psi_t\rangle$  by a sensing process characterized by operator  $\tilde{\mathcal{U}}$ , <sup>27</sup> and then a quantum noise channel with its operator  $\tilde{N}$  act on state  $|\psi_t\rangle$ , and the final state <sup>28</sup> thus becomes

$$\tilde{\rho_t} = P_0 |\psi_t\rangle \langle \psi_t| + (1 - P_0)\tilde{N} |\psi_t\rangle \langle \psi_t| \tilde{N}^{\dagger}$$
(S1)

29 as shown in Fig. S1.

$$|\psi_0\rangle \xrightarrow{\tilde{\mathcal{U}}} |\psi_t\rangle \xrightarrow{\tilde{N}: (1-P_0)} \tilde{\rho}_t$$

Figure S1: The chart of the state changes by sensing process characterized by operator  $\tilde{\mathcal{U}}$  and quantum noise channel  $\tilde{N}$ .

#### 30 1.1 Fidelity

31 The fidelity of the final state is

$$\tilde{F} = \langle \psi_t | \tilde{\rho}_t | \psi_t \rangle = P_0 + (1 - P_0) |\langle \psi_t | \tilde{N} | \psi_t \rangle|^2.$$
 (S2)

<sup>32</sup> Our method requires identifying the quantum principal component of this state. We thus <sup>33</sup> analyze the quantum principle component of the final state and compare the fidelity of it <sup>34</sup> with that of the full state fidelity in Eq. (S2).

Firstly, we expand the final state  $\tilde{N}|\psi_t\rangle$  by its original state  $|\psi_t\rangle$  and its perpendicular state  $|\psi_t^{\perp}\rangle$  as

$$\tilde{N}|\psi_t\rangle = \alpha|\psi_t\rangle + \beta|\psi_t^{\perp}\rangle,$$
 (S3)

37 with  $\langle \psi_t^{\perp} | \psi \rangle = \langle \psi | \psi_t^{\perp} \rangle = 0$ , then the final state can be expressed in the basis of  $|\psi\rangle$ ,  $|\psi_t^{\perp}\rangle$  as

$$\tilde{\rho}_{t} = P_{0} |\psi\rangle \langle \psi_{t}| + (1 - P_{0}) \tilde{N} |\psi_{t}\rangle \langle \psi_{t}| \tilde{N}^{\dagger} 
= (P_{0} + |\alpha|^{2} (1 - P_{0})) |\psi_{t}\rangle \langle \psi_{t}| + |\beta|^{2} (1 - P_{0}) |\psi_{t\perp}\rangle \langle \psi_{t\perp}| 
+ \alpha\beta^{*} (1 - P_{0}) |\psi_{t}\rangle \langle \psi_{t\perp}| + \alpha^{*}\beta (1 - P_{0}) |\psi_{t\perp}\rangle \langle \psi_{t}| 
= \begin{bmatrix} P_{0} + |\alpha|^{2} (1 - P_{0}) & \alpha\beta^{*} (1 - P_{0}) \\ \alpha^{*}\beta (1 - P_{0}) & |\beta|^{2} (1 - P_{0}) \end{bmatrix}$$
(S4)
$$= \begin{bmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{bmatrix}.$$

38 The eigenvalues and its eigenvectors can be obtained by some mathematical calculation as

$$\lambda_{+} = \frac{1 + \sqrt{1 - 4|\beta|^{2}(1 - P_{0})P_{0}}}{2},$$

$$\eta_{+} = \frac{1}{\sqrt{\Delta\lambda}} \binom{\sqrt{\lambda_{+} - \rho_{22}}}{\sqrt{\lambda_{+} - \rho_{22}}},$$
(S5)

39 and

$$\lambda_{-} = \frac{1 - \sqrt{1 - 4|\beta|^{2}(1 - P_{0})P_{0}}}{2},$$

$$\eta_{-} = \frac{1}{\sqrt{\Delta\lambda}} \begin{pmatrix} \rho_{12} \\ \sqrt{\rho_{11} - \lambda_{-}} \end{pmatrix},$$
(S6)

