Bayesian approach for electron quantum state tomography

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1 Introduction

In signal processing image restoration problems have been well investigated. Recent related works aims for example to tackle high dimension problem and real-time performances. But very few of these researches have been implemented fo tomography problems in mesoscopic physics domain. In this article, we propose specifically designed algorithm for an electron quantum state Wigner function restoration. In this introduction, first we present the experimental measurements performed, then we explain why a linear inverse problem need to be solved. In following sections methods solving this problem are presented.

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To represent electron states we use a time-energy Wigner function. This function is a quasi-probability distribution of finding a electron or an hole at a given energy and time. When we make two electron states, a source and a probe, interfere with an Hong-Ou-Mandel interferometer, they interference results in a variation of the current noise ΔS. This noise variation is directly proportional to the overlap between the two Wigner functions.

$$\Delta S \propto \int_{-\infty}^{+\infty} d\epsilon \int_{0}^{T} dt \Delta W_S(\epsilon, t) \Delta W_P(\epsilon, t) \tag{1}$$

If one electron state is a source that we want to characterize and the other is a complete collection of known probe, than accumulating all ΔS is a tomography protocol. In order to accumulate data the source is periodic of pulsation Ω. The experimentally easiest probes to generate are the n sine harmonic of the source. And these sine probes are shifted in energy of a constant value ϵ_0 thanks to a constant DC current. For the n harmonic, of amplitude V_n and phase ϕ_0 the overlap integral is with f the Fermi-Dirac distribution function.

$$\frac{\Delta S_{II,n}(\epsilon_0, \phi_0 = 180°) - \Delta S_{II,n}(\epsilon_0, \phi_0 = 0°)}{eV_n} = \frac{2e^2}{h}\frac{\Omega}{2\pi} \int_{\epsilon=-\infty}^{\epsilon=+\infty} d\epsilon \int_{t=0}^{t=\frac{2\pi}{\Omega}} dt \Delta W_S(\epsilon, t) \cos(n\Omega t) \left(\frac{f(\epsilon - \frac{n\hbar\Omega}{2} - \epsilon_0) - f(\epsilon + \frac{n\hbar\Omega}{2} - \epsilon_0)}{n\Omega} \right) \tag{2}$$

The first term of above equation is the noise variation normalized by the experimental parameters, we note it $\Delta \tilde{S}_n(\epsilon_0)$. The integral over time shows that for each probe we are measuring a component of the time-Fourier transform of the Wigner function. This time-Fourier transform corresponds to the Glauber function and is noted G_n. Finally after integrating over time, the remaining expression is a convolution of the Glauber function.

2 Previous method

As a first approach the deconvolution problem is solved using a Wiener filter. The convolution can be expressed as

$$\Delta\tilde{s}_n(\epsilon_0) = \int_{-\infty}^{+\infty} d\epsilon h_n(\epsilon_0 - \epsilon) g_n(\epsilon) + n(\epsilon_0) \tag{3}$$

This equation can be expressed as a simple product equation taking the Fourier transform of each function. Let $\bar{t}$ be the conjugate Fourier variable of ϵ :

$$\Delta\tilde{S}_n(\bar{t}) = H_n(\bar{t}) G_n(\bar{t}) + N_n(\bar{t}) \tag{4}$$

The Wiener filter is the function $F_W(\bar{t})$ which minimize, over all noise realization $N(\bar{t})$, the mean of

$$||F_W(\bar{t})\Delta\tilde{S}_n(\bar{t}) - G_n(\bar{t})||_2^2 \tag{5}$$

Solving for all $\bar{t}$ the equation:

$$\frac{d}{dF_W(\bar{t})}\left(||F_W(\bar{t})\Delta\tilde{S}_n(\bar{t}) - G_n(\bar{t})||_2^2\right) = 0 \tag{6}$$

one can demonstrate that

$$F_W(\bar{t}) = \frac{H_n^*(\bar{t})}{|H_n(\bar{t})|^2 + \left|\frac{N_n(\bar{t})}{G_n(\bar{t})}\right|^2} \tag{7}$$

