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## Methods of Error Estimation for Delay Power Spectra in 21 cm Cosmology

JIANRONG TAN<sup>1,2</sup>, ADRIAN LIU<sup>2</sup>, NICHOLAS S. KERN<sup>3</sup>, ZARA ABDURASHIDOVA,<sup>4</sup> JAMES E. AGUIRRE,<sup>1</sup>  
PAUL ALEXANDER,<sup>5</sup> ZAKI S. ALI,<sup>4</sup> YANGA BALFOUR,<sup>6</sup> ADAM P. BEARDSLEY,<sup>7</sup> GIANNI BERNARDI,<sup>8,9,6</sup>  
TASHALEE S. BILLINGS,<sup>1</sup> JUDD D. BOWMAN,<sup>7</sup> RICHARD F. BRADLEY,<sup>10</sup> PHILIP BULL,<sup>11</sup> JACOB BURBA,<sup>12</sup> STEVEN CAREY,<sup>5</sup>  
CHRISTOPHER L. CARILLI,<sup>13</sup> CARINA CHENG,<sup>4</sup> DAVID R. DEBOER,<sup>4</sup> MATT DEXTER,<sup>4</sup> ELOY DE LERA ACEDO,<sup>5</sup>  
JOSHUA S. DILLON<sup>4</sup>, JOHN ELY,<sup>5</sup> AARON EWALL-WICE,<sup>4</sup> NICOLAS FAGNONI,<sup>5</sup> RANDALL FRITZ,<sup>6</sup>  
STEVE R. FURLANETTO,<sup>14</sup> KINGSLEY GALE-SIDES,<sup>5</sup> BRIAN GLENDENNING,<sup>13</sup> DEEPTHI GORTHI,<sup>4</sup> BRADLEY GREIG,<sup>15</sup>  
JASPER GROBBELAAR,<sup>6</sup> ZIYAAD HALDAY,<sup>6</sup> BRYNA J. HAZELTON,<sup>16,17</sup> JACQUELINE N. HEWITT,<sup>18</sup> JACK HICKISH,<sup>4</sup>  
DANIEL C. JACOBS,<sup>7</sup> AUSTIN JULIUS,<sup>6</sup> JOSHUA KERRIGAN,<sup>12</sup> PIYANAT KITTIWISIT,<sup>19</sup> SAUL A. KOHN,<sup>1</sup>  
MATTHEW KOLOPANIS,<sup>7</sup> ADAM LANMAN,<sup>12</sup> PAUL LA PLANTE,<sup>4</sup> TELALO LEKALAKE,<sup>6</sup> DAVID MACMAHON,<sup>4</sup>  
LOURENCE MALAN,<sup>6</sup> CRESSHIM MALGAS,<sup>6</sup> MATTHYS MAREE,<sup>6</sup> ZACHARY E. MARTINOT,<sup>1</sup> EUNICE MATSETELA,<sup>6</sup>  
ANDREI MESINGER,<sup>20</sup> MATHAKANE MOLEWA,<sup>6</sup> MIGUEL F. MORALES,<sup>16</sup> TSHGOFALANG MOSIANE,<sup>6</sup> STEVEN G. MURRAY,<sup>7</sup>  
ABRAHAM R. NEBEN,<sup>3</sup> BOJAN NIKOLIC,<sup>5</sup> CHUNEETA D. NUNHOKEE,<sup>4</sup> AARON R. PARSONS,<sup>4</sup> NIPANJANA PATRA,<sup>4</sup>  
SAMANTHA PIETERSE,<sup>6</sup> JONATHAN C. POBER,<sup>12</sup> NIMA RAZAVI-GHODS,<sup>5</sup> JON RINGUETTE,<sup>16</sup> JAMES ROBNETT,<sup>13</sup>  
KATHRYN ROSIE,<sup>6</sup> PETER SIMS,<sup>12</sup> SAURABH SINGH,<sup>2</sup> CRAIG SMITH,<sup>6</sup> ANGELO SYCE,<sup>6</sup> NITHYANANDAN THYAGARAJAN,<sup>7,13</sup>  
PETER K. G. WILLIAMS,<sup>21,22</sup> AND HAOXUAN ZHENG<sup>18</sup>

<sup>1</sup>*Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104, USA*

<sup>2</sup>*Department of Physics and McGill Space Institute, McGill University, Montreal, QC, Canada H3A 2T8*

<sup>3</sup>*Department of Physics, Massachusetts Institute of Technology, Cambridge, MA, USA*

<sup>4</sup>*Department of Astronomy, University of California, Berkeley, CA*

<sup>5</sup>*Cavendish Astrophysics, University of Cambridge, Cambridge, UK*

<sup>6</sup>*SKA-SA, Cape Town, South Africa*

<sup>7</sup>*School of Earth and Space Exploration, Arizona State University, Tempe, AZ*

<sup>8</sup>*Department of Physics and Electronics, Rhodes University, PO Box 94, Grahamstown, 6140, South Africa*

<sup>9</sup>*INAF-Istituto di Radioastronomia, via Gobetti 101, 40129 Bologna, Italy*

<sup>10</sup>*National Radio Astronomy Observatory, Charlottesville, VA*

<sup>11</sup>*School of Physics & Astronomy, Queen Mary University of London, London, UK*

<sup>12</sup>*Department of Physics, Brown University, Providence, RI*

<sup>13</sup>*National Radio Astronomy Observatory, Socorro, NM*

<sup>14</sup>*Department of Physics and Astronomy, University of California, Los Angeles, CA*

<sup>15</sup>*School of Physics, University of Melbourne, Parkville, VIC 3010, Australia*

<sup>16</sup>*Department of Physics, University of Washington, Seattle, WA*

<sup>17</sup>*eScience Institute, University of Washington, Seattle, WA*

<sup>18</sup>*Department of Physics, Massachusetts Institute of Technology, Cambridge, MA*

<sup>19</sup>*School of Chemistry and Physics, University of KwaZulu-Natal, Westville Campus, Durban, South Africa*

<sup>20</sup>*Scuola Normale Superiore, 56126 Pisa, PI, Italy*

<sup>21</sup>*Center for Astrophysics, Harvard & Smithsonian, 60 Garden St., Cambridge, MA*

<sup>22</sup>*American Astronomical Society, 1667 K Street NW, Suite 800, Washington, DC 20006*

## ABSTRACT

Precise measurements of the 21 cm power spectrum are crucial for understanding the physical processes of hydrogen reionization. Currently, this probe is being pursued by low-frequency radio interferometer arrays. As these experiments come closer to making a first detection of the signal, error estimation will play an increasingly important role in setting robust measurements. Using the delay power spectrum approach, we have produced a critical examination of different ways that one can estimate error bars on the power spectrum. We do this through a synthesis of analytic work, simulations of toy models, and tests on small amounts of real data. We find that, although computed independently,

Corresponding author: Jianrong Tan

[jianrong@sas.upenn.edu](mailto:jianrong@sas.upenn.edu)

the different error bar methodologies are in good agreement with each other in the noise-dominated regime of the power spectrum. For our preferred methodology, the predicted probability distribution function is consistent with the empirical noise power distributions from both simulated and real data. This diagnosis is mainly in support of the forthcoming HERA upper limit, and also is expected to be more generally applicable.

## 1. INTRODUCTION

The Epoch of Reionization (EoR)—when neutral hydrogen in the intergalactic medium (IGM) was ionized by photons from early galaxies and active galactic nuclei—remains one of the most exciting frontiers in modern astrophysics and cosmology. Precise measurements of this era will significantly enhance our understanding on the origin of very first stars, the process of galaxy formation and the thermal history of the IGM (Barkana & Loeb 2001; Dayal & Ferrara 2018). Some measurements, such as those of the optical depth of Cosmic Microwave Background (CMB) photons (Planck Collaboration et al. 2020), the Gunn-Peterson trough in distant quasar spectra (Becker et al. 2001; Fan et al. 2006; Bolton et al. 2011; Becker et al. 2015), quasar damping wings (Davies et al. 2018), and the decrease in the number density and the clustering trends of Ly- $\alpha$  emitters at high redshifts (Stark et al. 2010; Ouchi et al. 2010; Bosman et al. 2018), have already established the basic parameters of the EoR. Collectively, they suggest that reionization is a process which probably began at  $z \gg 10$  and ended around  $z \approx 6$ . However, the aforementioned probes paint an indirect and incomplete picture of the EoR. For example, CMB measurements are integral constraints over redshift, making the extraction of detailed information technically difficult (often involving subtle kinetic Sunyaev-Zel’dovich effect or polarization measurements); Ly $\alpha$  photons suffer from severely saturated absorption that makes it difficult for them to probe earlier times than the end of reionization; and low-mass galaxies (i.e., those thought to be responsible for supplying a large fraction of ionizing photons) are too faint to be directly detected. A complementary probe capable of making direct observations of the EoR is therefore desirable.

A strong candidate for a direct probe of reionization is the 21 cm line. Arising from the “spin flip” transition in the hyperfine structure of atomic hydrogen, the 21 cm line is a promising way to directly trace the evolution of HI regimes on different spatial scales and to eventually provide a comprehensive three-dimensional picture throughout the history of reionization (Furlanetto et al. 2006; Morales & Wyithe 2010; Pritchard & Loeb 2012; Liu & Shaw 2020). Current experimental efforts are focused on slightly more modest—but still ambitious—observables. One example is the global 21 cm signal,

which is a single spectrum of 21 cm absorption or emission averaged over the entire angular area of the sky (Bowman et al. 2008; Singh et al. 2018). Recently, the Experiment to Detect the Global Epoch of reionization Step team (EDGES) reported a tentative detection of a 21 cm absorption signature at  $z \sim 17$  (Bowman et al. 2018a), although this result remains controversial (Hills et al. 2018; Bowman et al. 2018b; Bradley et al. 2019; Singh & Subrahmanyan 2019; Sims & Pober 2020). Global signal measurements are complemented by experimental efforts to map spatial fluctuations in the 21 cm brightness temperature field. Most such efforts currently focus on a measurement of the power spectrum, i.e., the variance in Fourier space. Power spectrum measurements have the potential to significantly improve constraints on cosmological and astrophysical parameters of reionization models, and to potentially even discover new fundamental physics (e.g., McQuinn et al. 2006; Pober et al. 2014; Greig & Mesinger 2015; Pober et al. 2015; Kern et al. 2017; Greig & Mesinger 2017; Hassan et al. 2017; Park et al. 2019; Ghara et al. 2020). Typically, these measurements are pursued by low-frequency radio interferometer arrays, such as the Murchison Widefield Array<sup>1</sup> (MWA; Tingay et al. 2013; Bowman et al. 2013), the Low Frequency Array<sup>2</sup> (LOFAR; van Haarlem et al. 2013), the Donald C. Backer Precision Array for Probing the Epoch of Reionization<sup>3</sup> (PAPER; Parsons et al. 2010), the Hydrogen Epoch of Reionization Array<sup>4</sup> (HERA; DeBoer et al. 2017), and the Square Kilometre Array<sup>5</sup> (SKA; Mellema et al. 2013; Koopmans et al. 2015). Although no experiment has yet to claim a detection of the 21 cm power spectrum at redshifts relevant to the EoR, steady progress has been made in recent years in the form of increasingly stringent and robust upper limits (Dillon et al. 2014, 2015; Beardsley et al. 2016; Patil et al. 2017; Barry et al. 2019; Kolopanis et al. 2019; Li et al. 2019; Mertens et al. 2020; Trott et al. 2020).

<sup>1</sup> <http://www.mwatelescope.org>

<sup>2</sup> <http://www.lofar.org>

<sup>3</sup> <http://eor.berkeley.edu>

<sup>4</sup> <https://reionization.org>

<sup>5</sup> <https://www.skatelescope.org>

In this paper, we tackle the crucial problem of error estimation in the context of 21 cm power spectrum measurements. While an extensive literature on power spectrum error estimation exists for CMB measurements and galaxy surveys, there are several challenges that are unique to 21 cm cosmology. Chief amongst these is the fact that any measured signals will be strongly contaminated by the foregrounds, which are generally 4 to 5 orders of magnitude stronger in temperature (de Oliveira-Costa et al. 2008; Jelić et al. 2008; Bernardi et al. 2009). To overcome this obstacle, some collaborations pursue a strategy of foreground subtraction, where models of foreground emission are subtracted from the data (e.g., Harker et al. 2009; Bernardi et al. 2011; Cho et al. 2012; Chapman et al. 2012; Shaw et al. 2015). Different approaches to foreground subtraction make different assumptions (see Liu & Shaw 2020 for examples), but all face the same problem of attempting to subtract a large contaminant from a large raw signal to reveal a small cosmological signature. With empirical constraints on the low-frequency radio sky being relatively scarce and generally imprecise, the chances of mis-subtraction are high. Errors in such a subtraction process as well as the effects of subtraction residuals must therefore be propagated through to a final power spectrum estimate.

In this paper, however, we do not tackle the problem of error propagation in the context of foreground subtraction; instead, we consider error estimation in the context of foreground avoidance, where one aims to make cosmological measurements exclusively in Fourier modes where foregrounds are expected to be subdominant. Key to this is the notion of the foreground wedge, a regime in Fourier space beyond which spectrally smooth foregrounds cannot extend if observed using an ideal interferometer (Datta et al. 2010; Parsons et al. 2012b; Vedantham et al. 2012; Morales et al. 2012; Trott et al. 2012; Thyagarajan et al. 2013; Hazelton et al. 2013; Liu et al. 2014a). The limitation of foregrounds to the wedge is a theoretically robust notion (Liu & Shaw 2020), and in principle one can make foreground-free measurements simply by avoiding the regime. In practice, observations are never made using perfect interferometers, and instrumental systematics such as having non-identical antenna elements, cable reflections, and cross couplings (e.g., Kern et al. 2019, 2020a) complicate one’s foreground mitigation efforts. These complications can result in the appearance of contaminants outside of the foreground wedge, and in this paper we define and tackle the problem of error estimation in two regimes: a noise-dominated regime and a signal-dominated regime (whether these signals could be foregrounds, systematics, or any other coherent signals).

Through a combination of analytic work, simulations of toy models, and tests on small amounts of real data, we critically examine different ways in which one can place error bars on 21 cm delay power spectra. Our goal is to produce a “buyer’s guide” that enumerates the advantages and disadvantages of various error estimation methods. Understanding these strengths and weaknesses are crucial for setting upper limits, diagnosing systematics, interpreting the results of null tests, and for the design and optimization of future telescopes (Morales 2005; McQuinn et al. 2006; Parsons et al. 2012a). Although we will focus primarily on the delay power spectrum-style analysis (Parsons et al. 2012b) in support of recent HERA upper limits (HERA Collaboration 2021), we expect many of our results to be more generally applicable.

This paper is organized as follows: in Section 2, we review the basics of power spectrum estimation using the delay spectrum technique, establishing our notation. In Section 3 we propose several methods for estimating errors in 21 cm delay power spectra. These approaches are then compared and contrasted using simulations and real data in Section 4. We then discuss the strengths and weaknesses of each error estimation method in Section 5 before summarizing our conclusions in Section 6. For readers’ convenience, we provide dictionaries for a number of quantities defined in this paper in Tables 1 and 2.

## 2. POWER SPECTRUM ESTIMATION VIA THE DELAY SPECTRUM

In this section we review the delay spectrum approach to 21 cm power spectrum estimation (Parsons et al. 2012b) using the the language of the quadratic estimator (QE) formalism (Liu & Tegmark 2011) that we adopt in this paper.

The delay spectrum technique enables power spectra to be estimated using just a single baseline of a radio interferometer, with fluctuations in the 21 cm signal probed primarily in the line-of-sight direction via spectral information. The starting point is the visibility  $V(\mathbf{b}, \nu)$  measured by an interferometer’s baseline  $\mathbf{b}$  at frequency  $\nu$ . Under the flat-sky limit, it is given by

$$V(\mathbf{b}, \nu) = \int I(\boldsymbol{\theta}, \nu) A(\boldsymbol{\theta}, \nu) \exp\left(-i2\pi\frac{\nu}{c}\mathbf{b} \cdot \boldsymbol{\theta}\right) d^2\theta, \quad (1)$$

where  $c$  is the speed of light,  $\boldsymbol{\theta}$  is the angular sky position,  $I(\boldsymbol{\theta}, \nu)$  is the source intensity function, and  $A(\boldsymbol{\theta}, \nu)$  is the primary beam function. If we express  $I(\boldsymbol{\theta}, \nu)$  in terms of its Fourier transform  $\tilde{I}(\mathbf{u}, \eta)$ , i.e.,

$$I(\boldsymbol{\theta}, \nu) = \int \tilde{I}(\mathbf{u}, \eta) e^{i2\pi(\mathbf{u} \cdot \boldsymbol{\theta} + \eta\nu)} d^2u d\eta, \quad (2)$$

then our visibility equation becomes

$$V(\mathbf{b}, \nu) = \int \tilde{I}(\mathbf{u}, \eta) A(\boldsymbol{\theta}, \nu) e^{i2\pi(\mathbf{u}\cdot\boldsymbol{\theta} + \eta\nu - \mathbf{b}_\lambda\cdot\boldsymbol{\theta})} d^2u d\eta d^2\theta$$

$$= \int \tilde{I}(\mathbf{u}, \eta) \tilde{A}(\mathbf{b}_\lambda - \mathbf{u}, \nu) e^{i2\pi\eta\nu} d^2u d\eta, \quad (3)$$

where we have defined  $\mathbf{b}_\lambda \equiv \frac{\nu}{c}\mathbf{b}$  as the normalized baseline vector for baseline  $\mathbf{b}$  in units of wavelength. In the angular directions, we see that a visibility has a response to  $\mathbf{u}$  modes centred around  $\mathbf{b}_\lambda$ . If the primary beam  $A$  is fairly broad,  $\tilde{A}$  will be highly compact and the majority of the integral will be sourced from  $\mathbf{u} \approx \mathbf{b}_\lambda$ . We will use this fact later. From this, one sees that a visibility  $V(\mathbf{b}, \nu)$  is a linear function of  $\tilde{I}(\mathbf{u}, \eta)$ . This quantity is directly related to the cylindrical power spectrum  $P(\mathbf{u}, \eta)$ , which decomposes power into Fourier wavenumbers perpendicular to the line of sight ( $\mathbf{u}$ ) and parallel to the line of sight ( $\eta$ ), and is formally defined as

$$\langle \tilde{I}^*(\mathbf{u}, \eta) \tilde{I}(\mathbf{u}', \eta') \rangle \equiv \delta^D(\mathbf{u} - \mathbf{u}') \delta^D(\eta - \eta') P(\mathbf{u}, \eta). \quad (4)$$

Such a power spectrum can be recast into more conventional cosmological coordinates via the relations<sup>6</sup>

$$\mathbf{k}_\perp = \frac{2\pi\mathbf{u}}{D_c}; \quad k_\parallel = \frac{2\pi\nu_{21}H_0E(z)}{c(1+z)^2}\eta, \quad (5)$$

where  $D_c$  is the line-of-sight comoving distance,  $\nu_{21}$  is the rest frequency of the 21 cm line,  $H_0$  is the Hubble parameter today, and  $E(z) \equiv \sqrt{\Omega_\Lambda + \Omega_m(1+z)^3}$ , with  $\Omega_\Lambda$  and  $\Omega_m$  as the normalized dark energy and matter density, respectively.

Since the power spectrum is a quadratic function of the Fourier representation of the sky, we expect that one should be able to estimate the power spectrum by forming some quadratic function of visibilities. However, directly squaring some functions of the visibilities will incur a noise bias because noise that is symmetrically distributed about zero will have a positive contribution that does not average down with cumulative samples. Fortunately, the noise bias can be avoided by cross-multiplying nominally identical measurements rather than by squaring a single measurement. For instance, one might choose to form quadratic combinations of data from adjacent time samples of a single baseline's time stream, or perhaps to cross-multiply the time streams from two redundant baselines that satisfy  $\mathbf{b}_1 = \mathbf{b}_2 = \mathbf{b}$  for some  $\mathbf{b}$ . In this paper, we will consider power spectrum measurements that are formed from

<sup>6</sup> In addition to mapping the arguments of  $P$ , there is also an additional multiplicative constant; see Liu et al. (2014a) for explicit expressions.

cross-multiplications in *both* time and different copies of an identical baseline. Utilizing both types of cross-multiplications has the advantage of avoiding skewness in the probability distributions of the measured power spectra, simplifying the interpretation of our results. This is discussed in Appendix A. In this section, however, we will—for simplicity—suppress explicit reference to the data time stream and use notation that explicitly refers to cross-correlating different baselines. Given a pair of redundant baselines  $\mathbf{b}_1$  and  $\mathbf{b}_2$ , we stack their measuring visibilities at multiple frequencies  $\nu_1, \nu_2, \dots$  at single time instants into two data vectors  $\mathbf{x}_1$  and  $\mathbf{x}_2$ , such that

$$\mathbf{x}_1 = \begin{pmatrix} V(\mathbf{b}_1, \nu_1) \\ V(\mathbf{b}_1, \nu_2) \\ \vdots \end{pmatrix}; \quad \mathbf{x}_2 = \begin{pmatrix} V(\mathbf{b}_2, \nu_1) \\ V(\mathbf{b}_2, \nu_2) \\ \vdots \end{pmatrix}. \quad (6)$$

To make an explicit connection between visibilities and power spectra, we must examine the statistical properties of these data vectors. For quadratic statistics the key quantity is the covariance matrix  $\mathbf{C}^{12} \equiv \langle \mathbf{x}_1 \mathbf{x}_2^\dagger \rangle$ , which can be written as

$$\mathbf{C}_{ij}^{12} \equiv \langle V(\mathbf{b}_1, \nu_i) V^*(\mathbf{b}_2, \nu_j) \rangle$$

$$= \int P(\mathbf{u}, \eta) \tilde{A}(\mathbf{b}_{\lambda 1i} - \mathbf{u}, \nu_i) \tilde{A}^*(\mathbf{b}_{\lambda 2j} - \mathbf{u}, \nu_j)$$

$$\times e^{i2\pi\eta(\nu_i - \nu_j)} d^2u d\eta$$

$$\approx \int P(\bar{\mathbf{b}}_\lambda, \eta) e^{i2\pi\eta(\nu_i - \nu_j)} d\eta$$

$$\times \int \tilde{A}^*(\mathbf{b}_{\lambda 1i} - \mathbf{u}, \nu_i) \tilde{A}(\mathbf{b}_{\lambda 2j} - \mathbf{u}, \nu_j) d^2u, \quad (7)$$

where  $\mathbf{b}_{\lambda 1i}$  and  $\mathbf{b}_{\lambda 2j}$  are the normalized baseline vectors for baseline  $\mathbf{b}_1$  and  $\mathbf{b}_2$  evaluated at frequencies  $\nu_i$  and  $\nu_j$ , respectively, and  $\bar{\mathbf{b}}_\lambda$  is the mean of the two. In deriving Equation (7), we first substituted Equation (3) for the expressions of visibilities in the angle bracket, and then factored the evaluated cylindrical power spectrum out of the integral over  $\mathbf{u}$ . Next we replace the continuous integral on power spectra with discrete sums over a series of piecewise constant bandpowers  $P(\bar{\mathbf{b}}_\lambda, \eta_\alpha)$ , such that

$$\mathbf{C}_{ij}^{12} \approx \sum_\alpha P(\bar{\mathbf{b}}_\lambda, \eta_\alpha) \int_{\eta_\alpha} e^{i2\pi\eta_\alpha(\nu_j - \nu_i)} d\eta$$

$$\times \int \tilde{A}(\mathbf{b}_{\lambda 1i} - \mathbf{u}, \nu_i) \tilde{A}^*(\mathbf{b}_{\lambda 2j} - \mathbf{u}, \nu_j) d^2u$$

$$\approx \sum_\alpha P(\bar{\mathbf{b}}_\lambda, \eta_\alpha) e^{i2\pi\eta_\alpha(\nu_i - \nu_j)} \Delta\eta$$

$$\times \int e^{-i2\pi(\mathbf{b}_{\lambda 1i} - \mathbf{b}_{\lambda 2j})\cdot\boldsymbol{\theta}} A(\boldsymbol{\theta}, \nu_i) A^*(\boldsymbol{\theta}, \nu_j) d^2\theta$$

$$\equiv \sum_\alpha P(\bar{\mathbf{b}}_\lambda, \eta_\alpha) \mathbf{Q}_{ij}^{12, \alpha}, \quad (8)$$

Henceforth, we will adopt the notation  $P_\alpha \equiv P(\bar{\mathbf{b}}_\lambda, \eta_\alpha)$  to mean the value of the cylindrical power spectrum  $P(\mathbf{u}, \eta)$  evaluated at  $\mathbf{u} = \bar{\mathbf{b}}_\lambda$  and  $\eta = \eta_\alpha$ . The index  $\alpha$  discretely runs over a series of bins in  $\eta$ , and as long as these bins are narrow compared to the scales over which the power spectrum changes, a piecewise constant treatment is appropriate.