40 where

$$\Delta \lambda = \lambda_{+} - \lambda_{-} = \sqrt{1 - 4|\beta|^{2}(1 - P_{0})P_{0}},$$

$$\lambda_{+} - \rho_{22} = \frac{(\rho_{11} - \rho_{22}) + \Delta \lambda}{2},$$

$$\lambda_{-} - \rho_{11} = -\frac{(\rho_{11} - \rho_{22}) + \Delta \lambda}{2},$$

41 with

$$(\lambda_{+} - \rho_{22})^{2} + |\rho_{12}|^{2} = (\lambda_{+} - \rho_{22})\Delta\lambda,$$
  
$$(\lambda_{-} - \rho_{11})^{2} + |\rho_{12}|^{2} = -(\lambda_{-} - \rho_{11})\Delta\lambda.$$

 $_{42}$  We thus rewrite the  $\tilde{\rho_t}$  as

$$\tilde{\rho}_{t} = \lambda_{+}\eta_{+}\eta_{+}^{\dagger} + \lambda_{-}\eta_{-}\eta_{-}^{\dagger} 
= \lambda_{+}|+\rangle\langle+|+\lambda_{-}|-\rangle\langle-| 
= K \begin{pmatrix} \lambda_{+} & 0 \\ 0 & \lambda_{-} \end{pmatrix} K^{\dagger},$$
(S7)

 $_{43}$  and  $\lambda_{+}$  part is indeed the principle component of the final state, where the diagonalization  $_{44}$  transformed matrix

$$K = (\eta_{+}, \eta_{-}) = \frac{1}{\sqrt{\Delta \lambda}} \begin{pmatrix} \sqrt{\lambda_{+} - \rho_{22}} & \frac{\rho_{12}}{\sqrt{\rho_{11} - \lambda_{-}}} \\ \frac{\rho_{12}^{*}}{\sqrt{\lambda_{+} - \rho_{22}}} & -\sqrt{\rho_{11} - \lambda_{-}} \end{pmatrix}$$
(S8)

with det K=-1 as can be checked. Actually, the diagonalization is a basis change process, that is, in the new basis  $|\pm\rangle$ , the density matrix  $\tilde{\rho}_t$  is diagonalized as Diag $\{\lambda_+, \lambda_-\}$ . Then, we have the relation

$$|+\rangle = K^{\dagger}|\psi_t\rangle \Rightarrow |\psi_t\rangle = K|+\rangle,$$
  
$$|-\rangle = K^{\dagger}|\psi_t^{\perp}\rangle \Rightarrow |\psi_t^{\perp}\rangle = K|-\rangle.$$

<sup>48</sup> The fidelity of the principle component of the final state [state optimized by quantum com-<sup>49</sup> puting (QC)] can be obtained as

$$F = \langle \psi_t | \rho_{f+} | \psi_t \rangle = |\langle + | \psi_t \rangle|^2 = |\langle + | K | + \rangle|^2, \tag{S9}$$

50 where

$$\langle +|K|+\rangle = \frac{1}{\sqrt{\Delta\lambda}} \left( \sqrt{\lambda_{+} - \rho_{22}} \quad \frac{\rho_{12}}{\sqrt{\lambda_{+} - \rho_{22}}} \right) \frac{1}{\sqrt{\Delta\lambda}} \begin{pmatrix} \sqrt{\lambda_{+} - \rho_{22}} & \frac{\rho_{12}}{\sqrt{\rho_{11} - \lambda_{-}}} \\ \frac{\rho_{12}^{*}}{\sqrt{\lambda_{+} - \rho_{22}}} & -\sqrt{\rho_{11} - \lambda_{-}} \end{pmatrix}$$

$$= \frac{1}{(\Delta\lambda)^{\frac{3}{2}}} \left[ (\lambda_{+} - \rho_{22})^{\frac{3}{2}} + \frac{|\rho_{12}|^{2}}{\sqrt{\rho_{11} - \lambda_{-}}} + \frac{|\rho_{12}|^{2}}{\sqrt{\lambda_{+} - \rho_{22}}} - \frac{|\rho_{12}|^{2}\sqrt{\rho_{11} - \lambda_{-}}}{(\lambda_{+} - \rho_{22})} \right].$$