Than computing $\tilde{G}_n(\bar{t}) = F_W(\bar{t})\Delta\tilde{S}_n(\bar{t})$ is the best estimator of $G_n(\bar{t})$. The solution is quite straight forward but as one can remark we need the prior knowledge of both the noise density spectrum $|N_n(\bar{t})|^2$ and the density spectrum of the solution $|G_n(\bar{t})|^2$. For the noise spectrum we can assume white noise and deduce its value thanks to error bar of repeated measurement. So up to this point we drop the $\bar{t}$ dependence of N_n. But $|G_n(\bar{t})|^2$ is unknown. For a lot of physical signal one can approximate it by a power law, but in our case this does not correspond to a physical property of the signal. The chosen solution has been to note that on the data above a certain $\bar{t}_c$ the values of $\Delta\tilde{S}_n(\bar{t})$ saturates around $|N_n|^2$. So for $\bar{t} \leq \bar{t}_c$ we assume $|G_n(\bar{t})|^2 \approxeq \frac{\Delta\tilde{S}_n(\bar{t})}{h_n(\bar{t})}$. And for $\bar{t} \geq \bar{t}_c$ we assume $|G_n(\bar{t})|^2 \leq |G_n(\bar{t}_c)|^2 \approxeq \frac{\Delta\tilde{S}_n(\bar{t}_c)}{h_n(\bar{t}_c)} \approxeq \frac{N_n}{h_n(\bar{t}_c)}$. This lead to the filter

$$\begin{aligned} F_W(\bar{t}) &= \frac{H_n^*(\bar{t})}{|H_n(\bar{t})|^2\left(1 + \left|\frac{N_n}{\Delta\tilde{S}_n(\bar{t})}\right|^2\right)} \text{ when } \bar{t} \leq \bar{t}_c & (8) \\ &= \frac{H_n^*(\bar{t})}{|H_n(\bar{t})|^2 + |H_n(\bar{t}_c)|^2} \text{ when } \bar{t} \geq \bar{t}_c & (9) \end{aligned}$$

The implemented algorithm is then:

Algorithm *Wiener filtering*

1. using FFT compute $H_n(\bar{t})$ and from measurement data $\Delta\tilde{S}_n(\bar{t})$, N_n

2. plot $\Delta\tilde{S}_n(\bar{t})$ and N_n, then choose a cut-off $\bar{t}_c$

3. repeat

3.1. adjust $\bar{t}_c$

3.2. compute $F_W(\bar{t})$ thanks to formula

3.3. compute $\tilde{G}_n(\bar{t}) = F_W(\bar{t})\Delta\tilde{S}_n(\bar{t})$

3.4. using IFFT compute $\tilde{G}_n(\epsilon)$,

3.5. **until** it doesn't look over-smooth or under-smooth

Finally the relevant physical quantity is the excess Wigner function $\Delta\tilde{W}(\epsilon, t)$ which is computed with:

$$\Delta\tilde{W}(\epsilon, t) = \tilde{G}_0(\epsilon) + \sum_{n=1}^{n_{\max}} 2\cos(n\Omega t)\,\tilde{G}_n(\epsilon) \tag{10}$$

This function is plotted in figure 1 This is a good first result to begin with. But there are some issues that can be improved. First there are no clear justification of the existence of a cut-off $\bar{t}_c$. Secondly the assumptions on the noise N_n does not take into account that we have possibly different errors bars for each ϵ. Finally it is not obvious how to add prior information in the direct ϵ space. For example we know that the $\tilde{G}_n(\epsilon)$ are decreasing towards 0 value for large ϵ.

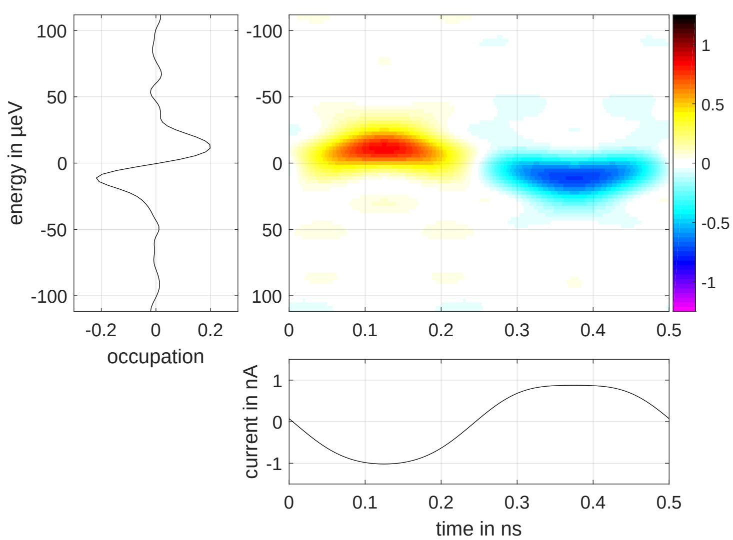

Figure 1: Wigner function extracted thanks to Wiener filter algorithm from a sinus drive measurement. Marginal distribution display usual physical quantity occupation number and current