Equation (8) shows the cross-baseline covariance matrix of visibilities encodes information about the power spectrum bandpowers via a family of response matrices  $\mathbf{Q}^{12,\alpha}$  (with a different matrix for every value of the bandpower index  $\alpha$ ). Since the covariance is an ensemble-averaged quadratic function of the data, one might venture that estimators for the bandpowers can be constructed by forming quadratic combinations of the data, i.e.,

$$\hat{P}_\alpha = \mathbf{x}_1^\dagger \mathbf{E}^{12,\alpha} \mathbf{x}_2, \quad (9)$$

where  $\mathbf{E}^{12,\alpha}$  is a matrix that can be chosen (within certain limitations) by the data analyst. Taking the ensemble average on both sides and inserting Equation (8) then yields

$$\langle \hat{P}_\alpha \rangle = \sum_\beta \text{tr}(\mathbf{E}^{12,\alpha} \mathbf{Q}^{21,\beta}) P_\beta \equiv \sum_\beta W_{\alpha\beta} P_\beta, \quad (10)$$

where  $\mathbf{W}$  is the window function matrix. To ensure that our estimated bandpowers are correctly normalized, we require that each row of  $\mathbf{W}$  sum to unity.

In the HERA power spectrum pipeline, we pick a family of  $\mathbf{E}^{12}$  matrices of the form

$$\mathbf{E}^{12,\alpha} \equiv M_\alpha \mathbf{R}_1 \mathbf{Q}^{\text{DFT},\alpha} \mathbf{R}_2, \quad (11)$$

where the matrix  $\mathbf{Q}_{ij}^{\text{DFT},\alpha} \equiv e^{i2\pi\eta_\alpha(\nu_i - \nu_j)}$  is responsible for taking the Fourier transform of the two copies of the data vectors in the quadratic estimator. The matrices  $\mathbf{R}_1$  and  $\mathbf{R}_2$  are weighting matrices that act on visibilities from  $\mathbf{b}_1$  and  $\mathbf{b}_2$ , respectively. In this paper, we use  $\mathbf{R} = \mathbf{T}\mathbf{Y}$ , where both  $\mathbf{T}$  and  $\mathbf{Y}$  are diagonal matrices. The former is used to impose a Blackman-Harris tapering function on the spectral data, and the latter propagates data flags. With a quadratic estimator of this form, the normalization scalar,  $M_\alpha$ , should take the form

$$M_\alpha = \frac{1}{\sum_\beta \text{tr}(\mathbf{R}_1 \mathbf{Q}^{\text{DFT},\alpha} \mathbf{R}_2 \mathbf{Q}^{12,\beta})} \quad (12)$$

which ensures that the rows of  $\mathbf{W}$  sum to unity, and therefore that the bandpowers are properly normalized. In our case, we do use this normalization, but we approximate the  $\mathbf{Q}^{12,\beta}$  term in the denominator. Rather than evaluating the full integral in Equation (8), we make the approximation that  $\mathbf{b}_{\lambda 1i} \approx \mathbf{b}_{\lambda 2i}$ . In fact, this is the motivation for the use of  $\mathbf{Q}^{\text{DFT},\alpha}$  in Equation (11) rather

than  $\mathbf{Q}^{12}$ ; notice that if  $\mathbf{b}_{\lambda 1i} = \mathbf{b}_{\lambda 2i}$ , then  $\mathbf{Q}^{12} \propto \mathbf{Q}^{\text{DFT}}$ . Over large bandwidths, this will fail for long baselines, since  $\mathbf{b}_\lambda \equiv \nu \mathbf{b}/c$ .

The approximation that we have just made is equivalent to the delay spectrum approximation (Parsons et al. 2012b; Liu et al. 2014a). To see this, we can write our estimator in the continuous limit. Our current form for  $\mathbf{E}^{12,\alpha}$  is separable into the product of two matrices that each involve only one of the two baselines. In particular, if  $\gamma(\nu)$  is the functional form of the Blackman-Harris taper, then we have  $\mathbf{E}_{ij}^{12,\alpha} = \gamma_1(\nu_i) e^{i2\pi\eta_\alpha(\nu_i - \nu_j)} \gamma_2(\nu_j)$ , and its action on each baseline's visibilities in Equation (9) is to compute the quantity

$$\sum_i V(\mathbf{b}, \nu_i) \gamma(\nu_i) e^{-2\pi\eta \nu_i \Delta\nu}, \quad (13)$$

which is just a discrete approximation to

$$\tilde{V}(\mathbf{b}, \eta) = \int V(\mathbf{b}, \nu) \gamma(\nu) e^{-i2\pi\eta\nu} d\nu. \quad (14)$$

Note Equation (14) is an equivalent expression of the delay transform in Parsons et al. (2012b). Therefore

$$\begin{aligned} \hat{P}_\alpha &= \mathbf{x}_1^\dagger \mathbf{E}^{12,\alpha} \mathbf{x}_2 \\ &\propto \sum_{ij} V^*(\mathbf{b}_1, \nu_i) \gamma_1(\nu_i) V(\mathbf{b}_2, \nu_j) \gamma_2(\nu_j) e^{i2\pi\eta_\alpha(\nu_i - \nu_j)} \\ &= \tilde{V}^*(\mathbf{b}_1, \eta_\alpha) \tilde{V}(\mathbf{b}_2, \eta_\alpha). \end{aligned} \quad (15)$$

Equation (15) just indicates that the quadratic estimator is proportional to the product of delay-transformed visibilities. This is an estimator that is based on Fourier transforming the visibility spectra from individual baselines, rather than combining information from different baselines. In principle, only the latter can probe truly rectilinear Fourier modes on the sky, since  $\mathbf{k}_\perp \propto \mathbf{b}_\lambda$  (which is a frequency-dependent quantity), and thus to probe the same  $\mathbf{k}_\perp$  at multiple frequencies—which is needed to perform the Fourier transform along the line-of-sight direction—one needs multiple baselines. The delay spectrum approach uses the fact that  $\mathbf{b}_\lambda$  evolves only slowly with frequency for short baselines to form an approximate power spectrum estimator. We make this approximation throughout this paper, as this is the choice that has been made for the next iteration of power spectrum upper limits from HERA observations. In recognition of this, we will henceforth use  $\tau$  to index our line-of-sight Fourier modes (as is customary for delay spectra) instead of  $\eta$  (which is generally used to denote true rectilinear line-of-sight wavenumbers) (Morales et al. 2012, 2019).

In the language of the delay spectrum, the foreground wedge becomes particularly simple to describe: smooth

Quantity	Definition/Meaning	First Appearance
$\mathbf{b}; \mathbf{b}_p$	Baseline vector; Vector of the $p$ th index baseline	Equation (1)
$\boldsymbol{\theta}$	Angular sky position	Equation (1)
$\nu; \nu_i$	Frequency; Frequency of the $i$ th index channel	Equation (1)
$\mathbf{b}_\lambda; \mathbf{b}_{\lambda p i}$	Normalized baseline vector in units of wavelength; Normalized vector for baseline $\mathbf{b}_p$ at frequency $\nu_i$	Equation (3)
$\mathbf{u}$	Fourier dual to $\boldsymbol{\theta}$	Equation (2)
$\eta; \eta_\alpha$	Fourier dual to $\nu$ ; the $\alpha$ th index $\eta$ mode	Equation (2)
$\tau; \tau_\alpha$	Delay, i.e., Fourier dual to $\nu$ on a single baseline; the $\alpha$ th index delay mode	Equation (16)
$A(\boldsymbol{\theta}, \nu)$	Primary beam function at position $\boldsymbol{\theta}$ and frequency $\nu$	Equation (1)
$\tilde{A}(\mathbf{u}, \nu)$	Spatial Fourier Transform Dual of primary beam function	Equation (3)
$\gamma(\nu)$	Spectral tapering function at frequency $\nu$	Equation (14)
$N_{\text{time}}; N_{\text{blp}}$	Number of time instants; Number of baseline-pairs	Equation (18)
$N_{\text{boot}}$	Number of bootstrapping sample sets	Equation (24)
$I(\boldsymbol{\theta}, \nu)$	Sky source intensity function at position $\boldsymbol{\theta}$ and frequency $\nu$	Equation (1)
$\tilde{I}(\mathbf{u}, \eta)$	Fourier transform of $I$ at angular wavenumber $\mathbf{u}$ and line-of-sight wavenumber $\eta$	Equation (2)
$V(\mathbf{b}, \nu)$	Visibility measured by baseline $\mathbf{b}$ at frequency $\nu$	Equation (1)
$P(\mathbf{u}, \eta)$	Cylindrical power spectrum at angular wavenumber $\mathbf{u}$ and line-of-sight wavenumber $\eta$	Equation (4)
$P_\alpha$	The $\alpha$ th bandpower $P_\alpha \equiv P(\bar{\mathbf{b}}_\lambda, \eta_\alpha)$	Equation (8)
$\hat{P}_\alpha$	The estimator for the $\alpha$ th bandpower $P_\alpha$	Equation (9)
$M_\alpha$	The normalization scalar of the estimator for the $\alpha$ th bandpower	Equation (11)
$\tilde{V}(\mathbf{b}_p, \tau_\alpha), \tilde{x}_p(\tau_\alpha)$	Delay spectra of baseline $\mathbf{b}_p$ at delay mode $\tau_\alpha$	Equation (15)
$\tilde{V}_{\text{signal}}(\mathbf{b}_p, \tau_\alpha), \tilde{s}_p(\tau_\alpha)$	The signal component of $\tilde{V}$ of baseline $\mathbf{b}_p$ at delay mode $\tau_\alpha$	Equation (16)
$\tilde{V}_{\text{noise}}(\mathbf{b}_p, \tau_\alpha), \tilde{n}_p(\tau_\alpha)$	The noise component of $\tilde{V}$ of baseline $\mathbf{b}_p$ at delay mode $\tau_\alpha$	Equation (16)
$P_{\tilde{x}_1 \tilde{x}_2}$	Power spectra formed from visibilities $\mathbf{x}_1$ and $\mathbf{x}_2$	Equation (30)

**Table 1.** Dictionary of highlighted scalars and functions.

Quantity	Definition/Meaning	Size	First Appearance
$\mathbf{x}_p$	Stacked visibilities at multiple frequencies of baseline $\mathbf{b}_p$	$N_{\text{freq}}$	Equation (6)
$\mathbf{C}^{pq}$	Covariance matrices $\mathbf{C}^{pq} \equiv \langle \mathbf{x}_p \mathbf{x}_q^\dagger \rangle$	$N_{\text{freq}} \times N_{\text{freq}}$	Equation (7)
$\mathbf{Q}^{pq, \alpha}$	Response of covariance $\mathbf{C}^{pq}$ to the $\alpha$ th bandpower	$N_{\text{freq}} \times N_{\text{freq}}$	Equation (8)
$\mathbf{E}^{pq, \alpha}$	Matrix for quadratic estimator of bandpower $P_\alpha$ , i.e., $\hat{P}_\alpha = \mathbf{x}_p^\dagger \mathbf{E}^{pq, \alpha} \mathbf{x}_q$	$N_{\text{freq}} \times N_{\text{freq}}$	Equation (9)
$\mathbf{W}$	Window function matrix	$N_{\text{delay}} \times N_{\text{delay}}$	Equation (10)
$\mathbf{R}_p$	Weighting matrix acting on $\mathbf{x}_p$	$N_{\text{freq}} \times N_{\text{freq}}$	Equation (11)
$\mathbf{Q}^{\text{DFT}, \alpha}$	Matrix taking Fourier Transform in the estimator	$N_{\text{freq}} \times N_{\text{freq}}$	Equation (11)
$\mathbf{U}^{pq}$	two-point correlation matrices $\mathbf{U}^{pq} \equiv \langle \mathbf{x}_p \mathbf{x}_q^T \rangle$	$N_{\text{freq}} \times N_{\text{freq}}$	Equation (33)
$\mathbf{G}^{pq}$	two-point correlation matrices $\mathbf{G}^{pq} \equiv \langle \mathbf{x}_p^* \mathbf{x}_q^\dagger \rangle$	$N_{\text{freq}} \times N_{\text{freq}}$	Equation (33)

**Table 2.** Dictionary of highlighted vectors and matrices.

spectrum foregrounds simply contaminate all modes below a particular delay, the value of which depends on the baseline length (Parsons et al. 2012b; Liu et al. 2014a; Liu & Shaw 2020). Suppose we decompose the delay transformed visibility into the signal component  $\tilde{V}_{\text{signal}}$  (mainly foregrounds, and we are neglecting the much weaker EoR signal here) and the noise component  $\tilde{V}_{\text{noise}}$ , such that

$$\begin{aligned} \tilde{V}(\mathbf{b}_1, \tau_\alpha) &\equiv \tilde{x}_1(\tau_\alpha) \\ &\equiv \tilde{V}_{\text{signal}}(\mathbf{b}_1, \tau_\alpha) + \tilde{V}_{\text{noise}}(\mathbf{b}_1, \tau_\alpha) \\ &\equiv \tilde{s}_1(\tau_\alpha) + \tilde{n}_1(\tau_\alpha). \end{aligned} \quad (16)$$

Since we are working on redundant baselines, we will henceforth drop the subscript on  $\tilde{s}$ , as the two baselines used in Equation (15) should measure identical signals. Mathematically, then, the statement that the smooth spectrum foregrounds contaminate only low delay modes is given by

$$\hat{P}_\alpha \approx \begin{cases} \tilde{s}^* \tilde{s} + \tilde{s}^* \tilde{n}_2 + \tilde{n}_1^* \tilde{s} & \text{if } |\tau_\alpha| < \tau_0 \\ \tilde{n}_1^* \tilde{n}_2 & \text{otherwise,} \end{cases} \quad (17)$$

where  $\tau_\alpha$  is the delay corresponding to the  $\alpha$ th bandpower, and  $\tau_0$  is some critical delay value that separates parts of the power spectrum that are foreground-dominated from those that are not. In general,  $\tau_0$  will depend on the properties of one’s instrument as well as the extent to which the assumption of smooth foregrounds is good. At delays less than  $\tau_0$ , we have assumed that the foreground signal is so large that the noise-noise cross term can be neglected.

Throughout the rest of this paper, we will appeal to Equation (17) for intuition when contemplating the behaviour of our power spectrum estimates at different delays. For now, we note two of its important properties. First, while the power spectrum of a signal  $\tilde{s}^* \tilde{s}$  will be always real valued, the overall estimator  $\hat{P}_\alpha$  is complex. It is possible to write down symmetrized estimators that give real power spectra. However, since the imaginary part is sourced by noise, it is a useful diagnostic quantity to examine. Second, even though the noise-noise terms may be negligible in the signal dominated regimes, there will still be a considerable uncertainty here that enters via the signal-noise cross terms.

Until now, we have focused on power spectra estimated from visibilities measured at single time instants. Given data from multiple times, we can average the power spectra estimated from individual measurements together. For a drift scan telescope, this averaging of power spectra from different time samples is tantamount to invoking statistical isotropy to justify the spherical averaging of power spectra over different wavevector  $\mathbf{k}$

directions. In addition to averaging in time, if we have multiple pairs of baselines within the same redundant group of baselines, we may average over the power spectrum estimates from multiple baseline pairs. The simplest way to do this is to perform an unweighted average:

$$\bar{\hat{P}}_\alpha = \frac{1}{N_{\text{time}} N_{\text{blp}}} \sum_{\text{time, blp}} \hat{P}_\alpha(\text{time, blp}), \quad (18)$$

where  $N_{\text{time}}$  is the number of time integrations,  $N_{\text{blp}}$  is the number of baseline pairs,  $\hat{P}_\alpha(\text{time, blp})$  is the power spectrum estimate (given by previous equations in this section) at a time instant and a baseline pair (“blp”), and  $\bar{\hat{P}}_\alpha$  is the average of estimates. The type of averaging performed here may be termed an “incoherent average”, to distinguish it from a “coherent average”, where one averages over visibilities (or converts them into a single image) before squaring them in power spectrum estimation. The latter provides greater sensitivity—if calibration errors and other systematic effects can be brought under control (Morales et al. 2019). The former retains the ability to inspect the contributions from particular baseline pairs and time until right before the final result, making some systematics easier to diagnose. However, note that by employing a suitable fringe-rate filtering of the time-stream data, it is in principle possible to recover the lost sensitivity from a “square-then-add” approach (Parsons et al. 2016). In this paper, we will focus on the error statistics of the incoherent average approach, as this is what is currently used in the HERA pipeline (HERA Collaboration 2021).

Before we move into the discussion on error estimation methods in the next section, it is worth noting that Equation (18) is not the optimal way to obtain average power spectra with the least variance. Generally, given a set of estimates  $\hat{P}_\alpha$  for bandpower  $P_\alpha$  with measurement errors  $\sigma$ , such that

$$\hat{P}_\alpha = DP_\alpha + \epsilon, \quad (19)$$

an linear estimator of  $P_\alpha$  is written as

$$\bar{\hat{P}}_\alpha = \mathbf{K} \hat{P}_\alpha. \quad (20)$$

Here  $\mathbf{D}$  is a column vector of 1s. We need to select  $\mathbf{K}$  such that  $\mathbf{K}\mathbf{D} = \mathbf{I}$  in order to achieve an unbiased constraint that satisfies  $\langle \bar{\hat{P}}_\alpha \rangle = P_\alpha$ . For an arbitrary matrix  $\mathbf{K}$ , the error bar  $\Sigma_\alpha \equiv \langle |\bar{\hat{P}}_\alpha - P_\alpha|^2 \rangle = \mathbf{K}\epsilon\epsilon\mathbf{K}^t$ , where the error covariance matrix  $\epsilon \equiv \langle \sigma\sigma^t \rangle$ . **The superscript “t” used here and along in this paper refers to the matrix transposition.** Note that Equation (18) is just a special case where  $\mathbf{K} = [\mathbf{D}^t\mathbf{D}]^{-1}\mathbf{D}^t$ . When  $\Sigma_\alpha$  is minimized (optimal),  $\bar{\hat{P}}_\alpha$  and the corresponding  $\Sigma_\alpha$  should take the



503 form of (Tegmark 1997; Dillon et al. 2014)

$$504 \quad \overline{\hat{P}}_\alpha = [\mathbf{D}^t \boldsymbol{\epsilon}^{-1} \mathbf{D}]^{-1} \mathbf{D}^t \boldsymbol{\epsilon}^{-1} \hat{P}_\alpha \quad (21)$$

$$505 \quad \Sigma_\alpha = [\mathbf{D}^t \boldsymbol{\epsilon}^{-1} \mathbf{D}]^{-1}, \quad (22)$$

507 which amounts to an inverse covariance weighting of  
508 the data in averaging it down. Equation (21) brings  
509 us the ability to propagate the full covariance informa-  
510 tion over samples to obtain an least-variance average  
511 result. The diagonal elements of  $\boldsymbol{\epsilon}$  are easily interpreted  
512 as the variance in each individual measurement, while  
513 the off-diagonal elements, reflected by the coherency be-  
514 tween time samples and baseline-pair samples, are far  
515 more complicated. If estimating the covariance matrix  
516  $\boldsymbol{\epsilon}$  of the pre-averaged data is difficult, one may opt to  
517 weight the data using some other matrix  $\boldsymbol{\Gamma}$  instead of  
518  $\boldsymbol{\epsilon}$  in Equation (21). In this case, the final variance  $\Sigma_\alpha$   
519 ends up being

$$520 \quad \Sigma_\alpha = [\mathbf{D}^t \boldsymbol{\Gamma}^{-1} \mathbf{D}]^{-1} \mathbf{D}^t \boldsymbol{\Gamma}^{-1} \boldsymbol{\epsilon} \boldsymbol{\Gamma}^{-t} \mathbf{D} [\mathbf{D}^t \boldsymbol{\Gamma}^{-t} \mathbf{D}]^{-1}. \quad (23)$$

521 In principle, one could model the off-diagonal elements  
522 of  $\boldsymbol{\epsilon}$ . This is particularly important in the cosmic-  
523 variance dominated regime where the sky signal—which  
524 is what sources a cosmic variance error—is slowly drift-  
525 ing through HERA’s field of view over the course of the  
526 day, thus inducing strong correlations between different  
527 time samples. In this paper we do not consider the mod-  
528 elling of off-diagonal covariances in  $\boldsymbol{\epsilon}$  (or between differ-  
529 ent  $\alpha$  values in  $\overline{\hat{P}}_\alpha$ ). We assume diagonal covariance  
530 matrices and set  $\boldsymbol{\Gamma} = \mathbf{I}$ , i.e., we use Equation (18) when  
531 computing the “incoherently-averaged” power spectra,  
532 and here we are acknowledging other possibilities only  
533 for completeness.

### 534 3. ERROR ESTIMATION METHODOLOGY

535 Placing robust error bars on power spectra is crucial  
536 to our data analysis, whether it is for setting upper lim-  
537 its, diagnosing experimental systematics, or eventually  
538 declaring a detection of the cosmological 21 cm signal.  
539 Generally, contributions to the error bars of observed  
540 power spectra come from three sources: the EoR sig-  
541 nal, noise, and foregrounds (Thyagarajan et al. 2013;  
542 Trott 2014; Dillon et al. 2014, 2015; Lanman & Pober  
543 2019). Of course, this is all complicated by the response  
544 of one’s instrument, and ultimately, one’s ability to place  
545 reliable error bars rests on one’s ability to understand  
546 the behaviour of each data source in the context of the  
547 instrument.

548 The intrinsic variance of the EoR signal, also known  
549 as “cosmic variance”, is the ensemble covariance on all  
550 possible realizations of the 21-cm temperature field. If

551 the field is Gaussian, then its cosmic variance is pro-  
552 portional to the square of the power spectrum ampli-  
553 tude over the number of independent modes. Lanman  
554 & Pober (2019), for example, estimate the cosmic vari-  
555 ance could go as high as  $\sim 35\%$  of the EoR signal for  
556 HERA-like fields of view with eight hours of local side-  
557 real time (LST) observations using only the shortest  
558 (14.6-m) baselines of HERA. This uncertainty due to  
559 cosmic variance is brought down to a few percent level  
560 for the spherically averaged power spectrum when us-  
561 ing all types of baselines. Importantly, as reionization  
562 evolves, the 21-cm temperature field is expected to be-  
563 come highly non-Gaussian, and the excess contribution  
564 from the non-Gaussian component could lift the cosmic  
565 variance in Gaussian part staggeringly, which is signifi-  
566 cant and should be considered for future high-sensitivity  
567 measurements (Mondal et al. 2016, 2017; Shaw et al.  
568 2019). In this paper, however, we assume that at our  
569 current levels of precision the cosmic variance is sub-  
570 dominant to noise and foregrounds.

571 For instrumental noise, we assume that the noise in  
572 the visibility from each baseline is independent and  
573 Gaussian-distributed. This is what one might expect  
574 based on the statistics of correlator outputs in a radio  
575 interferometer, but is also an assumption that we will  
576 see borne out in our empirical data in Section 4. With  
577 these well-understood statistical properties, the noise-  
578 dominated delays (recall Equation 17) are relatively easy  
579 to model, at least in principle.

580 The low-delay, foreground-dominated regimes are  
581 trickier to model. One key problem is that the statistics  
582 of foregrounds are not well-understood, particularly at  
583 the low frequencies relevant to us. There are different  
584 approaches that one can take to this roadblock. The  
585 first is where one attempts to make a measurement of  
586 the cosmological 21 cm signal only, by proactively sub-  
587 tracting (or simultaneously fitting) a foreground model.  
588 To properly set error bars on such a power spectrum, it is  
589 necessary to propagate uncertainties (accounting for the  
590 possibility of mis-subtractions) in the foreground model  
591 to the final errors (or in the case of a simultaneous fit-  
592 ting, to allow the errors on the cosmological signal to  
593 be appropriately inflated as one marginalizes over fore-  
594 ground uncertainties). While conceptually straightforward,  
595 these steps are difficult to implement in practice  
596 without a deep understanding of foreground statistics.