51 the differences between the quantum metrology (QM) state fidelity

$$\tilde{F} = P_0 + (1 - P_0) |\langle \psi_t | \tilde{N} | \psi_t \rangle|^2 = \rho_{11} = 1 - \rho_{22} \le 1$$

 $_{52}$  and its principle component fidelity  $F-\tilde{F}$  can be calculated numerically in parameters setup  $_{53}$  as

$$\alpha = \cos\frac{\Theta}{2}, \beta = e^{i\phi}\sin\frac{\Theta}{2}$$

54 with

$$P_0 \in [0,1], \ \Theta \in [0,2\pi], \ \phi \in [0,2\pi].$$

55 Both of them are  $\phi$ -independent, the numerical results as shown in Fig. S2 confirms that the 56 fidelity of principle component in come special parameter zone of  $\Theta$ ,  $P_0$  shall larger than the 57 QM state.

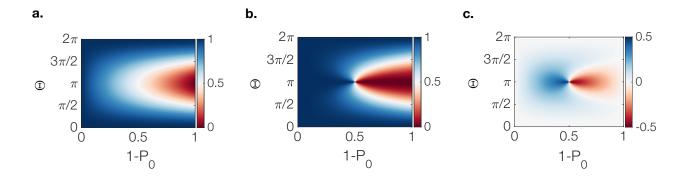


Figure S2: Fidelity results based on the theoretical model. a,b, State fidelity  $\tilde{F}$  without QC optimization and F with QC optimization as functions of  $1 - P_0$  and  $\Theta$ . c, Fidelity enhancement  $F - \tilde{F}$  achieved by the QM+QC method.

#### 58 1.2 Quantum Fisher Information

<sup>59</sup> We begin by considering measurement precision in a sensing process. For example, using a ruler to measure an unknown length d, we perform N independent measurements to obtain a set of samples  $\{d_i\}$ . Due to inevitable measurement errors, each  $d_i$  slightly deviates from the true value, and the precision of the estimation  $\hat{d}$  improves as this deviation decreases. In classical statistics, the Fisher information quantifies the lower bound of such estimation errors.

In QM, the sensing outcomes arise from quantum evolution rather than classical sampling. 66 The corresponding limit of precision is given by the quantum Fisher information (QFI), 67 which determines the minimum achievable variance in estimating a parameter  $\xi$  encoded in 68 a quantum state  $\rho(\xi)$ :

$$\operatorname{Var}[\hat{\xi}] \ge \frac{1}{n \mathcal{F}[\rho(\xi)]},$$
 (S10)

69 where n denotes the number of independent measurements. Here,  $\mathcal{F}[\rho(\xi)]$  measures the 70 sensitivity of the quantum state  $\rho(\xi)$  to changes in the parameter  $\xi$ , and is defined as

$$\mathcal{F}[\rho(\xi)] = \text{Tr}[\rho(\xi)L^2], \tag{S11}$$

71 with L being the symmetric logarithmic derivative (SLD) operator satisfying

$$\frac{\partial \rho(\xi)}{\partial \xi} = \frac{1}{2} \left( L \rho(\xi) + \rho(\xi) L \right). \tag{S12}$$

The core of calculating the QFI lies in solving the SLD. Here we employ the spectral decomposition of the density matrix, since the quantum states under consideration can be

74 mixed in general. The density operator is expressed in terms of its eigenvalues and eigenvec-75 tors as  $\rho = \sum_k s_k |k\rangle \langle k|$ , where  $s_k$  are the eigenvalues and  $|k\rangle$  the corresponding eigenvectors. 76 Projecting the SLD equation onto the eigenbasis  $\{|k\rangle\}$  gives

$$\langle i|\dot{\rho}|j\rangle = \frac{1}{2} \left( \langle i|L\rho|j\rangle + \langle i|\rho L|j\rangle \right) = \frac{s_i + s_j}{2} L_{ij}. \tag{S13}$$

77 This leads to the spectral decomposition form of the SLD:

$$L_{ij} = \begin{cases} \frac{2\langle i|\dot{\rho}|j\rangle}{s_i + s_j}, & s_i + s_j > 0, \\ 0, & s_i = s_j = 0. \end{cases}$$
 (S14)

78 For the diagonal elements (i = j) with  $s_i > 0$ ,

$$L_{ii} = \frac{\partial_{\xi} s_i}{s_i}.$$
 (S15)

79 The QFI can then be evaluated as

$$\mathcal{F}[\rho(\xi)] = \sum_{k: s_k > 0} \frac{(\partial_{\xi} s_k)^2}{s_k} + 2 \sum_{k,l: s_k + s_l > 0} \frac{(s_k - s_l)^2}{s_k + s_l} \left| \langle \psi_k | \partial_{\xi} \psi_l \rangle \right|^2.$$
 (S16)

80 For a pure state  $\rho = |\psi\rangle\langle\psi|$ , this expression reduces to

$$\mathcal{F} = 4(\langle \partial_{\xi} \psi | \partial_{\xi} \psi \rangle - |\langle \psi | \partial_{\xi} \psi \rangle|^2). \tag{S17}$$

In practical calculations, the partial derivative  $\dot{\rho}$  can be obtained numerically through a finite difference:

$$\partial_{\xi}\tilde{\rho}_{t} = \frac{\tilde{\rho}_{t}^{+} - \tilde{\rho}_{t}^{-}}{2\delta},\tag{S18}$$

where  $\tilde{\rho}_t^{\pm} = \tilde{U}_{\phi \pm \delta}(|\psi_0\rangle \langle \psi_0|)$ , and  $\delta$  is a small detuning parameter.

The optimization of quantum states on a quantum computer can be viewed as an anastates of the principal component analysis process, realized through eigen-decomposition. By identifying the eigenstate corresponding to the largest eigenvalue, one obtains the optimized quantum state  $\rho_{NR}$ .

#### 88 1.3 Noise model

Noise in quantum systems is inherently complex and diverse, and numerous theoretical mod-90 els have been developed to describe its various forms. Following the approach outlined in the 91 previous section, we have established a representative noise model to illustrate the optimiza-92 tion capability of the QM+QC method. In this section, we further extend our analysis by 93 introducing additional types of quantum noise channels. As shown in Fig. S3, we consider 94 three typical examples: the dephasing channel,

$$\rho \to E_0 \rho E_0^{\dagger} + E_1 \rho E_1^{\dagger}, \tag{S19}$$

95 where

110

$$E_0 = \sqrt{1 - p}I, \ E_1 = \sqrt{p}Z,$$
 (S20)

<sub>96</sub> the amplitude damping channel,

$$E_0 = \begin{bmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{bmatrix}, \quad E_1 = \begin{bmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{bmatrix}, \tag{S21}$$

97 and the depolarizing channel,

$$\rho \to (1-p)\rho + \frac{p}{3}(X\rho X + Y\rho Y + Z\rho Z). \tag{S22}$$

<sup>98</sup> Consistent with the main text, the enhancement in quantum Fisher information (QFI) is <sup>99</sup> employed as a quantitative measure to characterize the optimization performance achieved <sup>100</sup> by the QM+QC framework.

# SUPPLEMENTARY SECTION 2: RANDOM NOISE IN THE EXPERIMENT

We next consider the influence of an unstable magnetic field on the Ramsey interferome- $_{104}$  try experiment. In Ramsey interferometry, the population signal exhibits cosine interfer- $_{105}$  ence fringes that oscillate with the evolution time  $\tau$ . When the magnetic field experiences  $_{106}$  Gaussian-distributed fluctuations, either naturally or through controlled perturbations, these  $_{107}$  fluctuations modify the phase accumulation of the quantum superposition. Averaged over  $_{108}$  many repetitions, the net effect of such instability manifests as decoherence of the interference  $_{109}$  fringes.