597 Instead, in this paper we treat foregrounds as addi-  
598 tive systematics on the total sky emission. Crucially,  
599 this means we only require empirical knowledge of the  
600 foregrounds themselves, and not their full probability  
601 distribution. We simply quantify the error bars on a  
602 measurement of total sky emission due to instrumental

Name	Description	Definition
$\sigma_{\text{bs}}$	Error bar of the average power spectra by bootstrapping over the collection of samples	Equation (24)
$P_{\text{diff}}$	Power spectra from differenced visibility used as a form of error bar	Equation (26)
$P_{\text{N}}$	Analytic noise power spectrum	Equation (27)
$P_{\text{SN}}$	Error bar based on $P_{\text{N}}$ but including the extra signal-noise cross term	Equation (30)
$\sigma_{\text{QE-N}}$	Error bar from the output covariance in QE formalism including only noise-noise term	Equation (37)
$\sigma_{\text{QE-SN}}$	Error bar from the output covariance in QE formalism including noise-noise term and signal-noise term	Equation (38)
$\tilde{P}_{\text{SN}}$	Same as $P_{\text{SN}}$ but with an adjustment for noise double-counting	Equation (31)
$\tilde{\sigma}_{\text{QE-SN}}$	Same as $\sigma_{\text{QE-SN}}$ but with an adjustment for noise double-counting	Equation (39)

**Table 3.** Dictionary of error bars.

603 noise, rather than what the error bars on the cosmo-  
 604 logical signal due to foreground uncertainties and noise.  
 605 Some understanding of foregrounds is still needed for  
 606 setting our errors because of the signal-noise cross terms  
 607 in Equation (17). Implicit in this approach is a strat-  
 608 egy of foreground avoidance in the hunt for a cosmo-  
 609 logical signal detection, where it is hoped that the sep-  
 610 aration between foreground-dominated and foreground-  
 611 negligible regimes in Equation (17) is a clean one. It  
 612 is important to note, however, that we seek to compute  
 613 error bars that transition smoothly between the regimes  
 614 and are valid even if the conceptual separation is not a  
 615 clean one in practice.<sup>7</sup>

616 In addition to foregrounds, one can treat instrumental  
 617 systematics in the same way. In other words, interpret-  
 618 ing systematics as additive “signals”, the signal-noise  
 619 cross term in the variance of power spectra is sourced  
 620 by not just foregrounds, but also other systematics such  
 621 as cable reflections and cross couplings (Kern et al. 2019,  
 622 2020a). We can apply some models to remove sys-  
 623 tematics from the signal, but the residuals due to mis-  
 624 subtraction will still increase the total uncertainties via  
 625 the signal-noise cross term. **Note, however, that in this**  
 626 **paper we do not develop a comprehensive model to ac-**  
 627 **count for all systematics, which is particularly difficult**  
 628 **when unknown modeling errors are present in compli-**

629 **cated effects (e.g. direction-dependent gains). We will**  
 630 **instead argue that a procedure of using the measured**  
 631 **visibility itself to model the foregrounds and systematics**  
 632 **allows us to set robust upper bounds, provided certain**  
 633 **safeguards are in place to avoid biases. We will leave**  
 634 **more exquisite *a priori* characterizations of foregrounds**  
 635 **and systematics in the signal-noise cross terms for the**  
 636 **future.**

637 Finally, one might worry that the averaging of power  
 638 spectra from multiple measurements together like Equa-  
 639 tion (18) might complicate the statistics. Appendix B  
 640 shows an example of this. There, we show that when  
 641 averaging over redundant baseline-pairs, the variance  
 642 of average power spectra in the foreground-dominated  
 643 regime goes down roughly with  $N_{\text{blp}}^{-1/2}$  and not  $N_{\text{blp}}^{-1}$   
 644 because some baselines will appear in multiple base-  
 645 line *pairs*. In other words, in foreground-dominated  
 646 (or systematics-dominated) regimes, one cannot assume  
 647 that baseline pairs average together in an independent  
 648 fashion. This has consequences for certain methods of  
 649 error bar computation, such as the bootstrapping ap-  
 650 proach discussed in the next subsection, which will tend  
 651 to underestimate error bars in these regimes. To avoid  
 652 this, one might just use *pairs* in which each baseline  
 653 only appears once in all baseline *pairs*, or to compute  
 654 a correction factor on the final results. In contrast to  
 655 the foreground/signal-dominated regime, in the noise-  
 656 dominated regime one obtains correct final error bars  
 657 by assuming that the baseline-pair samples are indepen-  
 658 dent (even if they are not for the aforementioned rea-  
 659 sons). In this paper, to avoid averaging power spectra  
 660 over correlated samples, we will concentrate on the av-  
 661 eraging of power spectra of a single baseline-pair over  
 662 multiple time samples.

663 We will have a more extensive discussion of the mean-  
 664 ing of our error bars in Section 5. For concreteness,  
 665 however, we will now propose several different meth-  
 666 ods for generating error bars based on the HERA power  
 667 spectrum pipeline before performing quantitative com-

<sup>7</sup> We stress that our analysis does not cease to apply at a certain delay—it is simply the case that at high delays, there is less of a pressing need to construct detailed models for foreground subtraction, which to some extent mitigates the need to consider the complicated statistical properties of this subtraction. It is likely that our formalism can be generalized to encompass some foreground subtraction, but detailed work beyond the scope of this paper would be necessary. As an example, suppose one were to use information at  $\tau = 0$  and an instrument model to subtract off leakage from other low (but non-zero) delay modes. In such a scenario, one would need to account for the fact that the noise contributions between different delay modes are now coupled. This can in principle be accommodated with appropriate covariance matrix modeling, but we leave this to future work.

parisons in Section 4. For the convenience of our readers, we provide Table 3 as a quick preview.

### 3.1. Bootstrap

Bootstrapping is a natural method for computing the error bars on the final averaged power spectrum with only minimal *a priori* modeling assumptions. Within the 21 cm cosmology literature, it has previously been used to set error bars on power spectrum upper limits (Parsons et al. 2014; Ali et al. 2015; although see Cheng et al. 2018 for caveats on these limits). Bootstrapping is a process that goes hand in hand with the averaging step described in Equation (18). Rather than performing a single average, we repeatedly form a new set of pre-averaged data by resampling the original set with replacement (i.e., allowing repeated entries). A new estimate of the final average,  $\bar{P}^{(k)}$ , can be produced from the  $k$ th draw. The scatter in the realizations of the final averaged power spectrum is then quoted as an error bar  $\sigma_{\text{bs}}$ , such that

$$\sigma_{\text{bs}}^2 = \frac{1}{N_{\text{boot}}} \sum_k \left[ \bar{P}^{(k)} - \frac{1}{N_{\text{boot}}} \sum_l \bar{P}^{(l)} \right]^2, \quad (24)$$

where  $N_{\text{boot}}$  is the number of bootstrapping sample sets. In essence, one is using the data itself as an empirical estimate of the distribution from which the data is drawn (Efron & Tibshirani 1994; Press et al. 2007).

If the input data samples are independent and identically distributed, bootstrapping will give the same error bars as the true ones from ensemble average. However, this assumption is likely to be violated with our data. Consider the two axes that we have at our disposal. One possibility is to bootstrap over different time samples. Over short timescales, different time integrations have relatively uncorrelated noise realizations. However, as our drift scan telescope moves across different local sidereal time (LST) values, the sky brightness seen by the telescope changes, leading to slow changes in the noise level for a sky-noise dominated telescope. An alternative to bootstrapping over time is to bootstrap over different copies of an identical (“redundant”) baseline group. Here, the downside is that it remains an open question as to how truly redundant current interferometric arrays are (Dillon et al. 2020), and precisely what the consequences of non-redundancy are (Choudhuri et al. 2021). With correlated data samples, bootstrapping tends to underestimate the true error bars on a final averaged power spectrum (Cheng et al. 2018). On the other hand, non-stationary effects such as non-redundancy can inflate bootstrap errors rather than revealing the fact that the data in fact come from multiple distributions.

In later sections, we will compute error bars that come from bootstrapping over different LSTs, but will interpret these results with caution given the caveats we have just outlined. Of course, these caveats by no means diminish the value of bootstrap errors as yet another consistency check, particularly when one is diagnosing systematic effects (e.g., Kolopanis et al. 2019).

### 3.2. Direct Noise Estimation By Visibility Differencing

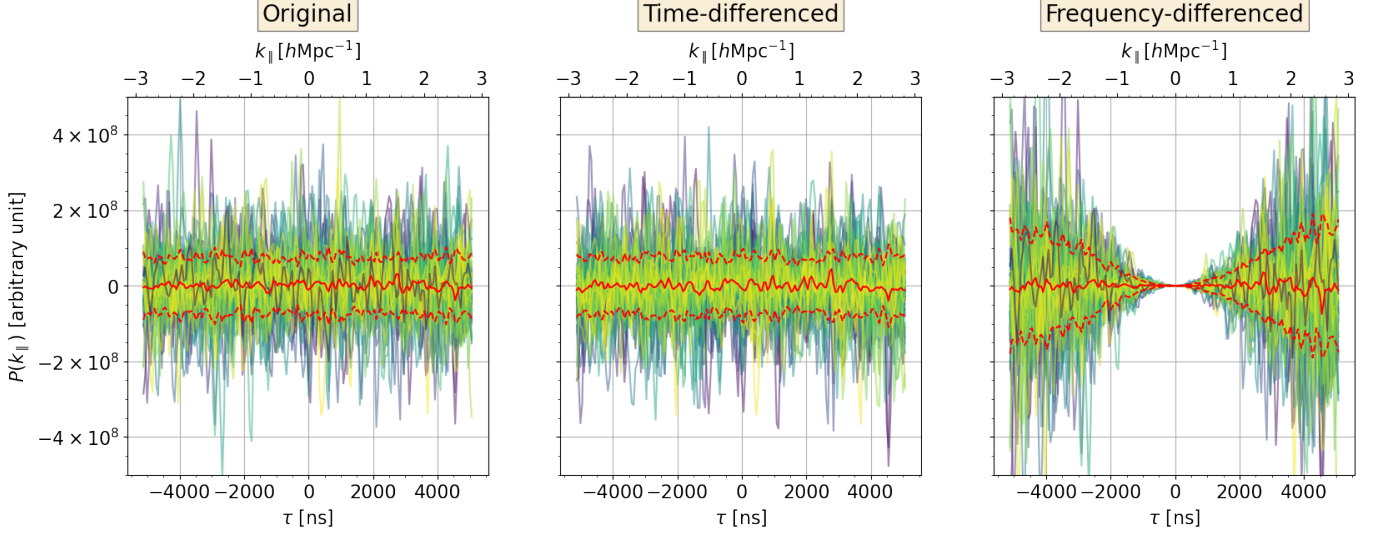
The foreground and EoR signal varies relatively slowly in time (or frequency), such that after differencing the integrated visibility between very close LSTs (or frequencies), the normalized residual,

$$V_{\text{diff}} = \frac{V(\mathbf{b}, \nu, t_1) - V(\mathbf{b}, \nu, t_2)}{\sqrt{2}} \quad \text{or} \quad V_{\text{diff}} = \frac{V(\mathbf{b}, \nu_1, t) - V(\mathbf{b}, \nu_2, t)}{\sqrt{2}}, \quad (25)$$

is almost noise-like. We can propagate such  $V_{\text{diff}}$  through power spectrum estimation pipelines to generate a “noise-like” power spectrum  $P_{\text{diff}}$ , such that

$$P_{\text{diff}} \propto \tilde{V}_{\text{diff}}^* \tilde{V}_{\text{diff}}, \quad (26)$$

where appropriate proportionality/normalization constants allow  $P_{\text{diff}}$  to have the same units as—and therefore be directly comparable to—power spectra. This quantity can be viewed as a random variable that represents random realizations of the noise in the system, which can be used to at least roughly estimate error bars in noise-dominated regimes (see Appendix C for more details). It can be computed from either time-differenced or frequency-differenced visibilities. However, by differencing neighbouring points in frequency, we are in fact applying a high-pass filter in the delay space, which means that power is suppressed at low delay modes. This is illustrated in Figure 1, and for this reason that the time-differencing method is preferred for empirical noise uncertainty estimation. However, it is important to note that many correlators do not dump data to disk fast enough for this to be feasible, as the sky changes non-negligibly on the timescale of a few seconds. The maximum time length of a single integration before reaching a decorrelation threshold depends on the baseline length, thus ones need particular simulations for their instruments to determine the suitable time scale (Wijnholds et al. 2018). For the upgraded HERA correlator, it will be able to produce time-differenced visibilities on the milli-second timescale for accurate, empirical noise estimates.



**Figure 1.** Here we generate  $\sim 60$  realizations of time streams of white-Gaussian-noise visibilities, and compute the time-differenced visibilities and frequency-differenced visibilities respectively. *Left:* Power spectra from the original visibilities. *Center:* Power spectra from time-differenced visibilities. *Right:* Power spectra from frequency-differenced visibilities. In each panel, we plot the power spectra from every realization, along with the mean (solid red) and the standard deviation (dashed red) of power spectra over all realizations. We see power spectra from frequency-differenced visibilities are highly suppressed at low delays.

### 3.3. Power Spectrum Method

With appropriate approximations (see Liu & Shaw 2020 for details), it is possible to write down an analytic expression for the noise power spectrum given a system temperature,  $T_{\text{sys}}$  in units of Kelvin:

$$P_N = \frac{X^2 Y \Omega_{\text{eff}} T_{\text{sys}}^2}{t_{\text{int}} N_{\text{coherent}} \sqrt{2 N_{\text{incoherent}}}}, \quad (27)$$

where  $X \equiv D_c$  and  $Y \equiv \frac{c(1+z)^2}{\nu_{21} H_0 E(z)}$  are conversion factors from sky angles and frequencies to cosmological coordinates,  $\Omega_{\text{eff}}$  is the effective beam area,  $t_{\text{int}}$  is the integration time,  $N_{\text{coherent}}$  is the number of samples averaged at the level of visibility while  $N_{\text{incoherent}}$  is the numbers of samples averaged at the level of power spectrum (Zaldarriaga et al. 2004; Pober et al. 2013; Cheng et al. 2018; Kern et al. 2020a). This is an estimate of the root-mean-square (RMS) of a power spectrum measurement in the limit that it is purely thermal noise dominated. The system temperature,  $T_{\text{sys}} = T_{\text{sky}} + T_{\text{rcvr}}$ , is the sum of the sky and receiver temperature and describes the total noise content of the visibilities formed between cross-correlating data from different antennas (Thompson et al. 2017).

There are many ways in which the key quantity  $T_{\text{sys}}$  can be estimated. For example, we can take advantage of the differenced visibilities discussed in the previous subsection. These differences can then be converted into

an estimate of  $T_{\text{sys}}$  via the relation

$$V_{\text{RMS}}(\{p, q\}) = \frac{2k_b \nu^2 \Omega_p T_{\text{sys}, \{p, q\}}}{c^2 \sqrt{B \Delta t}}, \quad (28)$$

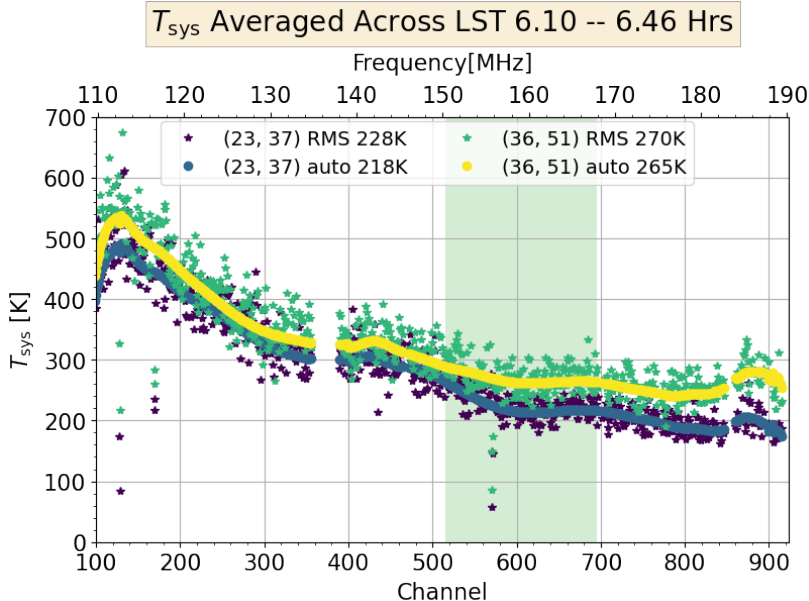
where  $k_b$  is the Boltzmann constant,  $\Omega_p$  is the integrated beam area,  $B$  is the bandwidth, and  $\Delta t$  is the integration time at a single time sample. The ‘‘RMS’’ subscript signifies taking the root-mean-square of the differenced visibilities and  $p$  and  $q$  are indices denoting two different antennas that form a baseline  $\{p, q\}$ . This serves to emphasize the fact that we can have a distinct system temperature for every baseline.

Another way to estimate  $T_{\text{sys}}$ —which we use in this paper—is to use auto-correlation visibilities, i.e., visibilities formed by correlating a single antenna’s data with itself. The system temperature on a non-auto correlation baseline  $\{p, q\}$  is then related to the geometric mean of the auto-correlation visibilities of the two constituent antennas as (Jacobs et al. 2015)

$$\sqrt{V(\{p, p\})V(\{q, q\})} = \frac{2k_b \nu^2 \Omega_p T_{\text{sys}, \{p, q\}}}{c^2}. \quad (29)$$

In Figure 2 we plot the system temperatures predicted using both methods for some HERA data. The lower scatter with the second method is why we recommend its usage.

The noise power spectrum  $P_N$  correctly describes the error bars *assuming that our instrument measures nothing but noise*. This may be a suitable approximation for noise-dominated delays. More generally, however,



**Figure 2.** Comparison of two ways to estimate the system temperature based on HERA data. The system temperatures of cross-correlation visibilities on two 14.6 m baselines [indexed by HERA antenna numbers (23, 37) and (36, 51)] are averaged across the LST range of 6.10 to 6.46 hours. The green regime, from frequency channel number #515 to 695, show the HERA data band used for analysis in this paper. The label “autos” and “RMS” indicate the method (either from products of auto-visibilitys or the RMS of differenced visibilitys) by which the curves of system temperatures are calculated. And the values of temperatures shown in labels are the average values over the band specified by the green regime. We see the results from two methods are consistent to 5%, though the curves from auto-correlations are far less scattered.

813 when a signal (be it foregrounds or systematics) exists,  
 814 the cross terms of Equation (17) provide an additional  
 815 contribution to the noise scatter/error bars.<sup>8</sup> This term  
 816 exists regardless of whether one’s foreground mitigation  
 817 strategy is based on subtraction or avoidance. In the  
 818 former case, the foreground residuals after subtracting  
 819 a model from data enter into the final expression; in the  
 820 latter case, the whole foreground contribution is propa-  
 821 gated as a systematic signal in the data. We show how  
 822 to take this into account in Appendix D, where we define  
 823  $P_{\text{SN}}$  as

$$824 \quad P_{\text{SN}}^2 \equiv \sqrt{2} \text{Re}(P_{\tilde{x}_1 \tilde{x}_2}) P_{\text{N}} + P_{\text{N}}^2 \quad (30)$$

825 which serves as a characterization of the error bars on  
 826 the total sky emission, consistent with the form derived  
 827 in Kolopanis et al. (2019). Here,  $\text{Re}(P_{\tilde{x}_1 \tilde{x}_2})$ , the real  
 828 part of power spectra formed from  $\mathbf{x}_1$  and  $\mathbf{x}_2$ , serves as  
 829 a stand-in for a signal-only power spectrum  $P_{\text{S}}$  assum-  
 830 ing that the signal dominates the noise (whether this  
 831 “signal” takes the form of foregrounds, systematics, or  
 832 the cosmological signal).

<sup>8</sup> We stress that this scatter/error is still due to instrumental noise and not the variance of the signal term. Even for a perfectly constant and known signal, the presence of the cross term alters the uncertainty, essentially having the signal term act as a multiplicative amplifier for noise fluctuations.

833 Using real data helps us approximate the true  $P_{\text{S}}$  when  
 834 we do not possess good *a priori* models. However, by  
 835 using real data our estimate of the first term of Equa-  
 836 tion (30) can in principle be negative because  $\tilde{x}_1$  and  
 837  $\tilde{x}_2$  contain different noise realizations. This can cause  
 838 problems, since the signal-only power spectrum is ex-  
 839 pected to be non-negative. We thus enforce a hard prior  
 840 on this term and set negative values of  $\text{Re}(P_{\tilde{x}_1 \tilde{x}_2})$  to  
 841 zero. In this way  $P_{\text{SN}}^2$  is always positive and the error  
 842 bar  $P_{\text{SN}}$  is at worst a conservative estimate. When we  
 843 average power spectra with error bars, this conservatism  
 844 leads to a substantial bias between  $P_{\text{SN}}$  and  $P_{\text{N}}$  in our fi-  
 845 nal error estimates in the noise-dominated regime. This  
 846 is due to  $\text{Re}(P_{\tilde{x}_1 \tilde{x}_2})$  in the first term of Equation (30)  
 847 is empirical—and therefore contains noise—which effec-  
 848 tively yields a double-counting of the noise-noise term  
 849 in the variance. This double-counting does not result in  
 850 an average bias if one does not enforce our prior, since  
 851 in a noise-dominated regime  $\text{Re}(P_{\tilde{x}_1 \tilde{x}_2})$  has zero mean.  
 852 Our prior ensures that  $P_{\text{SN}} > P_{\text{N}}$ . Despite this, we  
 853 will show that Equation (30) is a reasonable approxima-  
 854 tion over broad swaths of the power spectrum. More-  
 855 over, if we understand the statistics of noise fluctuations,  
 856 one can simply predict—and correct for—the double-  
 857 counting bias in  $P_{\text{SN}}$ . In the noise-dominated regime,  
 858  $P_{\text{N}}$  characterizes the scatter in  $\text{Re}(P_{\tilde{x}_1 \tilde{x}_2})$ . Thus one can  
 859 estimate the expectation value of the extra noise contri-

860 bution from the first term of Equation (30) by comput-  
861 ing

$$\begin{aligned}
& \sqrt{2} \langle \text{Re}(P_{\tilde{x}_1 \tilde{x}_2}) \rangle P_N \\
&= \sqrt{2} \left[ \frac{1}{\sqrt{2\pi} P_N} \int_0^\infty y \exp(-y^2/2P_N^2) dy \right] P_N \\
&= P_N^2 / \sqrt{\pi}. \tag{31}
\end{aligned}$$

866 The integral runs over only positive values since we are  
867 imposing a non-negative prior. Note that here where we  
868 have neglected any complicated window function effects  
869 in inserting the measured power spectrum, essentially  
870 assuming that all power is locally sourced at the delay  
871 where it is measured. In principle, these effects can be  
872 taken into account in a more general derivation within  
873 the quadratic estimator formalism, but we leave this for  
874 future work.

875 We see from Equation (31) that the excess of  $P_{\text{SN}}$   
876 above  $P_N$  in the noise-dominated regime is proportional  
877 to  $P_N$ ; thus, we can just subtract it from the initially  
878 computed  $P_{\text{SN}}$ . We then define a modified “ $P_{\text{SN}}$ ” free  
879 from the double-counting noise bias as<sup>9</sup>

$$\tilde{P}_{\text{SN}} \equiv P_{\text{SN}} - \left( \sqrt{1/\sqrt{\pi} + 1} - 1 \right) P_N. \tag{32}$$

881 The reduction of double-counting noise bias in this way  
882 also holds where signal dominates over noise. Since  $P_N$ ,  
883  $P_{\text{SN}}$ , and  $\tilde{P}_{\text{SN}}$  are all either power spectra or constructed  
884 from products of power spectra, we name this methodol-  
885 ogy of error estimation the “Power Spectrum Method”.

### 3.4. Covariance Method

887 The quadratic estimator formalism leads to a natu-  
888 ral way to write down an analytic form of error bars by  
889 propagating the input covariance matrices on visibili-  
890 ties into the output covariance matrices on bandpowers,  
891 which we name “Covariance Method” (see Appendix E  
892 for more details). Provided three set of matrices below  
893 containing the full frequency-frequency two-point corre-

<sup>9</sup> Here we derived the correction factor  $\sqrt{1/\sqrt{\pi} + 1} - 1 \approx 0.251$  assuming  $\text{Re}(P_{\tilde{x}_1 \tilde{x}_2})$  follows Gaussian distribution. This is appropriate assuming that enough power spectra formed from data at different times have been incoherently averaged together for the Central Limit Theorem to apply (we will examine this point further in Section 4.1). For a single snapshot in time, the measured power spectrum follows a Laplacian distribution (again, see Section 4.1) and the correction factor becomes  $\sqrt{3/2} - 1 \approx 0.225$ . Since the difference is small and in practice we operate in the Gaussianized regime anyway we use  $\sqrt{1/\sqrt{\pi} + 1} - 1$  in our definition.

894 lation information of complex visibilities

$$\begin{aligned}
& \mathbf{C}_{ij}^{12} \equiv \langle \mathbf{x}_{1,i} \mathbf{x}_{2,j}^* \rangle, \\
& \mathbf{U}_{ij}^{12} \equiv \langle \mathbf{x}_{1,i} \mathbf{x}_{2,j} \rangle, \\
& \mathbf{G}_{ij}^{12} \equiv \langle \mathbf{x}_{1,i}^* \mathbf{x}_{2,j}^* \rangle, \tag{33}
\end{aligned}$$

899 the variance in the real part of  $\hat{P}_\alpha$  is

$$\begin{aligned}
& \text{var} \left[ \text{Re}(\hat{P}_\alpha) \right] \\
&= \frac{1}{4} \left\{ \text{tr} \left[ (\mathbf{E}^{12,\alpha} \mathbf{U}^{22} \mathbf{E}^{21,\alpha*} \mathbf{G}^{11} + \mathbf{E}^{12,\alpha} \mathbf{C}^{21} \mathbf{E}^{12,\alpha} \mathbf{C}^{21}) \right. \right. \\
&+ 2 \times (\mathbf{E}^{12,\alpha} \mathbf{U}^{21} \mathbf{E}^{12,\alpha*} \mathbf{G}^{21} + \mathbf{E}^{12,\alpha} \mathbf{C}^{22} \mathbf{E}^{21,\alpha} \mathbf{C}^{11}) \\
&+ \left. \left. (\mathbf{E}^{21,\alpha} \mathbf{U}^{11} \mathbf{E}^{12,\alpha*} \mathbf{G}^{22} + \mathbf{E}^{21,\alpha} \mathbf{C}^{12} \mathbf{E}^{21,\alpha} \mathbf{C}^{12}) \right] \right\}, \tag{34}
\end{aligned}$$

905 and the variance in the imaginary part of  $\hat{P}_\alpha$  is

$$\begin{aligned}
& \text{var} \left[ \text{Im}(\hat{P}_\alpha) \right] \\
&= \frac{-1}{4} \left\{ \text{tr} \left[ (\mathbf{E}^{12,\alpha} \mathbf{U}^{22} \mathbf{E}^{21,\alpha*} \mathbf{G}^{11} + \mathbf{E}^{12,\alpha} \mathbf{C}^{21} \mathbf{E}^{12,\alpha} \mathbf{C}^{21}) \right. \right. \\
&- 2 \times (\mathbf{E}^{12,\alpha} \mathbf{U}^{21} \mathbf{E}^{12,\alpha*} \mathbf{G}^{21} + \mathbf{E}^{12,\alpha} \mathbf{C}^{22} \mathbf{E}^{21,\alpha} \mathbf{C}^{11}) \\
&+ \left. \left. (\mathbf{E}^{21,\alpha} \mathbf{U}^{11} \mathbf{E}^{12,\alpha*} \mathbf{G}^{22} + \mathbf{E}^{21,\alpha} \mathbf{C}^{12} \mathbf{E}^{21,\alpha} \mathbf{C}^{12}) \right] \right\}, \tag{35}
\end{aligned}$$

911 To get the final error bar on power spectra, we should  
912 accurately model input covariance matrices on visibil-  
913 ities and propagate them into output covariance ma-  
914 trix on bandpowers. Generally, we assume that the  
915 input covariance matrices can be decomposed as  $\mathbf{C} \equiv$   
916  $\mathbf{C}_{\text{signal}} + \mathbf{C}_{\text{noise}}$ .

917 Assuming the distributions of the real and imaginary  
918 parts of noise in visibilities are independently and iden-  
919 tically distributed (IID) at the same frequency and are  
920 uncorrelated between different frequency channels, our  
921 expressions simplify considerably. With these assump-  
922 tions,  $\mathbf{C}_{\text{noise}}^{11}$  and  $\mathbf{C}_{\text{noise}}^{22}$  are diagonal and  $\mathbf{C}_{\text{noise}}^{12}$ ,  $\mathbf{U}_{\text{noise}}^{11}$ ,  
923  $\mathbf{U}_{\text{noise}}^{22}$ ,  $\mathbf{U}_{\text{noise}}^{12}$ ,  $\mathbf{G}_{\text{noise}}^{11}$ ,  $\mathbf{G}_{\text{noise}}^{22}$  and  $\mathbf{G}_{\text{noise}}^{12}$  are all zero.  
924 Analogous to Equation (29), one can estimate the di-  
925 agonal terms of  $\mathbf{C}_{\text{noise}}^{11}$  and  $\mathbf{C}_{\text{noise}}^{22}$  using the amplitudes  
926 of auto-correlation visibilities. For a baseline  $\{p, q\}$  com-  
927 posed by two antennas  $p$  and  $q$ , its  $\mathbf{C}_{\text{noise}}$  is

$$\begin{aligned}
& \mathbf{C}_{\text{noise},i}^{\{p,q\},\{p,q\}}(t) \equiv \langle V_{\text{noise}}(\{p, q\}, \nu_i, t) V_{\text{noise}}^*(\{p, q\}, \nu_i, t) \rangle \\
& \approx \left| \frac{V(\{p, p\}, \nu_i, t) V(\{q, q\}, \nu_i, t)}{N_{\text{nights}} B \Delta t} \right|, \tag{36}
\end{aligned}$$

931 where  $B \Delta t$  is the product of the channel bandwidth and  
932 the integration time, and  $N_{\text{nights}}$  is the total number of  
933 nights of data analyzed from a drift scan telescope.

934 Inserting only  $\mathbf{C}_{\text{noise}}$  for  $\mathbf{C}$  in Equations (34) and (35),  
 935 we have another estimate on the noise power variance  
 936 as

$$\begin{aligned}
 937 \quad \text{var} \left[ \text{Re}(\hat{P}_\alpha) \right] &= \text{var} \left[ \text{Im}(\hat{P}_\alpha) \right] \\
 938 &= \frac{1}{2} \left\{ \text{tr} \left[ \mathbf{E}^{12,\alpha} \mathbf{C}_{\text{noise}}^{22} \mathbf{E}^{21,\alpha} \mathbf{C}_{\text{noise}}^{11} \right] \right\} \\
 939 &= \sigma_{\text{QE-N}}^2. \tag{37}
 \end{aligned}$$

941 By taking the trace on the products of matrices, we have  
 942 in fact taken a weighted average of covariance informa-  
 943 tion over frequencies. The quantity  $\sigma_{\text{QE-N}}$  should be  
 944 equal to  $P_{\text{N}}$  from the previous subsection, provided that  
 945 in computing  $T_{\text{sys}}$  using Equation (27) we average over  
 946 frequencies to obtain an effective  $T_{\text{sys}}$  in the same way.  
 947 In this way, we see that the analytic noise power spec-  
 948 trum essentially reduces to a special case of Equation  
 949 (37).

950 Of course, the fully covariant treatment here also im-  
 951 plicitly includes the signal-noise cross terms discussed in  
 952 previous sections. Including both  $\mathbf{C}_{\text{signal}}$  and  $\mathbf{C}_{\text{noise}}$  in  
 953  $\mathbf{C}$  gives

$$\begin{aligned}
 954 \quad \text{var} \left[ \text{Re}(\hat{P}_\alpha) \right] &= \text{var} \left[ \text{Im}(\hat{P}_\alpha) \right] \\
 955 &= \frac{1}{2} \left\{ \text{tr} \left[ \mathbf{E}^{12,\alpha} \mathbf{C}_{\text{noise}}^{22} \mathbf{E}^{21,\alpha} \mathbf{C}_{\text{noise}}^{11} \right. \right. \\
 956 &\quad \left. \left. + \mathbf{E}^{12,\alpha} \mathbf{C}_{\text{signal}}^{22} \mathbf{E}^{21,\alpha} \mathbf{C}_{\text{noise}}^{11} \right. \right. \\
 957 &\quad \left. \left. + \mathbf{E}^{12,\alpha} \mathbf{C}_{\text{noise}}^{22} \mathbf{E}^{21,\alpha} \mathbf{C}_{\text{signal}}^{11} \right] \right\} \\
 958 &= \sigma_{\text{QE-SN}}^2. \tag{38}
 \end{aligned}$$

960 Since we have assumed only  $\mathbf{C}_{\text{noise}}^{11}$  and  $\mathbf{C}_{\text{noise}}^{22}$  are non-  
 961 zero, the extra signal-noise cross terms entering into the  
 962 expression are just their couplings with the signal coun-  
 963 terparts. For that last contribution, we estimate  $\mathbf{C}_{\text{signal}}$   
 964 as

$$965 \quad \mathbf{C}_{\text{signal},ij}^{11} = \mathbf{C}_{\text{signal},ij}^{22} = \frac{1}{2} \left[ \mathbf{x}_{1,i} \mathbf{x}_{2,j}^* + \mathbf{x}_{2,i} \mathbf{x}_{1,j}^* \right]. \tag{39}$$

967 Note that this way of modelling  $\mathbf{C}_{\text{signal}}$  is Hermitian and  
 968 noise-bias free when taking the ensemble average, but  
 969 not positive definite. With a similar argument to  $P_{\text{SN}}$   
 970 in subsection 3.3, we enact a hard non-negative prior  
 971 on  $\mathbf{C}_{\text{signal}}$ , where rows and columns containing negative  
 972 diagonal elements are set to zero. This procedure can be  
 973 shown to give signal-noise cross terms in Equation (38)  
 974 that are always non-negative. However, this means that  
 975  $\sigma_{\text{QE-SN}}$  suffers from the same double-counting noise bias  
 976 with  $P_{\text{SN}}$ , and analogously we may construct a modified  
 977 “ $\sigma_{\text{QE-SN}}$ ” which is also free from the bias as

$$978 \quad \tilde{\sigma}_{\text{QE-SN}} = \sigma_{\text{QE-SN}} - \left( \sqrt{1/\sqrt{\pi} + 1} - 1 \right) \sigma_{\text{QE-N}}. \tag{40}$$

979 Generally speaking, the power spectrum method of  
 980 the previous subsection is a special case of the covariance  
 981 method of this subsection. For example, if we estimate  
 982  $P_{\text{N}}$  in a way that carefully accounts for the frequency  
 983 dependence of  $T_{\text{sys}}$ , we should find that when we in-  
 984 sert it into the expression for  $P_{\text{SN}}$  that  $P_{\text{SN}} = \sigma_{\text{QE-SN}}$ .  
 985 The covariance method has the advantage of providing  
 986 off-diagonal covariances between different bandpowers  
 987 in addition to variances.

### 988 3.5. Summary

989 The methods of error bar estimation introduced in this  
 990 section can be categorized into two groups:

- 991 •  $\sigma_{\text{bs}}, P_{\text{SN}}, \sigma_{\text{QE-SN}}$ : these estimate error bars on the  
 992 total emission, including both contributions from  
 993 signal-noise cross terms and noise-noise terms.
- 994 •  $P_{\text{diff}}, P_{\text{N}}, \sigma_{\text{QE-N}}$ : these estimate the error bar in  
 995 the limit of noise-dominated (or noise level), only  
 996 including contributions from the noise-noise terms.

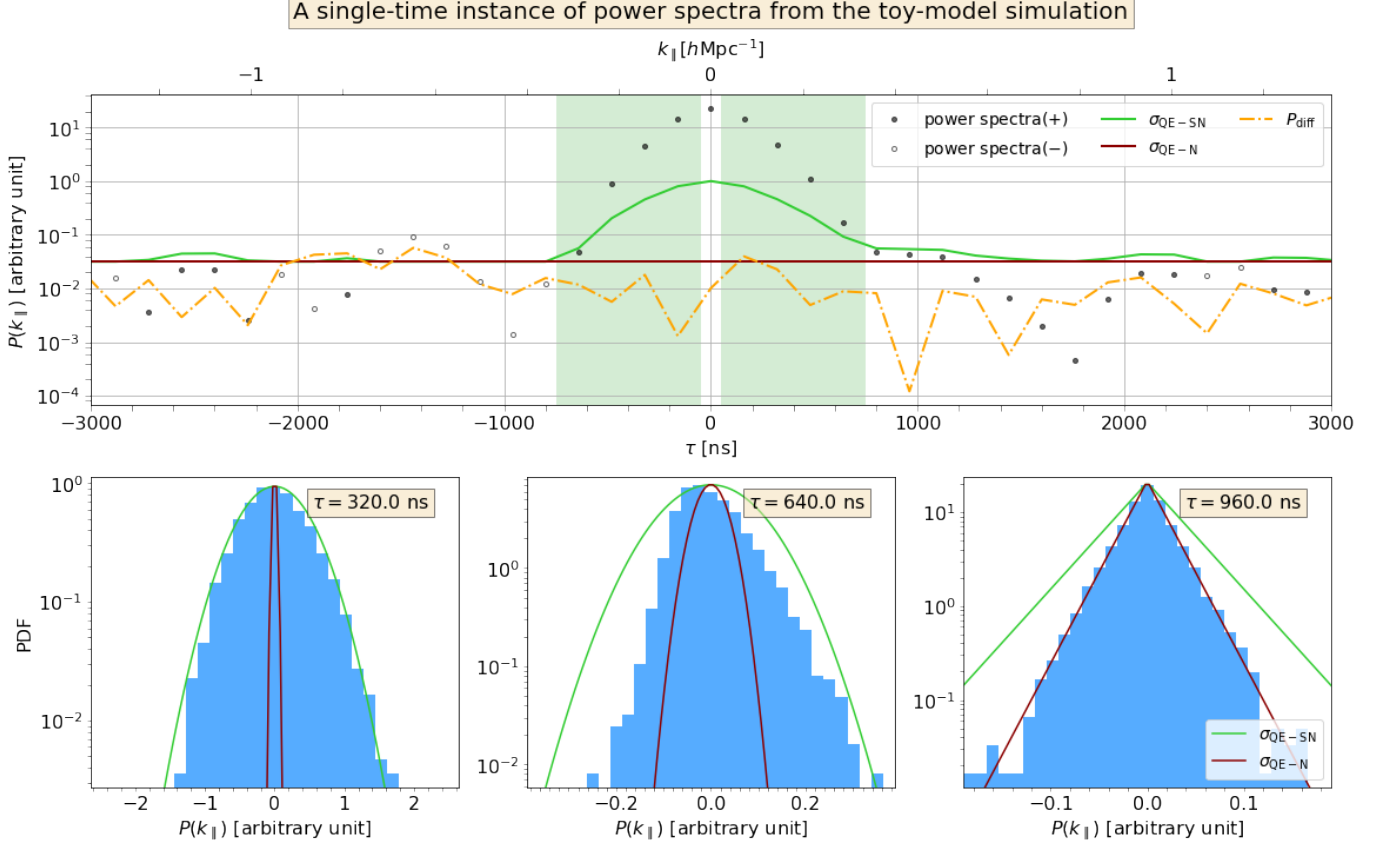
997 Before we jump into a quantitative discussion using the  
 998 HERA power spectrum pipeline to compute these error  
 999 bars in the next section, it is important to stress that  
 1000 there are other methods of error estimation that we do  
 1001 not cover in this paper. For example, LOFAR has used  
 1002 the Stokes V parameter as an estimator of noise level  
 1003 (Patil et al. 2017; Gehlot et al. 2019; Mertens et al. 2020)  
 1004 since the astrophysical sky is expected to exhibit only  
 1005 extremely weak circular polarization. However, reliably  
 1006 estimating Stokes V power requires more accurate po-  
 1007 larization calibration solutions than that are currently  
 1008 available for HERA (Kohn et al. 2019). Since one of our  
 1009 goals is to test our error estimation methods on HERA  
 1010 data, we will omit discussion of Stokes V techniques in  
 1011 this paper.

## 1012 4. TESTS

1013 In this section, we quantitatively examine the error  
 1014 estimation methods introduced in Section 3. We apply  
 1015 them to 21 cm delay power spectra estimated from both  
 1016 simulated data and HERA Phase I data. We directly  
 1017 compare the relative amplitudes of the error bars pre-  
 1018 dicted by each method, delay mode by delay mode. We  
 1019 also study how the error bars respond to systematics  
 1020 and foregrounds in different regimes of delay space.

### 1021 4.1. Simulations from a Toy Model

1022 We start with simulations from a toy model. This al-  
 1023 lows us to generate a large number of realizations, with  
 1024 which we can numerically test the validity of our error  
 1025 bars in the ensemble-averaged limit. Our simulated vis-  
 1026 ibilities include only the foregrounds and noise. For the



**Figure 3.** Error bars on single-baseline-pair power spectra at one timestamp from simulations described in Section 4.1. *Top:* We plot power spectra together with error bar types  $P_{\text{diff}}$ ,  $\sigma_{\text{QE-SN}}$  and  $\sigma_{\text{QE-N}}$ . The green shaded regime ranges from  $\pm 50$  ns to  $\pm 750$  ns, where the foreground power is dominant over the noise power. *Bottom:* We plot histograms of bandpowers from  $\sim 10000$  realizations at  $\tau = 320.0$  (strongly foreground-dominated regime),  $640.0$  (transition regime),  $960.0$  (noise-dominated regime) ns respectively, along with probability distribution function (PDF) curves predicted using the  $\sigma_{\text{QE-SN}}$  and  $\sigma_{\text{QE-N}}$  values at the same delay. At  $\tau = 320.0, 640.0$  ns, the PDF takes a Gaussian form. At  $\tau = 960.0$  ns, the PDF takes the form of a Laplacian. The  $P(k_{\parallel})$  values used in the histograms have been subtracted from the mean value of all realizations. We can see error bars are roughly comparable to each other in amplitudes in the noise-dominated regime. At  $\tau = 320.0$ , the envelope of the histogram matches exactly with the PDF using  $\sigma_{\text{QE-SN}}$ . At  $\tau = 960.0$ , the envelope of the histogram matches the PDF using  $\sigma_{\text{QE-N}}$ , while we see the PDF using  $\sigma_{\text{QE-SN}}$  is broader. Therefore, using  $\sigma_{\text{QE-SN}}$  will lead to a more conservative estimate of errors in this delay regime.

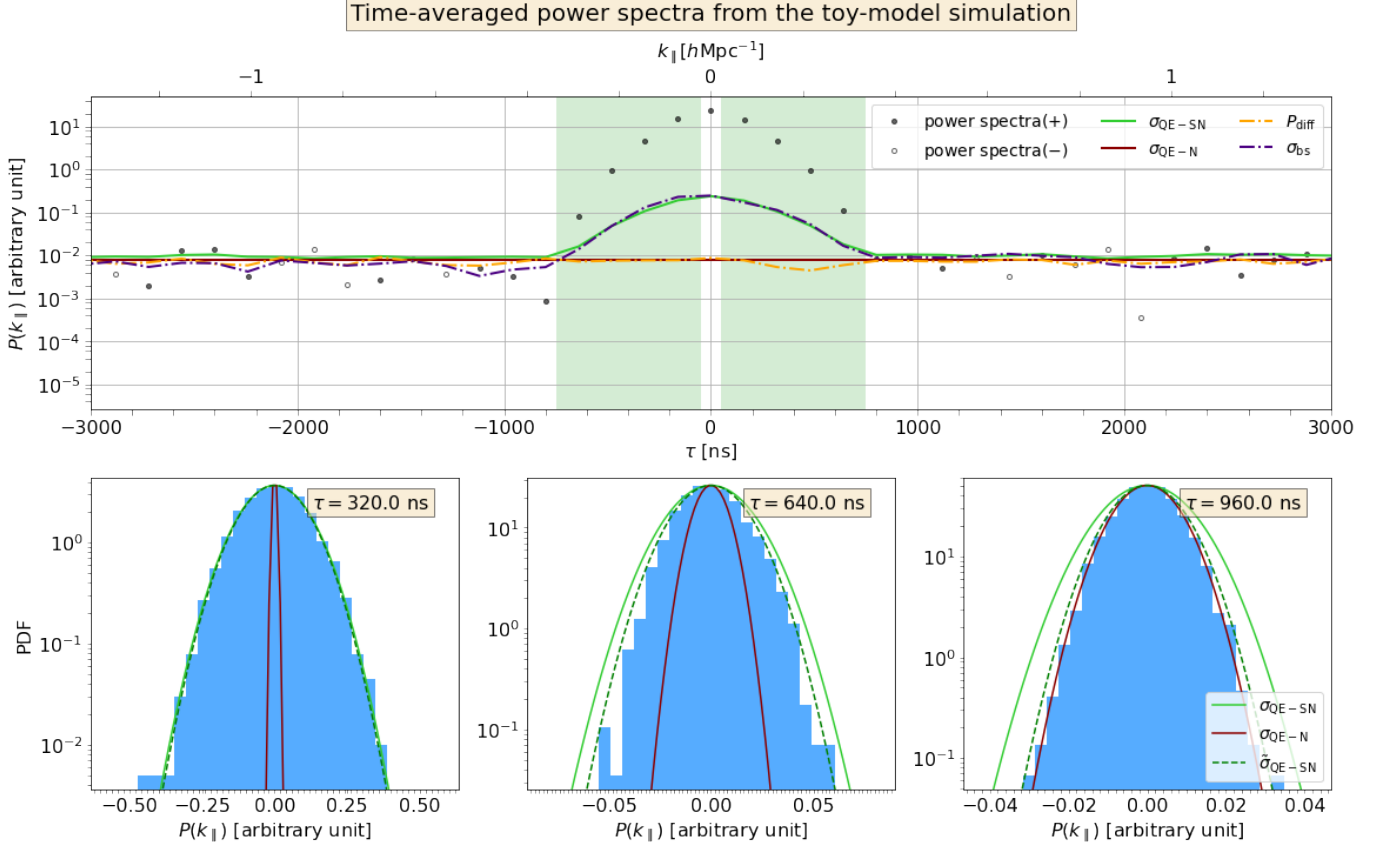
1027 foreground portion of the visibilities we draw a random  
 1028 visibility from a frequency-frequency covariance matrix  
 1029 of the form  $C_{ij} = A \exp[-(\nu_i - \nu_j)^2/l^2]$ , where  $A$  and  $l$   
 1030 characterize the amplitude and correlation length of the  
 1031 foreground signal, respectively. The adopted covariance  
 1032 model creates smoothly varying functions in frequency  
 1033 space, which is roughly in accordance with the relatively  
 1034 flat spectral structure of real foregrounds. Here we simu-  
 1035 late visibilities on two redundant baselines for 20 con-  
 1036 secutive timestamps. We set  $A = 25$  and  $l = 5\text{MHz}$ ,  
 1037 and the foreground visibilities are kept the same on each  
 1038 baseline and over all timestamps. The noise components  
 1039 of the visibilities on each baseline at each timestamp  
 1040 are independently drawn from the same white Gaussian  
 1041 distribution  $\mathcal{N}(0, \sigma^2 = 1)$ . We produce  $\sim 10000$  realiza-

1042 tions of such visibilities and then use `hera_pspec` code<sup>10</sup>  
 1043 to estimate the delay power spectra and to compute the  
 1044 error bars discussed previously.

1045 In Figure 3, we plot power spectra together with a  
 1046 few of the error bar types computed from one times-  
 1047 tamp of data from the simulations. We compute  $P_{\text{diff}}$   
 1048 by differencing visibilities between the one timestamp  
 1049 and the next. We use Equation (37) and (38) to cal-  
 1050 culate error bars of the ‘‘covariance method’’, while we  
 1051 evaluate  $C_{\text{noise}}$  using the exact covariance matrix from  
 1052 which noise visibilities are drawn, since we did not simu-  
 1053 late visibilities on auto-correlation baselines. In the  
 1054 top panel of Figure 3, the green shaded regime (which

<sup>10</sup> [https://github.com/HERA-Team/hera\\_pspec](https://github.com/HERA-Team/hera_pspec)





**Figure 4.** Error bars on time-averaged power spectra over 20 timestamps from simulations in Section 4.1. The figure follows similar conventions to Figure 3, except *Top*:  $\sigma_{bs}$  is added; *Bottom*: All PDFs take the forms of Gaussian and the ones specified by  $\tilde{\sigma}_{QE-SN}$  are appended. We observe good agreement between  $\sigma_{bs}$  and  $\sigma_{QE-SN}$  in the foreground-dominated regime, and the consistency of all types of labeled error bars in the noise-dominated regime. After the incoherent average, we see histograms at all delays become Gaussian. Additionally,  $\tilde{\sigma}_{QE-SN}$  is clearly different from  $\sigma_{QE-SN}$  where the signal is less dominant. Especially at  $\tau = 960.0$  ns, the PDF using  $\tilde{\sigma}_{QE-SN}$  is closer to the exact noise-dominated version using  $\sigma_{QE-N}$ .