Under an ideal static magnetic field B, the signal measured by a Ramsey sequence follows

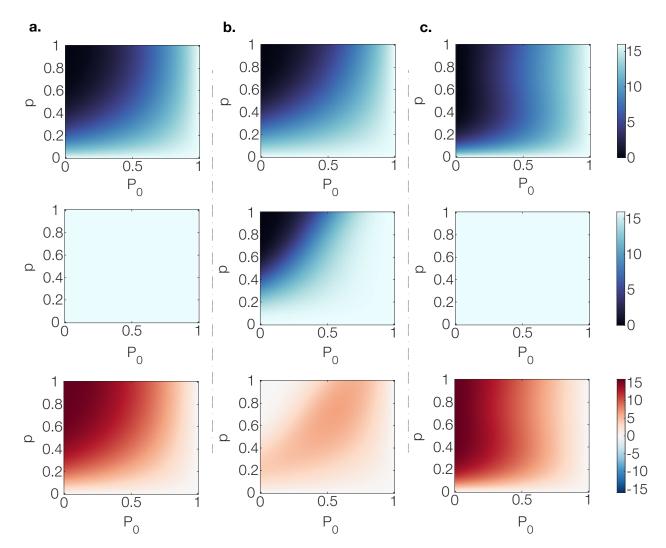


Figure S3: QM+QC results under different noise conditions. a–c, Quantum Fisher information (QFI) optimization results for the dephasing, amplitude-damping, and depolarizing channels, respectively. Each column, from top to bottom, shows: the QFI before QC optimization ( $\mathcal{F}_{QM}$ ), the QFI after QC optimization ( $\mathcal{F}_{QM+QC}$ ), and the corresponding QFI improvement ( $\Delta \mathcal{F} = \mathcal{F}_{QM+QC} - \mathcal{F}_{QM}$ ).

111 a simple cosine oscillation with time  $\tau$ :

$$\mathcal{P}(\tau) = \frac{1}{2} \left[ 1 + \cos(\Delta \omega \tau) \right], \tag{S23}$$

where  $\Delta \omega = \gamma (B - B_{\rm ref})$  is the frequency shift induced by the magnetic field deviation from a reference value  $B_{\rm ref}$ , and  $\gamma$  denotes the gyromagnetic ratio. The reference field  $B_{\rm ref}$  represents the static bias field typically present in magnetic-field sensing experiments.

In each experimental repetition, the magnetic field B is sampled from a Gaussian distribution  $\mathcal{N}[B_0, (B_0\varsigma)^2]$ , where  $B_0$  is the average value of the magnetic field to be measured and

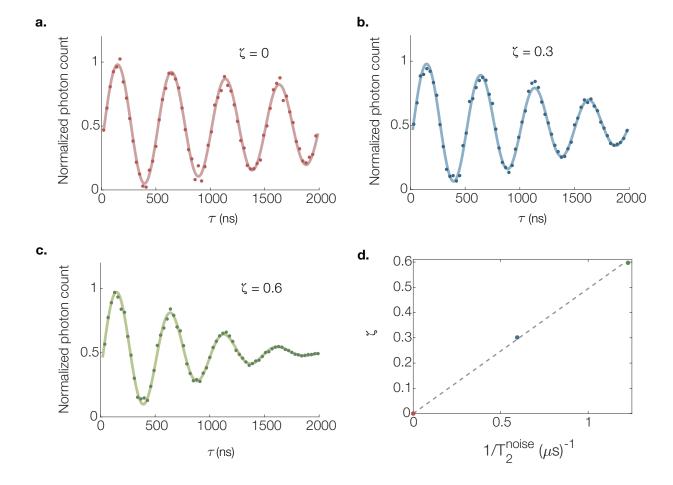


Figure S4: Effects of different noise intensities on Ramsey signals. a-c, The attenuation of the Ramsey signal under  $\varsigma = 0, 0.3, 0.6$ . We can obtain the equivalent decoherence time caused by noise by fitting it with a formula:  $e^{-\tau/T_2^*}e^{-\left(\tau/T_2^{noise}\right)^2}$ . d, Mapping relationship between equivalent decoherence time  $T_2^{noise}$  and noise intensity  $\sigma$ .