1055 ranges from  $\pm 50$  ns to  $\pm 750$  ns) is where the foreground  
 1056 power is dominant over the noise power. We see that  
 1057  $P_{diff}$  and  $\sigma_{QE-N}$  are insensitive to the foreground  
 1058 power in this regime, and when moving to higher delays, the  
 1059 noise levels characterized by  $P_{diff}$ ,  $\sigma_{QE-N}$ , and  $\sigma_{QE-SN}$   
 1060 are very close to one another. Compared to the other two,  
 1061  $P_{diff}$  shows much more scatter from delay to delay since  
 1062 it is a more empirical estimation of noise based on exam-  
 1063 ining what amounts to noise *realizations*. Notice also  
 1064 that as expected by construction, the  $\sigma_{QE-SN}$  curve al-  
 1065 ways lies above  $\sigma_{QE-N}$ , due to the fact we enforce a zero  
 1066 clipping on the signal-noise cross term.

1067 In the bottom panel of Figure 3, we plot histograms  
 1068 of power spectra at three delays ( $\tau = 320.0, 640.0$  and  
 1069  $960.0$  ns) by accumulating data points from  $\sim 10000$   
 1070 realizations. The results here are therefore representative  
 1071 of ensemble-averaged expectations. At each delay, we  
 1072 also plot theoretical predictions for the probability dis-  
 1073 tribution functions (PDFs). Precisely what form these  
 1074 PDFs take will depend on the delay. In the low-delay

1075 regime, Equation (17) shows the variation comes from  
 1076 single powers of visibility noise, which we assume is  
 1077 Gaussian. (Recall that we are not modelling the signal  
 1078 as a random field, in the sense that it does not partici-  
 1079 pate in our ensemble average.) The result is a Gaussian  
 1080 PDF. At high delays Equation (17) shows that the power  
 1081 spectrum is the cross-multiplication of two independent  
 1082 realization of noise. The resulting PDF is a Laplacian.  
 1083 Both of these distributions take one free parameter (the  
 1084 standard deviation of power) and we show predictions  
 1085 where this standard deviation is specified by  $\sigma_{QE-SN}$  and  
 1086  $\sigma_{QE-N}$ . At  $\tau = 320.0$  and  $640.0$  ns, we plot Gaussian re-  
 1087 ference PDFs. At  $\tau = 960.0$  ns, we plot a Laplacian  
 1088 reference PDF. We see at  $\tau = 320.0$  ns, where fore-  
 1089 ground power is overwhelmingly dominant, the shape of  
 1090 the histogram is indeed Gaussian-like, and its envelope  
 1091 matches the PDF curves using  $\sigma_{QE-SN}$ . At  $\tau = 960.0$   
 1092 where noise is dominant, the shape of the histogram is  
 1093 indeed Laplacian-like, and its envelope matches the PDF  
 1094 curves using  $\sigma_{QE-N}$  (since  $\sigma_{QE-N}$  does not suffer from

1095 the conservatism of  $\sigma_{\text{QE-SN}}$  discussed in Section 3.3).  
 1096 With  $\tau = 640.0$  ns we have a transition case between  
 1097 the two extremes. The distribution of power spectra  
 1098 will be skewed since neither the signal nor the noise  
 1099 dominates in this occasion (for a mathematical proof of  
 1100 the skewness see Appendix F). The histogram does not  
 1101 match the PDF predicted by either standard deviation,  
 1102 but note from the widths of the PDFs that an error bar  
 1103 given by  $\sigma_{\text{QE-SN}}$  is a conservative error, as we designed  
 1104 it to be.

1105 In Figure 4, we present the same types of error bars  
 1106 plus a bootstrapped one on power spectra which were  
 1107 formed by incoherently averaging over 20 timestamps.  
 1108 We see in the green regime that  $\sigma_{\text{bs}}$  agrees with  $\sigma_{\text{QE-SN}}$ .  
 1109 All the different kinds of error bars agree well with each  
 1110 other in the noise dominated regime, and with the ex-  
 1111 tra time averaging step (compared to Figure 3)  $P_{\text{diff}}$  ex-  
 1112 hibits less scatter. Again, we plot histograms of the  
 1113 averaged power spectra from Monte-Carlo simulations  
 1114 against Gaussian PDF curves at  $\tau = 320.0, 640.0$  and  
 1115  $960.0$  ns. One feature to note from the histogram is that  
 1116 each distribution has become nearly Gaussian. This is  
 1117 simply due to the Central Limit Theorem as power spec-  
 1118 tra are averaged together incoherently. In addition to  
 1119  $\sigma_{\text{QE-SN}}$  and  $\sigma_{\text{QE-N}}$ , we also plot the PDFs using  $\tilde{\sigma}_{\text{QE-SN}}$   
 1120 which eliminates the double-counting bias in  $\sigma_{\text{QE-SN}}$ . It  
 1121 is as expected that the PDF using  $\tilde{\sigma}_{\text{QE-SN}}$  is more close  
 1122 to the one using  $\sigma_{\text{QE-N}}$  at the noise-dominated delay  
 1123 mode.

#### 1124 4.2. Application to HERA Phase I Data

1125 The HERA Phase I data used for analysis in this pa-  
 1126 per consists of 18 observing nights taken in the Karoo  
 1127 Desert, South Africa from December 10th to 28th, 2017.  
 1128 The HERA array consisted of  $\sim 40$  functional anten-  
 1129 nas during observations, which were taken across a 100  
 1130 to 200 MHz band comprised of 1024 channels and dual  
 1131 polarization “X” and “Y” feeds. [See Table 1 of Kern  
 1132 et al. (2020b) for more details on the array and corre-  
 1133 lator specifications during the observations.] The data  
 1134 used in this work were first preprocessed with the HERA  
 1135 analysis pipeline (internally called H1C IDR2.2<sup>11</sup>). This  
 1136 includes automated metric evaluation and data flag-  
 1137 ging for faulty antennas and radio frequency interference  
 1138 (RFI). In addition, the data are redundantly calibrated  
 1139 (Dillon et al. 2020), absolutely calibrated (Kern et al.  
 1140 2020b), binned and averaged across observing nights,  
 1141 in-painted over RFI gaps in frequency and then treated  
 1142 for known instrumental systematics (Kern et al. 2020a).

<sup>11</sup> [http://reionization.org/manual\\_uploads/HERA069\\_IDR2.2\\_Memo\\_v3.html](http://reionization.org/manual_uploads/HERA069_IDR2.2_Memo_v3.html)

1143 We pick a slice of HERA Phase I visibilities taken from  
 1144 a 14.6-m redundant baseline group during an LST range  
 1145 of 5.75 to 6.10 hours. The visibilities in each timestamp  
 1146 are integrated over  $\sim 10$  seconds. We select visibilities  
 1147 falling within a 150.3 to 167.8 MHz band to compute  
 1148 power spectra. We use pseudo-Stokes I visibilities  $V_{\text{PI}}$ ,  
 1149 which are constructed by combining the visibilities from  
 1150 a cross correlation of two X feeds (“XX”) and a cross-  
 1151 correlation two Y feeds (“YY”) as follows:

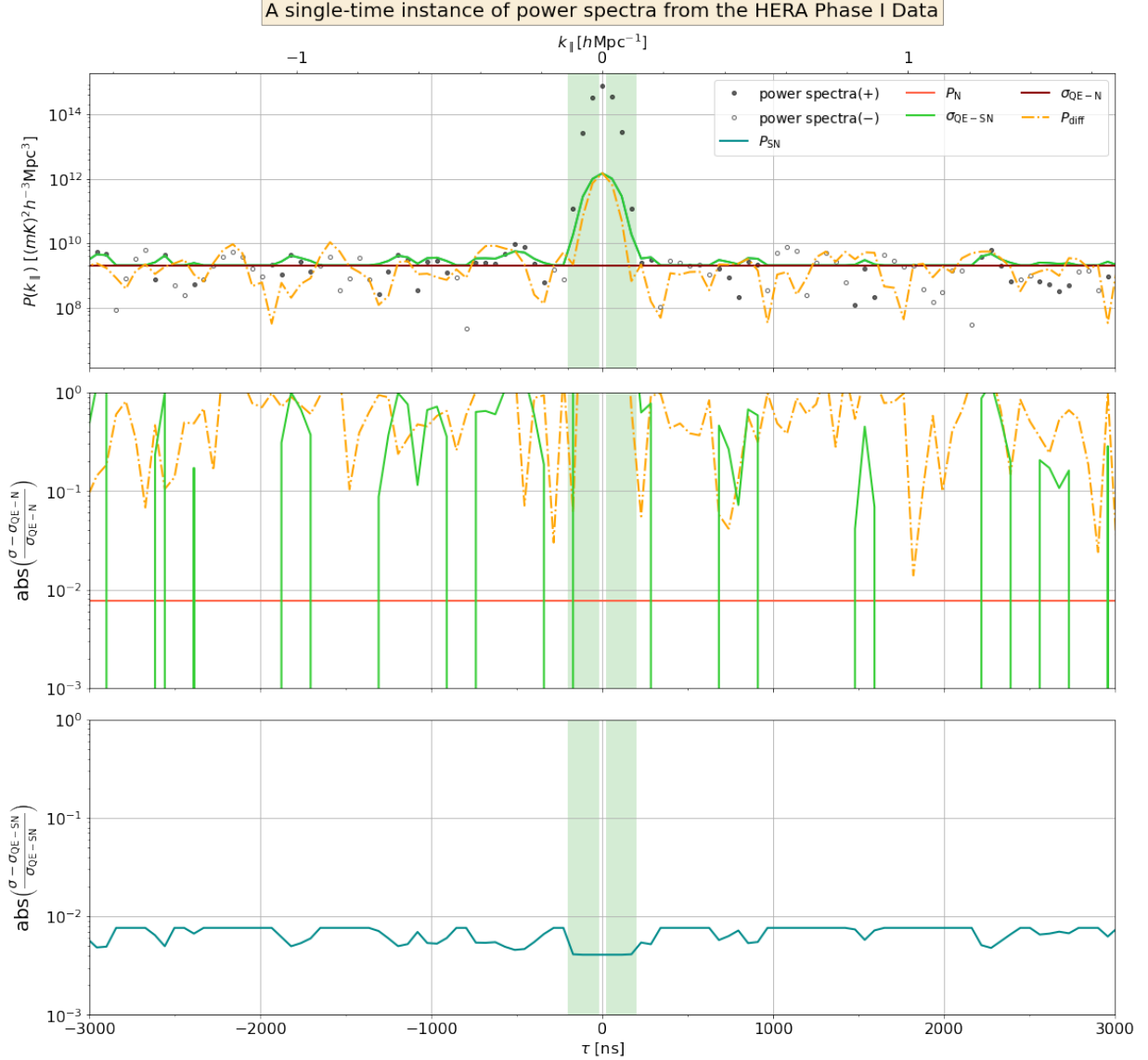
$$1152 \quad V_{\text{PI}} = \frac{1}{2} (V_{\text{XX}} + V_{\text{YY}}) . \quad (41)$$

1153 In forming the delay power spectra we cross correlate  
 1154 visibilities from different baselines (e.g.,  $\mathbf{b}_1\text{-}\mathbf{b}_2$ ,  $\mathbf{b}_1\text{-}\mathbf{b}_3$ ,  $\mathbf{b}_2\text{-}$   
 1155  $\mathbf{b}_3$ , etc.) and between odd and even timestamps (e.g.,  
 1156  $t_1\text{-}t_2$ ,  $t_3\text{-}t_4$ ,  $t_5\text{-}t_6$ , etc.) to form delay power spectra. In  
 1157 this way, we obtain power spectra on 253 baseline-pairs  
 1158 at 30 timestamps.

1159 We show the power spectra from one baseline-pair  
 1160 at one timestamp in Figure 5, together with error bar  
 1161 types  $P_{\text{diff}}$ ,  $\sigma_{\text{QE-SN}}$ ,  $\sigma_{\text{QE-N}}$ ,  $P_{\text{SN}}$ , and  $P_{\text{N}}$ . The  $P_{\text{diff}}$  errors  
 1162 are computed from time-differenced visibilities, e.g., for  
 1163 power spectra at the cross timestamp  $t_1 - t_2$  we form  
 1164  $V_{\text{diff}} \propto V(t_2) - V(t_1)$  and then we cross multiply  $V_{\text{diff}}$   
 1165 from two different baselines to obtain the correspond-  
 1166 ing  $P_{\text{diff}}$  for that baseline pair. We calculate  $\sigma_{\text{QE-SN}}$   
 1167 and  $\sigma_{\text{QE-N}}$  using Equations (38) and (37) with  $\mathbf{C}_{\text{signal}}$   
 1168 and  $\mathbf{C}_{\text{noise}}$  specified by Equation (39) and (36). Equa-  
 1169 tions (30) and (27) give the expressions for  $P_{\text{SN}}$  and  $P_{\text{N}}$ .  
 1170 See `hera_pspec` for detailed implementation.

1171 In the top panel of Figure 5, we see all error bars  
 1172 agree well with each other in the noise-dominated regime  
 1173 (the red curve for  $P_{\text{N}}$  is almost exactly underneath the  
 1174 brown curve for  $\sigma_{\text{QE-N}}$ , making the former difficult to  
 1175 see; the same is true for the teal curve for  $P_{\text{SN}}$  versus the  
 1176 bright green curve for  $\sigma_{\text{QE-SN}}$ ). The green shaded regime  
 1177 ranging from  $\pm 20$  ns to  $\pm 200$  ns is where foregrounds  
 1178 are expected to dominate. Here we see that  $P_{\text{diff}}$  also  
 1179 responds to the foreground power, similar to  $P_{\text{SN}}$  and  
 1180  $\sigma_{\text{QE-SN}}$ . This tells us that the time-differenced visibil-  
 1181 ities contain non-negligible foreground residuals, which  
 1182 is not surprising since the sky is expected to evolve non-  
 1183 negligibly over the  $\sim 10$  seconds of difference between  
 1184 our time samples.

1185 In Section 3, we argued that the “covariance method”  
 1186 and the “power spectrum method” should be equivalent  
 1187 to each other. In the middle and bottom panels of Fig-  
 1188 ure 5, we compute the relative difference in magnitudes  
 1189 between error bars, setting  $\sigma_{\text{QE-SN}}$  and  $\sigma_{\text{QE-N}}$  as the  
 1190 benchmarks respectively. We see that  $P_{\text{SN}}$  differs from  
 1191  $\sigma_{\text{QE-SN}}$  and  $P_{\text{N}}$  from  $\sigma_{\text{QE-N}}$  by less than 1%, so they  
 1192 are essentially equivalent in our pipeline. On the other  
 1193 hand,  $P_{\text{diff}}$  can differ from  $\sigma_{\text{QE-N}}$  at more than the 10%-

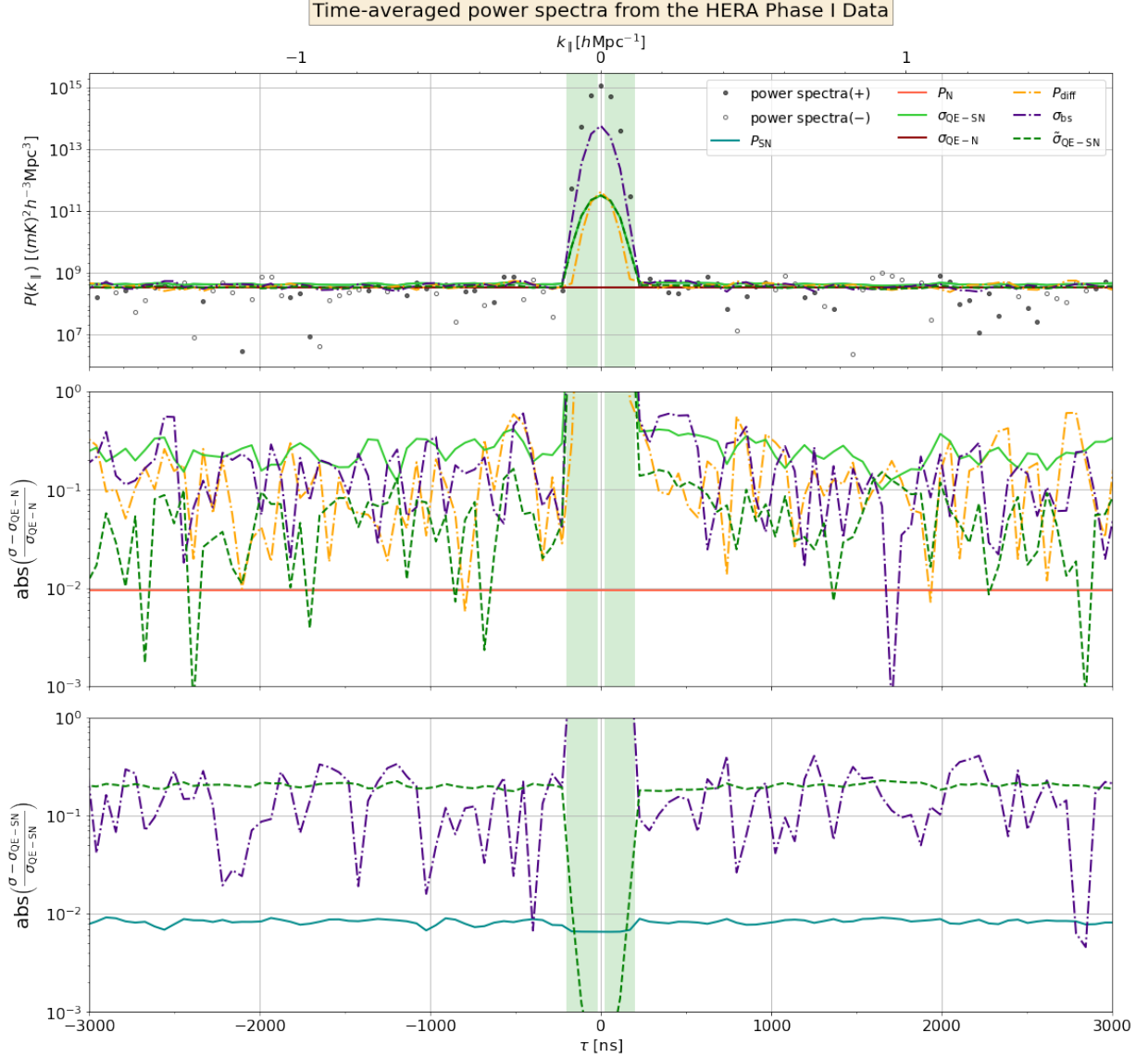


**Figure 5.** Error bars on single-baseline-pair power spectra at one timestamp from HERA Phase I data. The visibilities are selected from a band spanning 150.3 to 167.8 MHz. *Top:* Power spectra with error bars. The green shaded regime ranging from  $\pm 20$  ns to  $\pm 200$  ns is expected to be foreground dominated. *Middle:* Absolute relative difference between selected error bars with  $\sigma_{\text{QE-N}}$ . *Bottom:* Absolute relative difference between selected error bars with  $\sigma_{\text{QE-SN}}$ . We see numerically that  $P_{\text{SN}}$  differs from  $\sigma_{\text{QE-SN}}$  by less than 1% and that the same is true for  $P_{\text{N}}$  and  $\sigma_{\text{QE-N}}$ .

1194 level due to the fact that it is highly scattered. Note  
 1195 that  $\sigma_{\text{QE-SN}}$  and  $P_{\text{SN}}$  are also scattered at some delays,  
 1196 whereas they are equal to  $\sigma_{\text{QE-N}}$  and  $P_{\text{N}}$  at other delays.  
 1197 This is due to our imposition of a non-negative prior on  
 1198 the signal-noise cross term.

1199 In Figure 6, we show the power spectra with error bars  
 1200 on the same baseline-pair as Figure 5, but with the fur-  
 1201 ther step of incoherently averaging over 30 time samples.  
 1202 We still see that all error bars (with bootstrap errors  $\sigma_{\text{bs}}$   
 1203 added) agree well in the noise-dominated regime. At low  
 1204 delays,  $\sigma_{\text{bs}}$  peaks at an even higher value than  $\sigma_{\text{QE-SN}}$ .  
 1205 This is because the sky is not unchanged over different

1206 timestamps, so the bootstrapped error bars over time  
 1207 samples are inflated. After incoherently averaging, we  
 1208 still see  $P_{\text{SN}}$  differing from  $\sigma_{\text{QE-SN}}$  and  $P_{\text{N}}$  differing from  
 1209  $\sigma_{\text{QE-N}}$  by less than 1%. On the other hand,  $P_{\text{diff}}$  and  $\sigma_{\text{bs}}$   
 1210 differ from  $\sigma_{\text{QE-N}}$  at roughly the 10% level in the noise-  
 1211 dominated regime. We also see that in the limit of noise  
 1212 domination,  $\sigma_{\text{QE-SN}}$  has a relative bias over  $\sigma_{\text{QE-SN}}$  by  
 1213 about 30%. Therefore, using  $\sigma_{\text{QE-SN}}$  or  $P_{\text{SN}}$  leads to  
 1214 a conservative estimate of one's errors, as we expected.  
 1215 For comparing, we also plot results of  $\tilde{\sigma}_{\text{QE-SN}}$ , which  
 1216 eliminates the double-counting noise bias in  $\sigma_{\text{QE-SN}}$ .  
 1217 The relative difference between  $\tilde{\sigma}_{\text{QE-SN}}$  and  $\sigma_{\text{QE-N}}$  is re-

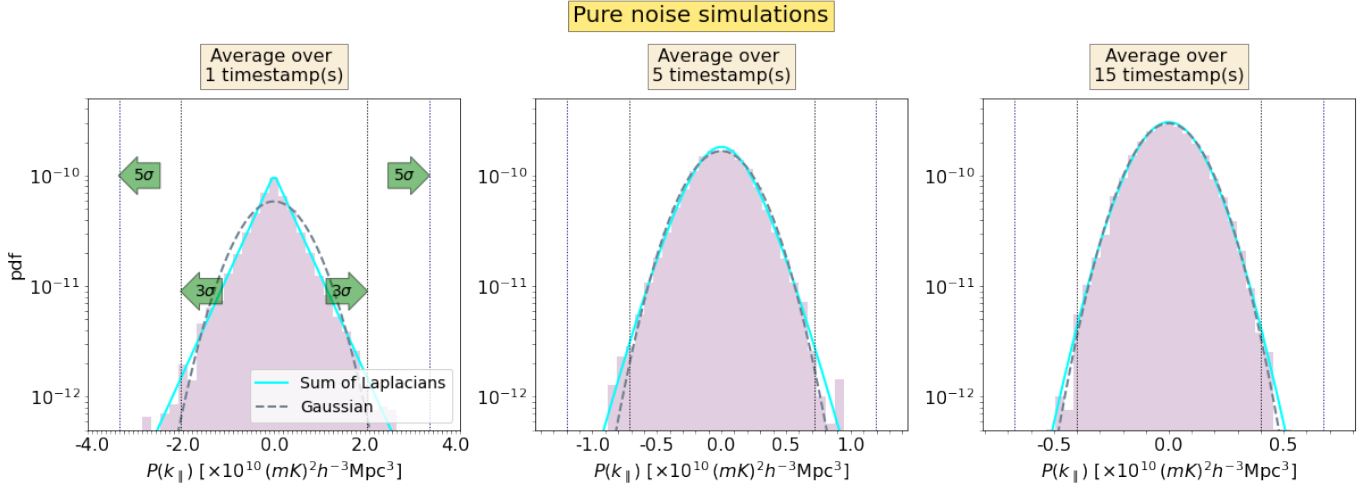


**Figure 6.** Error bars on single-baseline-pair power spectra incoherently averaged over 30 time samples from the same slice of HERA Phase I data as Figure 5. Our plotting conventions also follow those of Figure 5 for other conventions. We add results from  $\tilde{\sigma}_{\text{QE-SN}}$  in each panel. In the center panel we see the relative difference between  $\tilde{\sigma}_{\text{QE-SN}}$  and  $\sigma_{\text{QE-N}}$  drops remarkably from  $\sim 30\%$  to a few percent compared to the  $\sigma_{\text{QE-SN}}$ , demonstrating the effectiveness of our noise-double-counting bias removal. On the other hand, in the bottom panel we see that going from  $\sigma_{\text{QE-SN}}$  to  $\tilde{\sigma}_{\text{QE-SN}}$  results in significant changes only at the noise-dominated delays, and thus there one can always elect to use  $\tilde{\sigma}_{\text{QE-SN}}$  even in foreground-dominated regimes.

1218 duced to a few percents in the noise-dominated regime.  
 1219 While  $\tilde{\sigma}_{\text{QE-SN}}$  is not significantly modified from  $\sigma_{\text{QE-SN}}$   
 1220 in the foreground-dominated regime. Thus if we want  
 1221 a compromise on reflecting the properties of the signal-  
 1222 noise cross term while not introducing noise bias,  $\tilde{\sigma}_{\text{QE-SN}}$   
 1223 might be our choice.

1224 What we have established so far is the *relative* agree-  
 1225 ment (or lack thereof) between different types of error  
 1226 bars in different regimes. However, we have not yet es-  
 1227 tablished the *absolute* validity of these error bars on real  
 1228 data (i.e., we have not ruled out the possibility that they

1229 are all incorrect in the same way). For simulated power  
 1230 spectra we were able to compare the Monte-Carlo his-  
 1231 tograms with the PDF curves predicted from the error  
 1232 bars. The good match between the two gave us confi-  
 1233 dence in applying our error estimation methods. Might  
 1234 we perform similar analyses for power spectra from real  
 1235 data? Unfortunately, in real observations we only have  
 1236 one realization of the sky so that we cannot reach en-  
 1237 semble average limit by accumulating data points from  
 1238 a large number of realizations. Also, unlike simulated  
 1239 data with understood statistics, real data will contain



**Figure 7.** We plot the histograms of incoherently averaged power spectra over certain timestamps from pure noise simulations. The histogram in each column contains  $\sim 10000$  data points. We compute  $\sigma_{\text{QE-N}}$  and refer to Equation (G33) to evaluate the “Sum of Laplacians” PDF. Data points have been subtracted from the mean over all realizations. We also plot the equivalent Gaussian PDF with the same variance as the “Sum of Laplacians” PDF. The green arrows point to the dotted vertical lines representing “ $3\sigma$ ” and “ $5\sigma$ ”, where  $\sigma$  is the square root of the variance of the predicted PDF. We see the envelopes of the histograms match the PDFs predicted using (G33) very well. As a check, the fractions of outliers beyond  $3\sigma$  in each histogram are (1.27%, 0.57%, 0.25%), while the corresponding values from the predicted PDFs are (1.34%, 0.58%, 0.22%)—a very close agreement. And with more time samples to be incoherently averaged, the shape of the histogram becomes increasingly Gaussian, which is a consequence of the central-limit theorem. As expected, we also see the distribution get narrower with more samples averaged together.

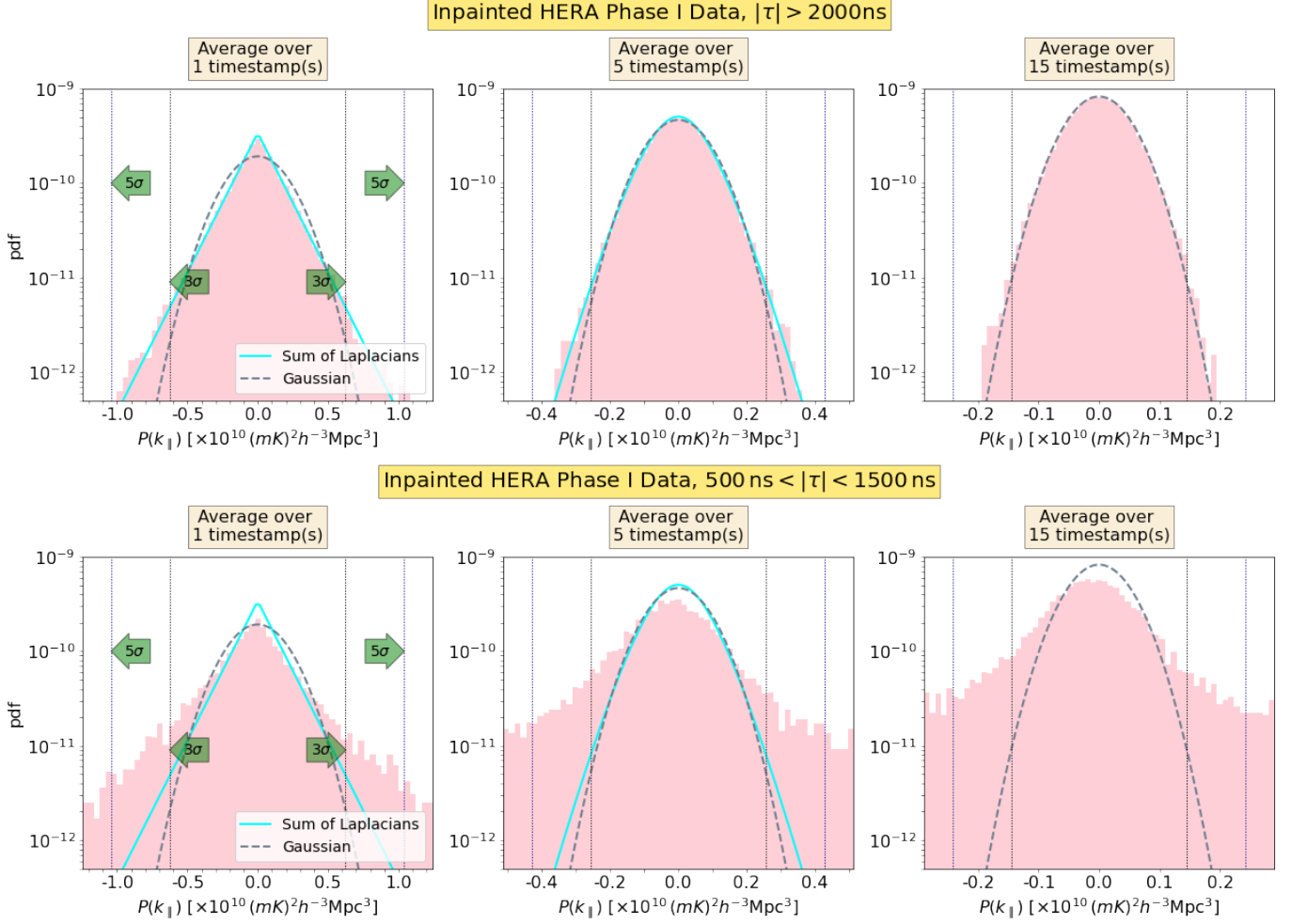
1240 systematics that make their statistics more complicated  
 1241 and difficult to understand (although this may change  
 1242 as the field of 21 cm cosmology continues to mature).

1243 For now, we may partially achieve our goal by checking  
 1244 the distributions of noise-like modes in our power spectra  
 1245 of real data. The noise-like modes refer to power  
 1246 spectra at higher delays where noise power is thought to  
 1247 be dominant and systematics are negligible. As we dis-  
 1248 cussed in Section 3, we expect the noise visibilities to be  
 1249 Gaussian-distributed. This makes it possible to analyt-  
 1250 ically compute the resultant statistics of power spectra.  
 1251 In Appendix G, we derive the mathematical form of the  
 1252 PDF of incoherently averaged noise-dominated power  
 1253 spectra. The final result, Equation (G33), shows that  
 1254 the correct PDF is a weighted sum of a series of Lapla-  
 1255 cian distributions. As a numeric test of the derivation,  
 1256 we produce Monte-Carlo histograms of incoherently aver-  
 1257 aged power spectra from pure Gaussian noise visibil-  
 1258 ities with an increasing number of averaged samples in  
 1259 Figure 7. We generate  $\sim 10000$  realizations of power  
 1260 spectra with multiple time samples, and evaluate the  
 1261 power spectra at a single timestamp, as well as what it  
 1262 would be if incoherently averaged over 5 or 15 times-  
 1263 tamps. For realizations at each time sample, we can  
 1264 calculate the error bar  $\sigma_{\text{QE-N}}$  of the power spectra and  
 1265 substitute them into Equation (G33). It is clear that the  
 1266 predicted PDF matches the envelope of the histograms  
 1267 and that the shape of the histograms of averaged power

1268 spectra become increasingly Gaussian when averaging  
 1269 is over more timestamps. This is again a result of the  
 1270 Central Limit Theorem.

1271 Confronting our results with real data, we use the  
 1272 power spectra from the same HERA Phase I data set  
 1273 as Figures 5 and 6 to generate the histograms. To ac-  
 1274 cumulate sufficient data points for a histogram, we view  
 1275 all noise-like modes in power spectra over different re-  
 1276 dundant baseline-pairs as independent realizations. And  
 1277 we carry out the incoherent average over the time axis.  
 1278 Because the noise level at different baseline pairs may  
 1279 differ, all power spectra are first normalized by being  
 1280 divided over their corresponding  $\sigma_{\text{QE-N}}$  and then sub-  
 1281 tracted from the mean of all data points. After the  
 1282 normalization, we have a uniform error bar  $\sigma_{\text{QE-N}}$  for  
 1283 all data points at each time sample. We then make his-  
 1284 tograms and compare their envelopes with the PDF of  
 1285 “Sum of Laplacians” predicted using Equation (G33).

1286 Before we jump to the results, we first take a look  
 1287 at the data set which includes RFI gap inpainting but  
 1288 without the removal of systematics. For histograms  
 1289 drawn in Figure 8, we evaluate the distributions of power  
 1290 spectra at delays larger than 2000 ns and at delays be-  
 1291 tween 500 and 1500 ns, respectively. In the former case,  
 1292 we see the shape of histograms are perfectly consistent  
 1293 with the predicted PDF, and the distributions become  
 1294 more Gaussian and narrower with increasing number  
 1295 of averaged samples, similar to what we saw in Fig-

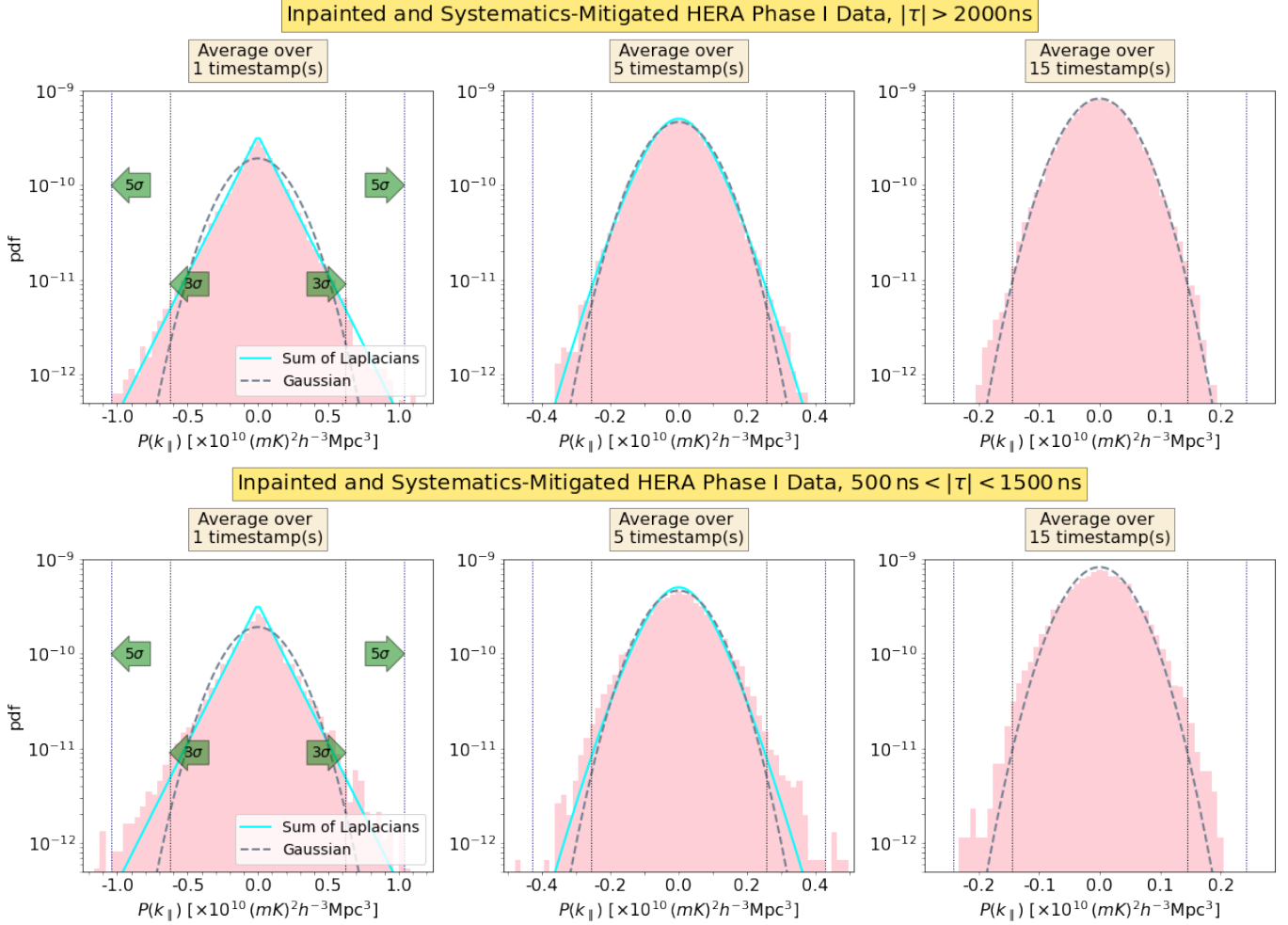


**Figure 8.** Histograms of power spectra at noise-like modes from the same HERA Phase I data used in Figure 5 and 6, including RFI gap inpainting, but without the removal of systematics. The data points are accumulated from power spectra at the same delays from different redundant baseline-pairs. Because their noise levels may differ, they are first normalized by dividing out their corresponding  $\sigma_{\text{QE-N}}$  and then having the mean of all data points subtracted off. In this way we have a uniform  $\sigma_{\text{QE-N}}$  for all points, and we use Equation (G33) to compute the “Sum of Laplacians” PDF. Refer to Figure 7 for other plotting conventions. *Top:* histograms from power spectra at all delays larger than 2000 ns, where there are  $\sim 27000$  points in each column. *Bottom:* histograms from power spectra at delays between 500 and 1500 ns, where there are  $\sim 9000$  points in each column. As a check, in the top panel, the fractions of outliers beyond  $3\sigma$  in each histogram are (1.49%, 0.65%, 0.40%), which are close to the corresponding values from the predicted PDFs (1.36%, 0.57%, 0.24%). In the bottom panel, the fractions of outliers beyond  $3\sigma$  in each histogram are (7.95%, 10.70%, 11.46%), which greatly exceed corresponding values from the predicted PDFs (1.36%, 0.57%, 0.24%).

1296 ure 7. While in the latter case, we observe the his-  
 1297 tograms are **flattened and much wider** compared to the  
 1298 predicted PDF and there exist evidently hefty wings on  
 1299 either ends. Numerically, the fractions of outliers be-  
 1300 yond  $3\sigma$  in each histogram are (7.95%, 10.70%, 11.46%),  
 1301 which greatly exceed corresponding values from pre-  
 1302 dicted PDFs (1.36%, 0.57%, 0.24%). This is a remark-  
 1303 able proof that significant systematics exist at lower de-  
 1304 lays in inpainted only data, as we expect.

1305 We produce histograms for the systematics-removed  
 1306 data, as we used for Figures 5 and 6, in Figure 9. At  
 1307 delays larger than 2000 ns, we still see a good match be-

1308 tween the Monte-Carlo histograms with the predicted  
 1309 PDFs. While at delays between 500 and 1500 ns, we see  
 1310 the deviations between histograms and PDFs are highly  
 1311 suppressed, compared to Figure 8. This is not surpris-  
 1312 ing since we have exerted systematics removal. Though  
 1313 there is still a little excess above PDFs in histograms  
 1314 on far ends, this does not substantially affect the error  
 1315 bars that one might quote on a power spectrum mea-  
 1316 surement (which serve as a summary statistic for the  
 1317 main bulk of the PDF rather than its wings). However,  
 1318 such deviations are worth keeping an eye on, especially  
 1319 when performing rigorous jackknife or null tests in an



**Figure 9.** Histograms of power spectra at noise-like modes from inpainted and systematics-mitigated HERA Phase I data. The power spectra used here come from exactly the same data set as Figure 5 and 6. As a check, in the top panel the fractions of outliers beyond  $3\sigma$  in each histogram are (1.48%, 0.63%, 0.39%), which are close to the corresponding values from the predicted PDFs (1.36%, 0.57%, 0.24%). And in the bottom panel, the fractions of outliers beyond  $3\sigma$  in each histogram are (2.19%, 1.32%, 0.80%), which slightly exceed the corresponding values from the predicted PDFs (1.36%, 0.57%, 0.24%), but at a much lower level than the disagreement seen in Figure 8.

1320 attempt to understand the systematics in one’s instru-  
 1321 ment. As noted above, the excessive wings of the histo-  
 1322 grams in the bottom panel of Figure 8 can serve as  
 1323 a diagnostic tool for systematics that lead to deviations  
 1324 from Gaussian noise-like visibilities. They may also be  
 1325 used to investigate the related question of how instru-  
 1326 mental systematics (e.g., Kern et al. 2019, 2020a) might  
 1327 affect the validity of one’s error bars. There are of course  
 1328 limitations of this analysis, but we show the systematics  
 1329 does not effectively change the noise properties of power  
 1330 spectra at high delays. Readers should interpret Figure  
 1331 8 and 9 as a quality check of HERA Phase I data, which  
 1332 shows the power spectra at high delays ( $> 2000$  ns) and  
 1333 at middle delays (500-1500 ns) after systematics miti-  
 1334 gation are close to the predicted behaviors of Gaussian  
 1335 noise visibilities. Thus  $\sigma_{\text{QE-N}}$  (along with other equiva-

1336 lent methods) validates itself a successful tool to charac-  
 1337 terize the noise statistics in real data. However, we will  
 1338 still quote  $\tilde{\sigma}_{\text{QE-SN}}$  as a more robust error bar on report-  
 1339 ing EoR upper limits at those delays. One should be  
 1340 aware that not all systematics can be cleanly corrected  
 1341 for, which mean that in principle the statistics can be  
 1342 much more complicated than the simple Gaussian distri-  
 1343 bution shown here. Along this theme, we urge readers  
 1344 to always perform consistency checks on the data, in-  
 1345 cluding but not limited to the ones we have performed  
 1346 here.

## 5. DISCUSSION

1347  
 1348 In previous sections, we have examined a number of  
 1349 different methods for assigning error bars to a HERA  
 1350 power spectrum. Here, we perform a comparison of the

different types of error bars, highlighting the advantages and disadvantages of each.

We first consider the error bars using the “covariance method” ( $\sigma_{\text{QE-N}}$  and  $\sigma_{\text{QE-SN}}$ ) to those computed using the “power spectrum method” ( $P_{\text{N}}$  and  $P_{\text{SN}}$ ).

- The “covariance method” error bars analytically take the covariance of the input visibilities and propagate them through to the output covariance of the bandpowers, via general formulae given by Equations (34) and (35). There are two weaknesses to this approach. First, the output errors will only be as good as the modeling of the input covariances. This modeling is particularly difficult for foregrounds and systematics, which can have statistical properties that are not entirely understood. In this paper, we adopt a strategy where we view systematics as non-random, and empirically estimate them from the real data. The other weakness of our “covariance method” is that our derivations rely on Gaussianity (Indeed, it would be strange for this method to only require an input *covariance*—a two-point function—if it were capable of capturing the effects of non-Gaussianity). This assumption will also be violated by foregrounds and systematics as well the cosmological signal (which is an effect that was modeled in [Mondal et al. 2016, 2017](#); [Shaw et al. 2019](#)).

Sidestepping these modeling restrictions on the “covariance method” are the noise-dominated bandpowers at high delays. In this regime, we use an input covariance matrix that is  $C_{\text{noise}}$  that is diagonal, with the diagonal elements set by the auto-correlation visibilities as Equation (36). The resulting error bars we call  $\sigma_{\text{QE-N}}$  (see Table 3 for a reminder of our notation). These error bars are confirmed by tests on simulations and real data in Figure 7 and Figure 9, which verify that the error bars do properly account for the spread seen in an ensemble of Monte Carlo simulations. Further bolstering our confidence in using the “covariance method” are their agreement with other error metrics at our disposal. Figures 5 and 6 show that in the noise-dominated regime, the error bars using the “covariance method” are in excellent agreement with the bootstrap errors  $\sigma_{\text{bs}}$ , error bars using the ‘power spectrum method’, and the power spectrum of differenced data  $P_{\text{diff}}$ .

- The agreement between these different error estimation methods raises the question of why one might favour the “covariance method” over others. Consider first a comparison between  $\sigma_{\text{QE-N}}$  and

$P_{\text{N}}$  from the “power spectrum method”. These two methods are in fact quite similar, because  $P_{\text{N}}$  is also an analytically propagated measurement of error, as one can see for instance in the derivation of [Zaldarriaga et al. \(2004\)](#). The difference is one of generality, whether in the inputs, the intermediate steps, and the outputs. On the input side,  $P_{\text{N}}$  assumes uncorrelated noise between visibilities whose amplitude is governed by the radiometer equation;  $\sigma_{\text{QE-N}}$  can accept an arbitrary input covariance (even though in our tests we take it to be diagonal). During the actual propagation of errors, the derivation of  $P_{\text{N}}$  assumes that fluctuations in  $uvv$  space are uncorrelated;  $\sigma_{\text{QE-N}}$  makes no such approximations. Finally, on the output side, the “power spectrum method” returns a single error bar; the ‘covariance method’ provides a full bandpower covariance matrix.

Of course, in reality not all delay modes are noise-dominated, and reliable error bars need to be placed even in signal-dominated regimes (whether this signal comes in the form of instrument systematics, foregrounds, or—ultimately—the cosmological signal). It is difficult to place rigorous error bars on bandpowers in these regimes: unless one has a physical model for all the systematics involved (with knowledge of their probability distributions), it is an ill-defined problem to ask how errors propagate. Unfortunately, the presence of unexplained (or at least not fully explained) systematics is the current state of affairs in 21 cm cosmology, and truly rigorous error bars will need to wait for future work on the modeling of systematics.

Even with well-defined (if not perfectly characterized) systematics, the meaning of one’s error bars is subtle. For instance, foregrounds such as a continuum of unresolved point sources can be appropriately treated as a random field. Given this, one’s approach might be to say that the unresolved point sources contribute some effective power spectrum to the measurement. With such a formalism, there is a fundamental limit to how well these foregrounds can be characterized, since they come with their own form of cosmic variance. In other words, if one is trying to place constraints on foregrounds, one must account for the fact that the particular realization of foregrounds that we see may not be representative of foregrounds in general. This sort of error is difficult to compute in general, as the squared nature of the power spectrum means that the non-Gaussian—and therefore non-trivial—four-point function of the foregrounds needs to be known.

A goal of characterizing the general statistical properties of all possible foregrounds, however, may be un-



necessarily ambitious. In particular, for a cosmological measurement one is not particularly concerned with the behaviour of a “typical” foreground; one is primarily concerned with how our particular realization of foregrounds affect our observations. As a concrete example, if our Galaxy’s synchrotron emission happens to be anomalously bright compared to a typical galaxy’s synchrotron emission, it is our own brighter foregrounds that we need to deal with! With such a mindset, it is more appropriate to consider all foregrounds as non-random components of our data. By this, we do not mean that the foregrounds need to be spatially or spectrally constant; rather, we mean that in hypothetical random draws for taking ensemble averages, the cosmological signal and the instrumental noise change with each new realization, but the foregrounds remain the same. If the foregrounds are not formally random, our error bars are the result of instrumental noise (and in principle cosmic variance of the cosmological signal, although this contribution is small for current upper limits).

It is important to stress, however, that even if our error bars are due to the randomness of instrumental noise, the resulting error bars are *not* simply what one obtains from imagining a noise-only measurement and propagating the noise fluctuations through to a power spectrum. This is because the power spectrum is a squared statistic. Thus, in the squaring of a measurement that contains both noise and a (non-random) signal, there are signal-noise cross-terms to contend with. These terms are zero in expectation, but do not have non-zero *variance*. This means that knowledge of the signal (whether from systematics or foregrounds) is needed to correctly account for instrumental noise errors in non-noise-dominated regimes.

- In short, even if we lower our ambitions and forgo incorporating knowledge about signal *statistics* into our error calculations, understanding the signal itself is necessary for computing noise-sourced error bars. This requirement is where noise-only computations like  $P_N$  and  $\sigma_{QE-N}$  fall short.
- This shortcoming is remedied by generalized versions of  $P_N$  and  $\sigma_{QE-N}$ , which we dub  $P_{SN}$  and  $\sigma_{QE-SN}$ . These are given by Equations (30) and (38). The key idea is that in signal dominated regimes, the measured data itself can be a good approximation to the signal. Thus, we may reinsert the data in an appropriate way to capture signal terms in our general expressions. Figures 3 and 4 show that these error bars work well in both signal-dominated and noise-dominated regimes.