 $_{117}$   $\varsigma$  is standard deviation in percentage. This leading to a corresponding Ramsey signal

$$\mathcal{P}_i(\tau) = \frac{1}{2} \left[ 1 + \cos \left( \gamma (B_i - B_{\text{ref}}) \tau \right) \right]. \tag{S24}$$

118 The ensemble-averaged signal can then be obtained by integrating over the Gaussian distri-119 bution of magnetic fields:

$$\bar{\mathcal{P}}(\tau) = \int_{-\infty}^{\infty} \frac{1}{2\sqrt{2\pi} B_0 \varsigma} \left[ 1 + \cos\left(\gamma (B - B_{\text{ref}})\tau\right) \right] e^{-\frac{1}{2} \left(\frac{B - B_0}{B_0 \varsigma}\right)^2} dB. \tag{S25}$$

120 Neglecting the constant term and using the linearity of integration, the Fourier transform of

121 the Gaussian function yields

$$\int \cos(\gamma (B - B_{\text{ref}})\tau) e^{-\frac{1}{2} \left(\frac{B - B_0}{B_0 \varsigma}\right)^2} dB \propto \cos(\gamma (B_0 - B_{\text{ref}})\tau) e^{-\frac{1}{2} (\gamma B_0 \varsigma \tau)^2}.$$
 (S26)

122 Consequently, the ensemble-averaged Ramsey signal takes the form

$$\bar{\mathcal{P}}(\tau) = \frac{1}{2} \left[ 1 + e^{-\frac{1}{2}(\gamma B_0 \varsigma \tau)^2} \cos(\gamma (B_0 - B_{\text{ref}})\tau) \right]. \tag{S27}$$

The result shows that while the Ramsey oscillation frequency remains unchanged, its amplitude is modulated by a Gaussian envelope  $e^{-\frac{1}{2}(\gamma B_0 \varsigma \tau)^2}$ . This behavior is equivalent to decoherence induced by quasi-static magnetic noise, and can thus be expressed as  $e^{-\frac{1}{2}(\tau/T_2^{\text{noise}})^2}$ , where the corresponding dephasing time is  $T_2^{\text{noise}} = 1/(\gamma B_0 \varsigma)$ .

#### 127 3 SUPPLEMENTARY SECTION 3: LOSS FUNCTION

As discussed in the main text, the objective of the loss function is to obtain a target operator by minimizing its value through iterative optimization. Here, we design an appropriate loss function to achieve the diagonalization of a density matrix. Any density matrix can be expressed in its spectral decomposition as  $\rho = \sum_{j=0}^{\mathcal{M}-1} \lambda_j |\psi_j\rangle \langle \psi_j|$ , where  $\{|\psi_j\rangle\}$  form an orthogonal basis and  $\mathcal{M} = 2^m$  denotes the Hilbert space dimension of an m-qubit system. Without loss of generality, the eigenvalues are arranged in descending order,  $\lambda_0 \geq \lambda_1 \geq 134 \cdots \geq \lambda_{\mathcal{M}-1}$ . If a unitary transformation U can be found such that it maps  $|\psi_j\rangle$  to the computational basis state  $|j\rangle$ , i.e.

$$\tilde{\rho}_t = U\rho U^{\dagger} = \sum_{j=0}^{\mathcal{M}-1} \lambda_j |j\rangle \langle j|, \qquad (S28)$$

then measurements in the computational basis  $\{|j\rangle\}$  directly yield the eigenvalues  $\lambda_j$  as outcome probabilities. For generic states, however, efficiently finding such a unitary U is generally intractable.

To formulate a practical loss function, we introduce a semidefinite, positive, and non-140 degenerate Hermitian operator P, whose eigenstates are the computational basis states  $|j\rangle$ 141 with corresponding eigenvalues  $s_j$ , such that  $P = \sum_{j=0}^{\mathcal{M}-1} s_j |j\rangle \langle j|$ . Unlike the eigenvalues 142 of  $\rho$ , we arrange the set  $\{s_j\}$  in ascending order,  $0 \le s_0 < s_1 < \cdots < s_{\mathcal{M}-1}$ , and impose 143 the normalization condition  $\sum_j s_j = 1$ . Such an operator is straightforward to construct. A 144 convenient choice is a diagonal matrix with elements  $\{0, 1, 2, \cdots, \mathcal{M}-1\}$ , normalized by 145 the factor  $\mathcal{M}(\mathcal{M}-1)/2$ . In the Pauli basis, it can be written as

$$P = \frac{1}{\mathcal{M}(\mathcal{M} - 1)} \sum_{j=1}^{n} 2^{j-1} (\sigma_z^j + 1),$$
 (S29)

where  $\sigma_z^j$  denotes the Pauli-Z operator acting on the jth qubit [1].