- Although we treat foregrounds and systematics as a single signal term that is directly estimated from measured data in this paper, we note that for future high-sensitivity detections, more elaborate modeling of both are needed. Of course, there is also the possibility of unknown systematic effects, which our formalism does not account for.
- However Moreover, two cautionary warnings are in order when applying Equations (30) and (38). The first is that because the measured data are now part of the error bars themselves, it can be dangerous to use these error bars to inform data weightings for downstream averages in one’s pipeline (e.g., in further incoherent time averaging of power spectra or in incoherent averaging of power spectra from different baselines). If the data weightings are coupled to the data themselves, our so-called quadratic estimators are no longer quadratic. As shown in Cheng et al. (2018), a blind application of the usual methods for normalizing quadratic estimators leads to power spectrum estimates that are biased low (“signal loss”). For this reason, while  $P_{SN}$  and  $\sigma_{QE-SN}$  are fine ways to compute error bars, we recommend that any error-motivated data weightings be based on  $P_N$  and  $\sigma_{QE-N}$  instead.
- The second warning is that there almost certainly exist regimes that are neither signal- nor noise-dominated, where signal and noise are comparable in magnitude. Here, it becomes necessary to contend with the fact that a noisy measurement of the signal can be unphysically negative. Said differently, if our estimate of the signal itself contains noise, we are in effect double counting the noise in our error computations. One approach is to enact a hard prior on the positivity of the signal. This is what was done in all computations of  $P_{SN}$  and  $\sigma_{QE-SN}$  in this paper. However, Figures 3 and 4 show that this has the effect of inflating the error bars. Given that this is a conservative bias on the errors, this may or may not be appropriate depending on one’s application.
- A slightly more accurate approach is to assume that instrumental noise is Gaussian distributed and to quantitatively predict and correct the noise bias in the errors. Implementing this correction gives  $\tilde{P}_{SN}$  and  $\tilde{\sigma}_{QE-SN}$ , which are given by Equations (32) and (40) respectively. Figures 3 and 4 show that this corrects the bias and gives error bars that are no longer overly conservative. However, because this correction is designed to give

Error Bar Type	Pros	Cons
Bootstrap ( $\sigma_{\text{bs}}$ )	Easy to implement with minimal <i>a priori</i> assumptions; can be useful as a reference statistics in diagnosis of systematics	Not strictly applicable in the presence of non-independent and non-statistically stationary data samples
Power spectra from differenced visibilities ( $P_{\text{diff}}$ )	Data product close to raw data	Provides noise <i>realizations</i> rather than direct error bars, resulting in considerable scatter
Power spectrum method ( $P_{\text{N}}$ and $P_{\text{SN}}$ )	Accurately captures variances/error bars in noise-dominated regimes (both $P_{\text{N}}$ and $P_{\text{SN}}$ ) and signal-dominated regimes ( $P_{\text{SN}}$ )	Does not contain covariance information between different bandpowers; $P_{\text{SN}}$ requires non-negativity prior on the signal, which slightly inflates errors; downstream data weightings using $P_{\text{SN}}$ at risk of signal loss
Covariance method ( $\sigma_{\text{QE-N}}$ and $\sigma_{\text{QE-SN}}$ )	Same accuracy as $P_{\text{N}}$ and $P_{\text{SN}}$ for variance information and additionally provides full covariance information	Derivation assumes data is Gaussian; $\sigma_{\text{QE-SN}}$ requires non-negativity prior on the signal, which slightly inflates errors; downstream data weightings using $\sigma_{\text{QE-SN}}$ at risk of signal loss
Modified covariance method ( $\tilde{\sigma}_{\text{QE-SN}}$ ) and modified power spectrum method $\tilde{P}_{\text{SN}}$	Eliminates conservative double counting of noise in noisy estimates of the signal	Occasional error predictions that are slightly smaller than instrumental noise expectations from $\sigma_{\text{QE-N}}$ and $P_{\text{N}}$

**Table 4.** A summary of the advantages and disadvantages of different error estimation methods in 21 cm power spectrum estimation.

1556 unbiased errors *in expectation*, it will occasionally  
 1557 give error bars that are slightly smaller than the  
 1558 error predicted by noise-only estimators such as  
 1559  $P_{\text{N}}$ . In practice, however, we find that this is a  
 1560 reasonably rare occurrence.

1561 With the aforementioned difficulties with error esti-  
 1562 mation in the presence of poorly characterized signals,  
 1563 one may be tempted to make use of more empirically  
 1564 based error estimates. These estimates also come with  
 1565 their strengths and weaknesses:

- 1566 • As discussed in Section 3.2,  $P_{\text{diff}}$  from frequency-  
 1567 differenced data suffers from a bias at low delays. Figure 1  
 1568 shows that even at reasonably high delays  $\sim 1500$  ns, the bias  
 1569 can be significant. Thus, while  $P_{\text{diff}}$  from frequency-differenced  
 1570 data is a useful asymptotic check at high delays, it is not  
 1571 a robust estimator of our errors. Implementing  
 1572  $P_{\text{diff}}$  using time-differenced data does not have the  
 1573 delay-dependent bias, as one can also see in Figure  
 1574 1. However, care must be taken to ensure that the  
 1575 time differencing is small enough to suppress any  
 1576 sky signal that is coherent between adjacent time  
 1577 samples (Dillon et al. 2015). In addition, with a  
 1578 differencing scheme one is ultimately constructing  
 1579 noise *realizations*, not noise statistics. The result-  
 1580 ing error bars thus show considerable scatter. In  
 1581 that sense, the analytically propagated error bars  
 1582

1583 vary in a more physically plausible—smoother—  
 1584 way with time and frequency.

- 1585 • The problem of a noisy error bar estimate per-  
 1586 sists with  $\sigma_{\text{bs}}$ . However, bootstrapping has several  
 1587 appealing features that makes it a crucial check  
 1588 on the analytically propagated error bars. First,  
 1589 no assumptions are made regarding Gaussianity of  
 1590 the input data. Thus, the fact that our  $\sigma_{\text{bs}}$  agree  
 1591 with our analytically propagated errors—which as-  
 1592 sumed the input noise in the visibilities—is an es-  
 1593 sential validation of our assumptions. In a similar  
 1594 way,  $\sigma_{\text{bs}}$  may potentially capture increased vari-  
 1595 ance due to systematics since it is a measure of  
 1596 uncertainties of total sky emission. However, the  
 1597 bootstrap method is known to suffer from some  
 1598 important limitations. For example, as noted in  
 1599 Appendix B, if systematics are correlated between  
 1600 samples, the bootstrap method tends to underes-  
 1601 timate errors. Also, bootstrapped error bars will  
 1602 be inflated from non-stationary effects such as sky  
 1603 brightness changes and non-redundancies between  
 1604 nominally identical baselines. Precisely how these  
 1605 non-stationary effects should be folded into one’s  
 1606 error estimation is reserved for future work, but  
 1607 the correct approach will certainly be more so-  
 1608 phisticated than a simple inflation of errors. That  
 1609 said, this increase in bootstrap errors due to non-

stationarity can serve as a useful diagnostic for further examination of unexpected systematics.

In Table 4 we summarize the discussion in this section with an succinct listing of the pros and cons of each error estimation method.

## 6. CONCLUSIONS

In this paper, we have systematically studied a variety of error bar methodologies in 21 cm power spectrum estimation. We have synthesized some of the common techniques in the literature, outlining their relative strengths and weaknesses in quantifying noise levels and in accounting for residual systematics. Specifically, we considered a variety of types of error estimators, including

- Power spectrum methods. This includes the standard  $P_N$  estimator for the noise power spectrum found in the literature (Zaldarriaga et al. 2004; Parsons et al. 2012a; Pober et al. 2013; Cheng et al. 2018; Kern et al. 2020b) and the  $P_{SN}$  estimator that involves cross products with signal power spectrum  $P_S$ , as detailed in Kolopanis et al. (2019). Here we set  $P_S$  to be the real values of experimentally observed power spectrum, which is a good approximation when the signal dominates the noise. Our implementation of  $P_{SN}$  leads to a double-counting bias compared to  $P_N$  which is considerable in noise-dominated regimes, and we show how a modified form  $\tilde{P}_{SN}$  can eliminate this bias.
- Covariance methods. This consists of propagating a data covariance matrix between frequencies per timestamp and per baseline-pair through the quadratic estimator (QE) formalism to the bandpower covariance matrix (Liu & Tegmark 2011; Dillon et al. 2014; Liu et al. 2014a,b), including error metrics described here:  $\sigma_{QE-N}$  for noise-dominated spectra and  $\sigma_{QE-SN}$  that include signal-noise terms. These have identical *variance* predictions as  $P_N$  and  $P_{SN}$  by construction but also provide bandpower covariance information.
- Other methods. Other methods studied in this work includes the bootstrapping method that can lead to misreported errors when not handled carefully (Cheng et al. 2018), as well as the method of using differenced visibilities as noise realizations propagated through a power spectrum estimator. We show that differencing in frequency is ill-advised for this approach. Differencing in time avoids some problems, but either differencing

scheme generates error estimates that are rather scattered. However, we stress the importance of these more empirically based methods are useful cross-checks (e.g., in the manner performed in this paper) that can also be helpful diagnostics for systematics (e.g., Kolopanis et al. 2019).

Using simulations and real HERA Phase I data, we show that these methods are generally in agreement with each other, demonstrating their robustness and their applicability to future delay power spectrum measurements from HERA. Importantly, we show that for bandpowers that are not completely dominated by noise, one needs to go beyond the standard thermal noise estimates and account for signal-noise cross terms in order to fully describe the uncertainty on the band power. In a series of Appendices, we also examine sources of skewness in probability distributions of measured power spectrum bandpowers (Appendices A and F), derive exact expressions for the probability distributions of incoherently summed delay power spectra (Appendix G), and examine whether common baselines in the cross multiplication of multiple baseline *pairs* affects assumptions about error independence (Appendix B). The insights gained in this paper regarding error estimation are applicable in 21 cm cosmology beyond HERA. They provide a foundation upon which to develop rigorous error estimation methods which will prove to be key in unlocking the potential of the 21 cm line as a powerful probe of our high redshift universe.

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1726

## APPENDIX

## 1727 A. SKEWNESS IN POWER SPECTRA ESTIMATED FROM MULTIPLE IDENTICAL BASELINES

1728 In this Appendix, we consider a source of skewness in probability distributions of delay spectra. In particular, we  
 1729 consider the noise properties of power spectra formed from a set of identical (“redundant”) baselines. We show that  
 1730 even if each baseline is measuring Gaussian random noise with mean zero, the resulting power spectra will exhibit some  
 1731 skewness. We emphasize, however, that this skewness vanishes if one additionally splits the data into two distinct set  
 1732 of time samples (e.g., even and odd time stamps) and estimates power spectra that are not only cross-baselines but  
 1733 also cross-times.

As a concrete example, suppose that on the  $i$ th copy of a particular baseline we measure  $\tilde{x}_i \equiv c_i + id_i$  after taking the delay transform, where  $c_i$  and  $d_i$  are independently Gaussian distributed random variables with variance  $\sigma^2/2$ . This represents the behavior of  $\tilde{x}_i$  at noise-dominated delays. If only two identical baselines were available, cross multiplying them to obtain a power spectrum would yield

$$\tilde{x}_1\tilde{x}_2^* = (c_1 + id_1)(c_2 - id_2) = (c_1c_2 + d_1d_2) + i(d_1c_2 - c_1d_2). \quad (\text{A1})$$

Consider the real part. Since  $c_1$  and  $c_2$  are independent random variables,  $c_1c_2$  is a symmetric distribution about zero (and in fact is given by  $K_0$ , the zeroth modified Bessel function of the second kind). The same reasoning holds for the  $d_1d_2$  term. Since  $\{c_i\}$  and  $\{d_i\}$  are independent, it follows that  $c_1c_2$  and  $d_1d_2$  are also independent. The result is that the probability distribution for  $c_1c_2 + d_1d_2$  is given by the convolution of the distributions for the individual terms. With the two contributing distributions both symmetric about zero, their convolution inherits this property, and is in fact given by the Laplacian distribution discussed in Section 4.1.

The situation is different when we have more than two baselines. Taking all possible pairwise combinations (excluding the multiplication of a baseline with itself to eliminate noise bias), we obtain

$$\text{Re}[\tilde{x}_1\tilde{x}_2^* + \tilde{x}_1\tilde{x}_3^* + \tilde{x}_2\tilde{x}_3^*] = (c_1c_2 + c_1c_3 + c_2c_3) + (d_1d_2 + d_1d_3 + d_2d_3), \quad (\text{A2})$$

where we have grouped our result into two terms that can be considered separately because  $\{c_i\}$  and  $\{d_i\}$  are independent. Consider the first term. It has zero mean:

$$\langle c_1c_2 + c_1c_3 + c_2c_3 \rangle = \langle c_1 \rangle \langle c_2 \rangle + \langle c_1 \rangle \langle c_3 \rangle + \langle c_2 \rangle \langle c_3 \rangle = 0 \quad (\text{A3})$$

because the different  $\{c_i\}$  are independent. However, the resulting distribution has a skewness to it, which can be seen by the fact that the third moment is non-zero:

$$\begin{aligned} \langle (c_1c_2 + c_1c_3 + c_2c_3)^3 \rangle &= \langle c_2^3c_1^3 + c_3^3c_1^3 + 3c_2c_3^2c_1^3 + 3c_2^2c_3c_1^3 + 3c_2c_3^2c_1^2 + 6c_2^2c_3^2c_1^2 + 3c_2^3c_3c_1^2 + 3c_2^2c_3^2c_1 + 3c_2^3c_3^2c_1 + c_2^3c_3^3 \rangle \\ &= 6\langle c_2^2c_3^2c_1^2 \rangle = 6\langle c_2^2 \rangle \langle c_3^2 \rangle \langle c_1^2 \rangle \neq 0 \end{aligned} \quad (\text{A4})$$

[Of course, in principle we should be taking the cube of Equation (A2) in its entirety, not just the first term. However, the independence of  $\{c_i\}$  and  $\{d_i\}$  means we reach the same conclusion.] The non-zero third moment shown here arises because the three terms that make up the sum are correlated as a triplet, even though each pair has no average covariance. For instance, the covariance between  $c_1c_2$  and  $c_1c_3$  is

$$\langle c_1c_2c_1c_3 \rangle - \langle c_1c_2 \rangle \langle c_1c_3 \rangle = \langle c_1^2 \rangle \langle c_2 \rangle \langle c_3 \rangle = 0. \quad (\text{A5})$$

This implies that even though  $c_1c_2$ ,  $c_1c_3$ , and  $c_2c_3$  are not independent, for the purposes of computing the variance of the final result, one obtains the same result even if one pretends that these contributions are independent. This result is explored in more detail in the first half of Appendix B

To summarize, the different moments of the distribution provide different insights into power spectrum estimation with different baseline pair combinations. The mean of the distribution is zero, indicating that there is no bias (as one might expect for cross-correlation spectra). The variance turns out to be the same expression as if we had completely independent baseline pairs, so the noise averages down with the number of baseline pairs as one might naively have expected them to (without worrying about correlations). However, the skewness is non-zero. This complicates the interpretation of null tests that implicitly assume that the probability distributions of noise-dominated delays are symmetric.

Importantly, these considerations do not apply when we consider the imaginary part, which is given by

$$\text{Im}[\tilde{x}_1\tilde{x}_2^* + \tilde{x}_1\tilde{x}_3^* + \tilde{x}_2\tilde{x}_3^*] = c_2d_1 + c_3d_1 - c_1d_2 + c_3d_2 - c_1d_3 - c_2d_3. \quad (\text{A6})$$

This has a third moment given by  $\langle (c_2d_1 + c_3d_1 - c_1d_2 + c_3d_2 - c_1d_3 - c_2d_3)^3 \rangle$ . To get terms that are non-zero under the expectation value, we require terms that contain *squares* of the random variables when we multiply out the polynomial. For example, the first term  $c_2d_1$  must be multiplied onto  $c_2d_3$ , because there is no other  $c_2$  term in the expression to pair to. This gives us  $c_2^2d_1d_3$ . However, we now need to multiply this onto  $d_1d_3$ , or we end up with a stray  $d_1$  and a stray  $d_3$ . But none of the terms are the product of two  $\{d_i\}$ , so no matter what terms we pair this up

with, it will average to zero. This logic applies to any of the terms, so the distribution of the imaginary part will not be skewed. Because of this, statistical tests involving the imaginary part of a power spectrum estimator can be more easily interpreted using symmetric distributions.

Our result here has implications for how one should avoid the noise bias in power spectrum measurements. Two commonly used methods for doing so are to cross-multiply either different identical baselines together or different time stamps together. Here we have shown that employing only one of these will incur a skewness. (While our discussion above focused on cross multiplying different baselines, the same conclusions hold if we consider cross multiplying more than two groups in time—after all, the indices in our mathematical expressions can simply be considered timestamp indices instead of baseline indices.) However, if we perform cross-multiplications across both time and baseline axes, the skewness vanishes. To see this, imagine that we split our data into odd and even time samples, labeled with superscripts “o” and “e” respectively. Equation (A2) then becomes

$$\text{Re}[\tilde{x}_1^e \tilde{x}_2^{o*} + \tilde{x}_1^e \tilde{x}_3^{o*} + \tilde{x}_2^e \tilde{x}_3^{o*}] = (c_1^e c_2^o + c_1^e c_3^o + c_2^e c_3^o) + (d_1^e d_2^o + d_1^e d_3^o + d_2^e d_3^o), \quad (\text{A7})$$

and cubing this expression as before to compute the third moment, one finds no non-zero terms after taking the ensemble average.

## B. VARIANCE OF AVERAGED POWER SPECTRA FROM DEPENDENT BASELINE-PAIR SAMPLES

In this Appendix, we consider the effect of having common baselines between different baseline *pairs* used to form power spectra. Inside a redundant baseline group consisting of  $N_{\text{bl}}$  different baselines, then we can construct up to  $N_{\text{blp}} = \frac{1}{2}N_{\text{bl}}(N_{\text{bl}} - 1)$  different baseline pairs and we can form a power spectrum using each pair. Consider the averaged power spectrum over these baseline pairs and the variance of this average. The form of the averaged power spectrum is

$$\bar{P} = \frac{\sum_{(p,q>p)} P_{pq}}{\frac{1}{2}N_{\text{bl}}(N_{\text{bl}} - 1)}, \quad (\text{B8})$$

where the sum is over all possible  $(p, q)$  pairs of baselines. The variance of the averaged power spectrum does not simply go down with  $N_{\text{blp}}^{-1}$  because the data being averaged together are not fully independent of each other. For example,  $P_{12}$  and  $P_{13}$  both carry information from baseline #1.

Let the signal be  $\tilde{s} \equiv a + bi$ , and  $\tilde{n}_p \equiv c_p + d_p i$  and  $\tilde{n}_q \equiv c_q + d_q i$  be the noise realizations in the  $p$ th and  $q$ th baselines. The signal  $\tilde{s}$  is identical in each baseline, since we are assuming that we are combining data from identical (“redundant”) baselines. The random variables  $c_p, d_p, c_q, d_q \dots$  are IID normal variables with variance  $\sigma^2$ . In the foreground-negligible regime, recall from Equation (17) that the average power spectrum is given by

$$\bar{P} = \frac{\sum_{(p,q>p)} n_p^* n_q}{\frac{1}{2}N_{\text{bl}}(N_{\text{bl}} - 1)} = \frac{\sum_{(p,q>p)} c_p c_q + d_p d_q}{\frac{1}{2}N_{\text{bl}}(N_{\text{bl}} - 1)} + i \frac{\sum_{(p,q>p)} c_p d_q - c_q d_p}{\frac{1}{2}N_{\text{bl}}(N_{\text{bl}} - 1)}. \quad (\text{B9})$$

We notice

$$\begin{aligned} \text{Var} \left( \sum_{(p,q>p)} c_p c_q \right) &= \left\langle \sum_{(p,q>p)} c_p c_q \sum_{(r,t>r)} c_r c_t \right\rangle - \left[ \left\langle \sum_{(p,q>p)} c_p c_q \right\rangle \right]^2 = \left\langle \sum_{(p,q>p)} c_p c_q \sum_{(r,t>r)} c_r c_t \right\rangle \\ &= \sigma^4 \left[ \sum_{(p,q>p,r,t>r)} (\delta_{pr} \delta_{qt} + \delta_{pt} \delta_{qr}) \right] = \frac{N_{\text{bl}}(N_{\text{bl}} - 1)}{2} \sigma^4, \end{aligned} \quad (\text{B10})$$

which means that the variance in the real part of  $\bar{P}$  is  $\frac{4\sigma^4}{N_{\text{bl}}(N_{\text{bl}} - 1)}$ . For the imaginary part we compute

$$\begin{aligned} \text{Var} \left( \sum_{(p,q>p)} c_p d_q - c_q d_p \right) &= \left\langle \sum_{(p,q>p)} \{c_p d_q - c_q d_p\} \sum_{(r,t>r)} \{c_r d_t - c_t d_r\} \right\rangle - \left[ \left\langle \sum_{(p,q>p)} \{c_p d_q - c_q d_p\} \right\rangle \right]^2 \\ &= \left\langle \sum_{(p,q>p)} \{c_p d_q - c_q d_p\} \sum_{(r,t>r)} \{c_r d_t - c_t d_r\} \right\rangle = \sigma^4 \left[ \sum_{(p,q>p,r,t>r)} (2\delta_{pr} \delta_{qt} - 2\delta_{pt} \delta_{qr}) \right] \\ &= N_{\text{bl}}(N_{\text{bl}} - 1) \sigma^4, \end{aligned} \quad (\text{B11})$$

so that the variance of the imaginary part of  $\bar{P}$  is also  $\frac{4\sigma^4}{N_{\text{bl}}(N_{\text{bl}}-1)}$ . Since the number of baseline pairs is given by  $N_{\text{bl}}(N_{\text{bl}}-1)/2$  and  $2\sigma^4$  is the variance we would expect to get from a single baseline pair, we can see that  $\bar{P}$  averages down in a manner that is identical to the scenario where the baseline pairs are independent.

In foreground-dominant regimes, the average power spectrum goes to

$$\bar{P} = \frac{\sum_{(p,q>p)} s^*s + s^*n_q + n_p^*s}{\frac{1}{2}N_{\text{bl}}(N_{\text{bl}}-1)} = \frac{\sum_{(p,q>p)} a^2 + b^2 + a(c_p + c_q) + b(d_p + d_q)}{\frac{1}{2}N_{\text{bl}}(N_{\text{bl}}-1)} + i \frac{\sum_{(p,q>p)} a(d_q - d_p) + b(c_p - c_q)}{\frac{1}{2}N_{\text{bl}}(N_{\text{bl}}-1)}. \quad (\text{B12})$$

The variance in the real part is  $\frac{4(a^2+b^2)\sigma^2}{N_{\text{bl}}}$  and the variance in the imaginary part is  $\frac{4(N_{\text{bl}}+1)(a^2+b^2)\sigma^2}{3N_{\text{bl}}(N_{\text{bl}}-1)}$ . They now go down roughly as  $N_{\text{blp}}^{-1/2}$  and are larger than the variance from independent samples by factors of  $(N_{\text{bl}}-1)$  and  $(N_{\text{bl}}+1)/3$  respectively.

### C. TIME-DIFFERENCED VISIBILITIES AS NOISE ESTIMATORS

In this Appendix, we establish the validity of using time-differenced visibilities as a way to estimate noise error bars. The key idea is that if we form residuals of data vectors  $x_p(\nu, t)$  by subtracting data from the  $p$ th baseline in adjacent time bins ( $t_1$  and  $t_2$ ) from each other, the result should be noise dominated. The same holds true for delay-transformed visibilities, where the residual can be written as  $\tilde{n}_p(\tau, t_2) - \tilde{n}_p(\tau, t_1)$ . Suppressing  $\tau$  and demoting the time variable to a subscript for notational brevity, we write  $\tilde{n}_{p,t} = c_{p,t} + d_{p,t}i$ , where  $c_p, d_p \dots$  are IID normal variables with variance  $\sigma^2$ . The power spectra constructed from such residuals are

$$\begin{aligned} P_{\text{diff}} &= \frac{(\tilde{n}_{1,t_2} - \tilde{n}_{1,t_1})^* (\tilde{n}_{2,t_2} - \tilde{n}_{2,t_1})}{\sqrt{2} \sqrt{2}} \\ &= \left[ \frac{(c_{1,t_2} - c_{1,t_1}) (c_{2,t_2} - c_{2,t_1})}{\sqrt{2} \sqrt{2}} + \frac{(d_{1,t_2} - d_{1,t_1}) (d_{2,t_2} - d_{2,t_1})}{\sqrt{2} \sqrt{2}} \right] \\ &\quad + \left[ \frac{(c_{1,t_2} - c_{1,t_1}) (d_{2,t_2} - d_{2,t_1})}{\sqrt{2} \sqrt{2}} - \frac{(c_{2,t_2} - c_{2,t_1}) (d_{1,t_2} - d_{1,t_1})}{\sqrt{2} \sqrt{2}} \right] i. \end{aligned} \quad (\text{C13})$$

From this, we see that

$$\left\langle [\text{Re}(P_{\text{diff}})]^2 \right\rangle = \left\langle \left[ \frac{(c_{1,t_2} - c_{1,t_1}) (c_{2,t_2} - c_{2,t_1})}{\sqrt{2} \sqrt{2}} + \frac{(d_{1,t_2} - d_{1,t_1}) (d_{2,t_2} - d_{2,t_1})}{\sqrt{2} \sqrt{2}} \right]^2 \right\rangle = \langle c_1^2 \rangle \langle c_2^2 \rangle + \langle d_1^2 \rangle \langle d_2^2 \rangle = 2\sigma^4. \quad (\text{C14})$$

This is again the variance expected for a noise-dominated power spectrum. Therefore, what we have shown is that  $|\text{Re}(P_{\text{diff}})|$  can serve as an estimator that *in expectation* is equal to the correct noise errors for the measured power spectrum  $P_{\tilde{x}_1\tilde{x}_2}$  in noise-dominated regimes. However, since this result only holds in expectation, we expect that in practice it will exhibit considerable scatter as an error estimate.

### D. SIGNAL DEPENDENT ERROR BAR FROM POWER SPECTRUM METHOD

In this Appendix we derive an expression for the variance on the power spectrum in the presence of foregrounds or systematics (or any ‘‘signal’’). A similar derivation is presented in [Kolopanis et al. \(2019\)](#). Given two delay spectra  $\tilde{x}_1 = \tilde{s} + \tilde{n}_1$  and  $\tilde{x}_2 = \tilde{s} + \tilde{n}_2$ , the power spectra formed from  $\tilde{x}_1^*\tilde{x}_2$  is

$$\begin{aligned} P_{\tilde{x}_1\tilde{x}_2} &= \tilde{s}^*\tilde{s} + \tilde{s}^*\tilde{n}_2 + \tilde{n}_1^*\tilde{s} + \tilde{n}_1^*\tilde{n}_2 \\ &= [a^2 + b^2 + a(c_1 + c_2) + b(d_1 + d_2) + c_1c_2 + d_1d_2] + [a(d_2 - d_1) + b(c_1 - c_2) + d_2c_1 - d_1c_2] i, \end{aligned} \quad (\text{D15})$$

where we have written  $\tilde{s} = a + bi$ ,  $\tilde{n}_1 = c_1 + d_1i$  and  $\tilde{n}_2 = c_2 + d_2i$ .

Consistent with the rest of the paper, we assume that  $a$  and  $b$  are not random variables, so that  $\langle s \rangle = s$ . The true sky power spectrum is then given by  $P_{\tilde{s}\tilde{s}} = a^2 + b^2$ , and  $c_1, d_1, c_2$  and  $d_2$  in noise parts are IID random normal variables. We then have

$$\begin{aligned} \text{Var}[\text{Re}(P_{\tilde{x}_1\tilde{x}_2})] &= \text{Var}[a^2 + b^2 + a(c_1 + c_2) + b(d_1 + d_2) + c_1c_2 + d_1d_2] \\ &= 2(a^2 + b^2)\langle c_1^2 \rangle + 2\langle c_1^2 \rangle^2 = \sqrt{2}P_{\tilde{s}\tilde{s}}P_{\text{N}} + P_{\text{N}}^2 = \sqrt{2}\langle \text{Re}(P_{\tilde{x}_1\tilde{x}_2}) \rangle P_{\text{N}} + P_{\text{N}}^2 = P_{\text{SN}}^2. \end{aligned} \quad (\text{D16})$$

In the above we have used the relation  $\text{var}(c_1c_2 + d_1d_2) = 2\langle c_1^2 \rangle^2 = P_{\text{N}}^2$ , where  $P_{\text{N}}$  is the analytic noise power spectrum. We have also used  $P_{\tilde{s}\tilde{s}} = \langle \text{Re}(P_{\tilde{x}_1\tilde{x}_2}) \rangle$ . This shows that  $P_{\text{SN}}$  is a general form for error bars in the existence of foregrounds or systematics (or again, any ‘‘signal’’).

## E. COVARIANCE METHOD

1857

1858 In this Appendix we provide more explicit derivations of the expressions quoted in Section 3.4 for the covariance  
1859 method of error estimation.

## E.1. Variance

1860

1861 If  $\hat{P}_\alpha$  is a complex number representing a power spectrum estimate of the  $\alpha$ th bandpower, its real part and imaginary  
1862 part are given by  $\frac{1}{2}(\hat{P}_\alpha + \hat{P}_\alpha^*)$  and  $\frac{1}{2i}(\hat{P}_\alpha - \hat{P}_\alpha^*)$  respectively. The variance in the real part of  $\hat{P}_\alpha$  is

$$1863 \quad \frac{1}{4} \left\{ \langle (\hat{P}_\alpha \hat{P}_\alpha) - \langle \hat{P}_\alpha \rangle \langle \hat{P}_\alpha \rangle \rangle + 2 \langle (\hat{P}_\alpha \hat{P}_\alpha^*) - \langle \hat{P}_\alpha \rangle \langle \hat{P}_\alpha^* \rangle \rangle + \langle (\hat{P}_\alpha^* \hat{P}_\alpha^*) - \langle \hat{P}_\alpha^* \rangle \langle \hat{P}_\alpha^* \rangle \rangle \right\}, \quad (\text{E17})$$

1864 while the variance in the imaginary part of  $\hat{P}_\alpha$  is

$$1865 \quad -\frac{1}{4} \left\{ \langle (\hat{P}_\alpha \hat{P}_\alpha) - \langle \hat{P}_\alpha \rangle \langle \hat{P}_\alpha \rangle \rangle - 2 \langle (\hat{P}_\alpha \hat{P}_\alpha^*) - \langle \hat{P}_\alpha \rangle \langle \hat{P}_\alpha^* \rangle \rangle + \langle (\hat{P}_\alpha^* \hat{P}_\alpha^*) - \langle \hat{P}_\alpha^* \rangle \langle \hat{P}_\alpha^* \rangle \rangle \right\}. \quad (\text{E18})$$

1866 Recall that  $\hat{P}_\alpha$  is defined as  $\hat{P}_\alpha = \mathbf{x}_1^\dagger \mathbf{E}^{12,\alpha} \mathbf{x}_2 = \sum_{ij} \mathbf{x}_{1,i}^* \mathbf{E}_{ij}^{12,\alpha} \mathbf{x}_{2,j}$ . We define three set of matrices containing the  
1867 whole two-point correlation information for the complex estimator  $\mathbf{C}^{12}$ ,  $\mathbf{U}^{12}$  and  $\mathbf{G}^{12}$ , such that

$$1868 \quad \mathbf{C}_{ij}^{12} \equiv \langle \mathbf{x}_{1,i} \mathbf{x}_{2,j}^* \rangle; \quad \mathbf{U}_{ij}^{12} \equiv \langle \mathbf{x}_{1,i} \mathbf{x}_{2,j} \rangle; \quad \mathbf{G}_{ij}^{12} \equiv \langle \mathbf{x}_{1,i}^* \mathbf{x}_{2,j}^* \rangle, \quad (\text{E19})$$

1870 Equipped with these definitions, we can generate the following equations

$$1871 \quad \begin{aligned} \langle \hat{P}_\alpha \hat{P}_\beta \rangle - \langle \hat{P}_\alpha \rangle \langle \hat{P}_\beta \rangle &= \sum_{ijkl} \langle \mathbf{x}_{1,i}^* \mathbf{E}_{ij}^{12,\alpha} \mathbf{x}_{2,j} \mathbf{x}_{1,k} \mathbf{E}_{kl}^{12,\beta} \mathbf{x}_{2,l} \rangle - \langle \mathbf{x}_{1,i}^* \mathbf{E}_{ij}^{12,\alpha} \mathbf{x}_{2,j} \rangle \langle \mathbf{x}_{1,k} \mathbf{E}_{kl}^{12,\beta} \mathbf{x}_{2,l} \rangle \\ 1872 &= \sum_{ijkl} \mathbf{E}_{ij}^{12,\alpha} \mathbf{E}_{kl}^{12,\beta} (\langle \mathbf{x}_{1,i}^* \mathbf{x}_{2,j} \mathbf{x}_{1,k} \mathbf{x}_{2,l} \rangle - \langle \mathbf{x}_{1,i}^* \mathbf{x}_{2,j} \rangle \langle \mathbf{x}_{1,k} \mathbf{x}_{2,l} \rangle) \\ 1873 &= \sum_{ijkl} \mathbf{E}_{ij}^{12,\alpha} \mathbf{E}_{kl}^{12,\beta} (\langle \mathbf{x}_{1,i}^* \mathbf{x}_{1,k} \rangle \langle \mathbf{x}_{2,j} \mathbf{x}_{2,l} \rangle + \langle \mathbf{x}_{1,i}^* \mathbf{x}_{2,l} \rangle \langle \mathbf{x}_{1,k} \mathbf{x}_{2,j} \rangle) \\ 1874 &= \sum_{ijkl} \mathbf{E}_{ij}^{12,\alpha} \mathbf{E}_{kl}^{12,\beta} (\mathbf{G}_{ik}^{11} \mathbf{U}_{jl}^{22} + \mathbf{C}_{li}^{21} \mathbf{C}_{jk}^{21}) \\ 1875 &= \sum_{ijkl} (\mathbf{E}_{ij}^{12,\alpha} \mathbf{U}_{jl}^{22} \mathbf{E}_{lk}^{21,\beta*} \mathbf{G}_{ki}^{11} + \mathbf{E}_{ij}^{12,\alpha} \mathbf{C}_{jk}^{21} \mathbf{E}_{kl}^{12,\beta} \mathbf{C}_{li}^{21}) \\ 1876 &= \text{tr}(\mathbf{E}^{12,\alpha} \mathbf{U}^{22} \mathbf{E}^{21,\beta*} \mathbf{G}^{11} + \mathbf{E}^{12,\alpha} \mathbf{C}^{21} \mathbf{E}^{12,\beta} \mathbf{C}^{21}), \end{aligned} \quad (\text{E20})$$

$$1878 \quad \begin{aligned} \langle \hat{P}_\alpha \hat{P}_\beta^* \rangle - \langle \hat{P}_\alpha \rangle \langle \hat{P}_\beta^* \rangle &= \sum_{ijkl} \langle \mathbf{x}_{1,i}^* \mathbf{E}_{ij}^{12,\alpha} \mathbf{x}_{2,j} \mathbf{x}_{1,k} \mathbf{E}_{kl}^{12,\beta*} \mathbf{x}_{2,l}^* \rangle - \langle \mathbf{x}_{1,i}^* \mathbf{E}_{ij}^{12,\alpha} \mathbf{x}_{2,j} \rangle \langle \mathbf{x}_{1,k} \mathbf{E}_{kl}^{12,\beta*} \mathbf{x}_{2,l}^* \rangle \\ 1879 &= \sum_{ijkl} \mathbf{E}_{ij}^{12,\alpha} \mathbf{E}_{kl}^{12,\beta*} (\langle \mathbf{x}_{1,i}^* \mathbf{x}_{2,j} \mathbf{x}_{1,k} \mathbf{x}_{2,l}^* \rangle - \langle \mathbf{x}_{1,i}^* \mathbf{x}_{2,j} \rangle \langle \mathbf{x}_{1,k} \mathbf{x}_{2,l}^* \rangle) \\ 1880 &= \sum_{ijkl} \mathbf{E}_{ij}^{12,\alpha} \mathbf{E}_{kl}^{12,\beta*} (\langle \mathbf{x}_{1,i}^* \mathbf{x}_{2,l}^* \rangle \langle \mathbf{x}_{1,k} \mathbf{x}_{2,j} \rangle + \langle \mathbf{x}_{1,i}^* \mathbf{x}_{1,k} \rangle \langle \mathbf{x}_{2,j} \mathbf{x}_{2,l}^* \rangle) \\ 1881 &= \sum_{ijkl} \mathbf{E}_{ij}^{12,\alpha} \mathbf{E}_{kl}^{12,\beta*} (\mathbf{G}_{il}^{12} \mathbf{U}_{kj}^{12} + \mathbf{C}_{ki}^{11} \mathbf{C}_{jl}^{22}) \\ 1882 &= \sum_{ijkl} (\mathbf{E}_{ij}^{12,\alpha} \mathbf{U}_{jk}^{21} \mathbf{E}_{kl}^{12,\beta*} \mathbf{G}_{li}^{21} + \mathbf{E}_{ij}^{12,\alpha} \mathbf{C}_{jl}^{22} \mathbf{E}_{lk}^{21,\beta} \mathbf{C}_{ki}^{11}) \\ 1883 &= \text{tr}(\mathbf{E}^{12,\alpha} \mathbf{U}^{21} \mathbf{E}^{12,\beta*} \mathbf{G}^{21} + \mathbf{E}^{12,\alpha} \mathbf{C}^{22} \mathbf{E}^{21,\beta} \mathbf{C}^{11}), \end{aligned} \quad (\text{E21})$$



1885 and

$$\begin{aligned}
1886 \quad \langle \hat{P}_\alpha^* \hat{P}_\beta^* \rangle - \langle \hat{P}_\alpha^* \rangle \langle \hat{P}_\beta^* \rangle &= \sum_{ijkl} \langle \mathbf{x}_{1,i} \mathbf{E}_{ij}^{12,\alpha*} \mathbf{x}_{2,j}^* \mathbf{x}_{1,k} \mathbf{E}_{kl}^{12,\beta*} \mathbf{x}_{2,l}^* \rangle - \langle \mathbf{x}_{1,i} \mathbf{E}_{ij}^{12,\alpha*} \mathbf{x}_{2,j}^* \rangle \langle \mathbf{x}_{1,k} \mathbf{E}_{kl}^{12,\beta*} \mathbf{x}_{2,l}^* \rangle \\
1887 \quad &= \sum_{ijkl} \mathbf{E}_{ij}^{12,\alpha*} \mathbf{E}_{kl}^{12,\beta*} (\langle \mathbf{x}_{1,i} \mathbf{x}_{2,j}^* \mathbf{x}_{1,k} \mathbf{x}_{2,l}^* \rangle - \langle \mathbf{x}_{1,i} \mathbf{x}_{2,j}^* \rangle \langle \mathbf{x}_{1,k} \mathbf{x}_{2,l}^* \rangle) \\
1888 \quad &= \sum_{ijkl} \mathbf{E}_{ij}^{12,\alpha*} \mathbf{E}_{kl}^{12,\beta*} (\langle \mathbf{x}_{1,i} \mathbf{x}_{1,k} \rangle \langle \mathbf{x}_{2,j}^* \mathbf{x}_{2,l}^* \rangle + \langle \mathbf{x}_{1,i} \mathbf{x}_{2,l}^* \rangle \langle \mathbf{x}_{2,j}^* \mathbf{x}_{1,k} \rangle) \\
1889 \quad &= \sum_{ijkl} \mathbf{E}_{ij}^{12,\alpha*} \mathbf{E}_{kl}^{12,\beta*} (\mathbf{G}_{jl}^{22} \mathbf{U}_{ik}^{11} + \mathbf{C}_{il}^{12} \mathbf{C}_{kj}^{12}) \\
1890 \quad &= \sum_{ijkl} (\mathbf{E}_{ji}^{21,\alpha} \mathbf{U}_{ik}^{11} \mathbf{E}_{kl}^{12,\beta*} \mathbf{G}_{lj}^{22} + \mathbf{E}_{ji}^{21,\alpha} \mathbf{C}_{il}^{12} \mathbf{E}_{lk}^{21,\beta} \mathbf{C}_{kj}^{12}) \\
1891 \quad &= \text{tr}(\mathbf{E}^{21,\alpha} \mathbf{U}^{11} \mathbf{E}^{12,\beta*} \mathbf{G}^{22} + \mathbf{E}^{21,\alpha} \mathbf{C}^{12} \mathbf{E}^{21,\beta} \mathbf{C}^{12}), \tag{E22}
\end{aligned}$$

1893 where  $\mathbf{E}_{ij}^{12,\alpha*} = \mathbf{E}_{ji}^{21,\alpha}$ . Setting  $\alpha = \beta$  in these equations then allows us to evaluate Equations (E17) and (E18).

### 1894 E.2. Covariance

1895 The covariance between the real part of  $\hat{P}_\alpha$  and the real part of  $\hat{P}_\beta$  is

$$1896 \quad \frac{1}{4} \left\{ (\langle \hat{P}_\alpha \hat{P}_\beta \rangle - \langle \hat{P}_\alpha \rangle \langle \hat{P}_\beta \rangle) + (\langle \hat{P}_\alpha \hat{P}_\beta^* \rangle - \langle \hat{P}_\alpha \rangle \langle \hat{P}_\beta^* \rangle) + (\langle \hat{P}_\alpha^* \hat{P}_\beta \rangle - \langle \hat{P}_\alpha^* \rangle \langle \hat{P}_\beta \rangle) + (\langle \hat{P}_\alpha^* \hat{P}_\beta^* \rangle - \langle \hat{P}_\alpha^* \rangle \langle \hat{P}_\beta^* \rangle) \right\}, \tag{E23}$$

1897 and the covariance between the imaginary part of  $\hat{P}_\alpha$  and the imaginary part of  $\hat{P}_\beta$  is

$$1898 \quad \frac{1}{4} \left\{ (\langle \hat{P}_\alpha \hat{P}_\beta \rangle - \langle \hat{P}_\alpha \rangle \langle \hat{P}_\beta \rangle) - (\langle \hat{P}_\alpha \hat{P}_\beta^* \rangle - \langle \hat{P}_\alpha \rangle \langle \hat{P}_\beta^* \rangle) - (\langle \hat{P}_\alpha^* \hat{P}_\beta \rangle - \langle \hat{P}_\alpha^* \rangle \langle \hat{P}_\beta \rangle) + (\langle \hat{P}_\alpha^* \hat{P}_\beta^* \rangle - \langle \hat{P}_\alpha^* \rangle \langle \hat{P}_\beta^* \rangle) \right\}. \tag{E24}$$

1899 These can be evaluated in the same way as the variances above.

## 1900 F. SKEWNESS IN DISTRIBUTIONS OF POWER SPECTRA AT INTERMEDIATE DELAYS

1901 In this Appendix, we consider the probability distribution functions of power spectra where neither signals (e.g.,  
1902 foregrounds) or noise are dominant and both must be considered. Using the same notation as Appendix D, the power  
1903 spectra formed from  $\tilde{x}_1 = \tilde{s} + \tilde{n}_1$  and  $\tilde{x}_2 = \tilde{s} + \tilde{n}_2$  is

$$\begin{aligned}
1904 \quad P_{\tilde{x}_1 \tilde{x}_2} &= \tilde{s}^* \tilde{s} + \tilde{s}^* \tilde{n}_2 + \tilde{n}_1^* \tilde{s} + \tilde{n}_1^* \tilde{n}_2 \\
1905 \quad &= [a^2 + b^2 + a(c_1 + c_2) + b(d_1 + d_2) + c_1 c_2 + d_1 d_2] + [a(d_2 - d_1) + b(c_1 - c_2) + d_2 c_1 - d_1 c_2] i. \tag{F25}
\end{aligned}$$

1907 Note that  $a$  and  $b$  are constants and  $c_1$ ,  $d_1$ ,  $c_2$  and  $d_2$  are IID randomly normal variables. For the real part of  $P_{\tilde{x}_1 \tilde{x}_2}$ ,  
1908 we have

$$1909 \quad \langle \text{Re}(P_{\tilde{x}_1 \tilde{x}_2}) \rangle = a^2 + b^2. \tag{F26}$$

1910 After subtracting from the mean, its third moment is

$$\begin{aligned}
1911 \quad \left\langle [\text{Re}(P_{\tilde{x}_1 \tilde{x}_2}) - (a^2 + b^2)]^3 \right\rangle &= \left\langle [a(c_1 + c_2) + b(d_1 + d_2) + c_1 c_2 + d_1 d_2]^3 \right\rangle = 6(a^2 c_1^2 c_2^2 + b^2 d_1^2 d_2^2) > 0. \tag{F27} \\
1912
\end{aligned}$$

1913 This non-vanishing third moment implies that the probability distribution of power spectra is skewed. This skewness  
1914 disappears for either signal-dominated or noise-dominated cases. These results are evident in the histograms shown in  
1915 Figure 3.

## 1916 G. PROBABILITY DISTRIBUTION FOR AN INCOHERENT SUM OF DELAY TRANSFORM-ESTIMATED 1917 POWER SPECTRA

1918 In this Appendix, we derive the probability distribution for noise in a power spectrum that has been formed by the  
1919 incoherent (i.e., after squaring) averaging of power spectra from individual time integrations. The resulting probability  
1920 distribution is used in Figures 7, 8, and 9 to validate our error bar methodology.

1921 For a noise-dominated delay power spectrum estimate, the power spectrum value  $u$  measured at one instant in time  
1922 is distributed as a double exponential:

$$1923 \quad p(x) = \frac{1}{\sigma\sqrt{2}} \exp\left(-\frac{\sqrt{2}|u|}{\sigma}\right), \quad (\text{G28})$$

1924 where it is assumed that the power spectra are estimated by cross-correlation—thus eliminating noise bias—and where  
1925  $\sigma$  is the standard deviation on the resulting power spectrum.

1926 Now suppose we average together a number of these power spectra. Let the power spectrum value at the  $i$ th time  
1927 step be given by  $u_i$ . The average value is then

$$1928 \quad z \equiv \sum_i w_i u_i, \quad (\text{G29})$$

1929 where  $\{w_i\}$  are a set of weights. Note that the error on each  $x_i$  may be different, so we define

$$1930 \quad p_i(u_i) = \frac{1}{\sigma_i\sqrt{2}} \exp\left(-\frac{\sqrt{2}|u_i|}{\sigma_i}\right). \quad (\text{G30})$$

1931 We now write down the probability distribution  $p_+(z)$  for  $z$ . First we define  $y_i \equiv w_i u_i$ , such that

$$1932 \quad p_i(y_i) = \frac{1}{w_i\sigma_i\sqrt{2}} \exp\left(-\frac{\sqrt{2}|y_i|}{w_i\sigma_i}\right). \quad (\text{G31})$$

1933 With this notation,  $z = \sum_i y_i$ , and we can write down  $z$  by using the fact that the probability distribution of a  
1934 sum of two random variables is the convolution of their individual distributions. By the convolution theorem, this is  
1935 equivalent to multiplying the Fourier transforms of the individual probability distributions  $\tilde{p}_i(k)$ , and thus

$$1936 \quad p_+(z) = \int \frac{dk}{2\pi} e^{ikz} \prod_i \tilde{p}_i(k) = \int \frac{dk}{2\pi} e^{ikz} \prod_i \frac{1}{1 + w_i^2 \sigma_i^2 k^2 / 2}, \quad (\text{G32})$$

1937 where we have used the fact that in our case,  $\tilde{p}_i(k) = (1 + w_i^2 \sigma_i^2 k^2 / 2)^{-1}$ . This integral can be evaluated by contour  
1938 integration, giving

$$1939 \quad p_+(z) = \sum_j \frac{e^{-|z|\sqrt{2}/w_j\sigma_j}}{w_j\sigma_j\sqrt{2}} \prod_{i \neq j} \frac{1}{1 - w_i^2 \sigma_i^2 / w_j^2 \sigma_j^2}. \quad (\text{G33})$$

1940 This is a weighted sum of double exponential distributions, and the curves in Figures 7, 8, and 9 labeled “Sum of  
1941 Laplacians” are plots of this formula.

1942 In closing, we note one peculiarity about this derivation—our contour integration assumed that none of the  $w_i\sigma_i$   
1943 values were exactly equal. In principle, this is a reasonable assumption, since for a drift scan telescope that is sky  
1944 noise dominated the noise power is continually changing from one time integration to the next. In practice, however,  
1945 if this change is happening slowly, two adjacent time integrations may have similar enough noise properties to make  
1946 Equation (G33) numerically problematic. If this is indeed the regime that one is in, it is advisable to instead use an  
1947 approximate expression by letting  $\sqrt{2}/w_i\sigma_i \equiv \kappa + \varepsilon_i$  and then Taylor expanding to leading order in  $\varepsilon_i$ .

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