We assert that a unitary operator U that minimizes the expectation value  $\text{Tr}[U\rho U^{\dagger}P]$  will diagonalize the density matrix  $\rho$  in the computational basis. The operator P can be any Hermitian matrix satisfying the conditions described above. The task therefore reduces to finding the optimal unitary U. In practice, we input the state  $\rho$  into a PQC represented by 151  $U(\boldsymbol{\theta})$ , and measure the expectation value of P at the circuit output. For instance, evaluating 152 the operator P defined in Eq. S29 requires only a simultaneous Pauli-Z measurement on 153 all qubits, which is experimentally straightforward. The corresponding objective function is 154 defined as

$$L(\boldsymbol{\theta}) = \text{Tr} \left[ U(\boldsymbol{\theta}) \rho U^{\dagger}(\boldsymbol{\theta}) \cdot P \right]. \tag{S30}$$

155 By minimizing this objective function over the parameter space using a suitable classical 156 optimization algorithm, one can obtain a good approximation to the target unitary U.

### 157 4 SUPPLEMENTARY SECTION 4: PQC MODEL

To realize QC optimization, we employ a PQC approach. For small systems, the PQC structure can be relatively simple. For instance, in the single-qubit case, only two rotation gates along distinct axes are sufficient, rendering the optimization process rather straightforward. However, as the number of qubits increases, the choice of PQC architecture becomes crucial, as it can substantially influence the convergence and final performance of the QC optimization. This aspect is further analyzed in the following section.

We first outline the complete PQC workflow. After the noisy sensing stage, the resulting quantum state  $\tilde{\rho}_t$  is transferred into a quantum processor (some transmission losses may loss occur in practice, although they do not affect the subsequent PQC procedure). The state then evolves under a parameterized unitary transformation  $U(\boldsymbol{\theta})$ , which forms the variational component of the hybrid quantum-classical optimization loop.

During the optimization process, the parameterized unitary operation is applied to the 170 input quantum state, after which the corresponding loss function is evaluated (the form and 171 physical meaning of this function were introduced in the previous section). To obtain the 172 gradient required for parameter updates, one of the circuit parameters is perturbed by a fixed 173 amount when implementing the parameterized operation. Unlike conventional differentiation

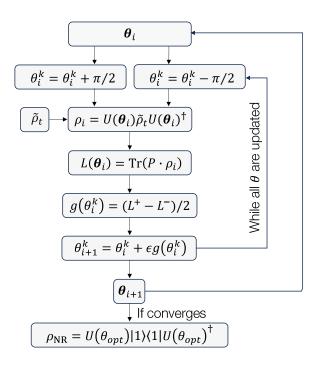


Figure S5: PQC Flowchart.

methods that rely on infinitesimal variations, it has been proven that for rotation operations, shifting a parameter by  $\pm \pi/2$  can yield an exact analytical gradient. The computed gradients are then used to iteratively update the circuit parameters toward the loss minimum.

As the optimization proceeds, the parameters are progressively refined, and for a well178 structured PQC model, the iterative process converges to a physically meaningful solution.
179 The key objective of this section is therefore to explore the characteristics of an effective
180 PQC design. In practice, the design considerations primarily involve the number of trainable
181 parameters, the arrangement of two-qubit entangling gates, the overall circuit depth, and the
182 specific choice of gate set.

We next introduce the circuit models explored in this work. To illustrate the importance 184 of PQC architecture design more intuitively, we first present a set of suboptimal circuit 185 configurations. As shown in Fig. S6a, although the fidelity increases markedly when the 186 circuit depth grows from one to two layers, further increasing the number of layers to four 187 yields almost no improvement. This observation indicates that the ansatz suffers from an 188 expressibility or train-ability limitation, and therefore does not constitute a suitable PQC 189 model for our purpose. Fig. S6b then presents a properly designed PQC architecture, which 190 exhibits distinct convergence behavior and achieves superior final optimization performance.

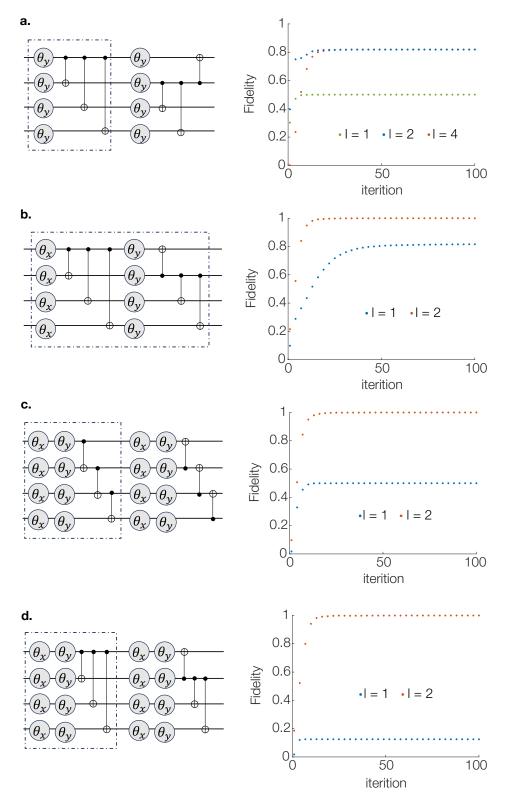


Figure S6: The impact of different PQC on the optimization process. a-d, The left side is a schematic diagram of PQC. The area within the dashed box is called a layer. The right side shows the optimization results for different number of layers l.

<sup>191</sup> These results highlight the crucial role of circuit structure in determining both convergence <sup>192</sup> speed and optimization accuracy.

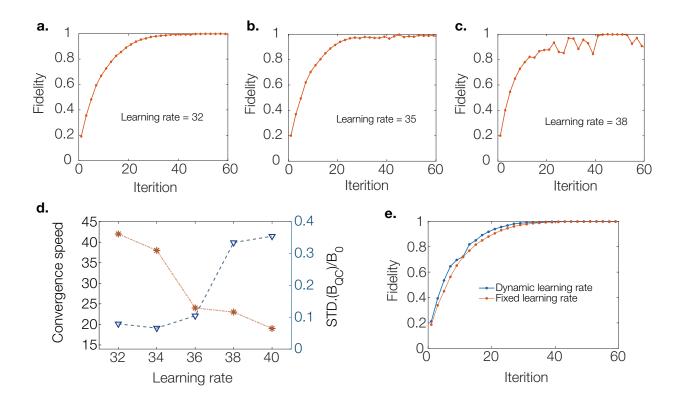


Figure S7: Impact of different learning rates on PQC performance. a-c, Evolution of fidelity during the optimization process for different learning rates. d, Relationship between convergence speed and the standard deviation of the optimized results as a function of learning rate. Here, convergence speed denotes the number of iterations required to reach convergence. e, Comparison between dynamic and fixed learning rates, showing that a dynamic learning-rate schedule achieves faster convergence without increasing the standard deviation.

As demonstrated above, different PQC architectures exhibit distinct optimization behaviors. Even for an identical circuit structure, however, the choice of optimization hyperparameters can strongly influence the convergence process. As shown in Fig. S7, we examine iteration step sizes of 32, 35, and 38, and observe that the corresponding convergence speeds differ noticeably. Although a larger step size can accelerate convergence, it cannot be increased arbitrarily. As illustrated in Fig. S7d, an excessively large step size causes pronounced oscillations after apparent convergence, leading to a higher standard deviation in the optimized results. This issue can be mitigated by adopting a dynamic learning rate. As shown in Fig. S7e, employing a properly designed learning-rate schedule that gradually decays with the number of iterations enables faster convergence while maintaining a low

203 standard deviation.

## $_{204}$ References

Tao Xin, Liangyu Che, Cheng Xi, Amandeep Singh, Xinfang Nie, Jun Li, Ying Dong,
 and Dawei Lu. Experimental quantum principal component analysis via parametrized
 quantum circuits. Phys. Rev. Lett., 126(11):110502, 2021.