3 Proposed Bayesian approach

In order to solve the deconvolution problem in the ϵ space, we used a Bayesian formulation. The quantity we are looking for is the more likely G_n knowing $\Delta\tilde{S}_n$ and the variance of N_n so called V_e. So we want to find $\tilde{G}_n$ which maximizes $p(G_n|\Delta\tilde{S}_n, V_e)$. This probability can be expressed as:

$$p(G_n|\Delta\tilde{S}_n, V_e) = \frac{1}{p(\Delta\tilde{S}_n)} p(\Delta\tilde{S}_n|G_n, V_e) p(G_n) \tag{11}$$

In this equation $p(\Delta\tilde{S}_n)$ is just a normalization constant it does not depend on G_n. $p(\Delta\tilde{S}_n|G_n, V_e)$ is the likelihood term. It tells you how much the solution G_n looks like your measurement after multiplication by the model. The last term $p(G_n)$ express all prior knowledge you have on the solution.

In our case the model, which links $\Delta\tilde{S}_n$ and G_n, is linear. And the values are naturally discretized by measurement points. So it can be expressed as a matrix product.

$$\Delta\tilde{S}_n = H_n G_n + N_n \tag{12}$$

Knowing the variances of all $N_n(\epsilon)$ leads us to express $p(\Delta\tilde{S}_n|G_n, V_e)$

$$p(\Delta\tilde{S}_n|G_n, V_e) \quad \propto \quad \exp\left(-\frac{1}{2}||\Delta\tilde{S}_n - H_n G_n||^2_{V_e}\right) \tag{13}$$

$$\text{with } ||x||^2_{V_e} \quad = \quad \sum_{\epsilon} \frac{x(\epsilon)^2}{V_e(\epsilon)} \tag{14}$$

Here we have already included the extra information that errors bars could be different between different ϵ compare to previous section. Than thanks to $p(G_n)$ we impose that G_n should take finite values and that $G_n(\epsilon)$ tends to zero when $|\epsilon|$ increase. To do so we define an envelope function V_f of amplitude v_f and width w such that $V_f(\epsilon) = v_f \exp\left(-\frac{\epsilon^2}{2w^2}\right)$. w is the energy ϵ band where there are excitations. We finally end up with:

$$p(G_n) \propto \exp\left(-\frac{1}{2}||G_n||^2_{V_f}\right) \tag{15}$$

Maximizing $p(G_n|\Delta\tilde{S}_n, V_e)$ is then equivalent to minimizing the criteria $||\Delta\tilde{S}_n - H_n G_n||^2_{V_e} + ||G_n||^2_{V_f}$. The solution is given by

$$\tilde{G}_n = (H' V_e^{-1} H + V_f^{-1})^{-1} H' V_e^{-1} \Delta\tilde{S}_n \tag{16}$$

Assuming that V_f follow an inverse-gamma distribution law of parameters α_f and β_f, the algorithm can update its value at each minimization. The obtained algorithm is the following.

Algorithm *Joint-Maximum A Posteriori (JMAP)*

1. choose amplitude v_f and width w of $V_f(\epsilon)$ envelope, and α_f order of Inverse-Gamma distribution.

2. compute $\tilde{G}_n = (H' V_e^{-1} H + V_f^{-1})^{-1} H' V_e^{-1} \Delta\tilde{S}_n$

3. repeat

3.1. compute $V_f(\epsilon) = \frac{\beta_f(\epsilon) + |\tilde{G}_n(\epsilon)|^2}{\alpha_f + 1/2}$ than update $\beta_f(\epsilon) = \alpha_f V_f(\epsilon)$

3.2. compute $\tilde{G}_n = (H' V_e^{-1} H + V_f^{-1})^{-1} H' V_e^{-1} \Delta\tilde{S}_n$

3.3. until $\tilde{G}_n$ is not varying

Comparing figure 2 and 1, we clearly see that JMAP algorithm remove wave structure at high $|\epsilon|$ values. This can be expected since we added this information. We also remark that the current marginal distribution looks more like a sine as expected from measurement parameters. This is an indicator that we improve the all Wigner function restoration.

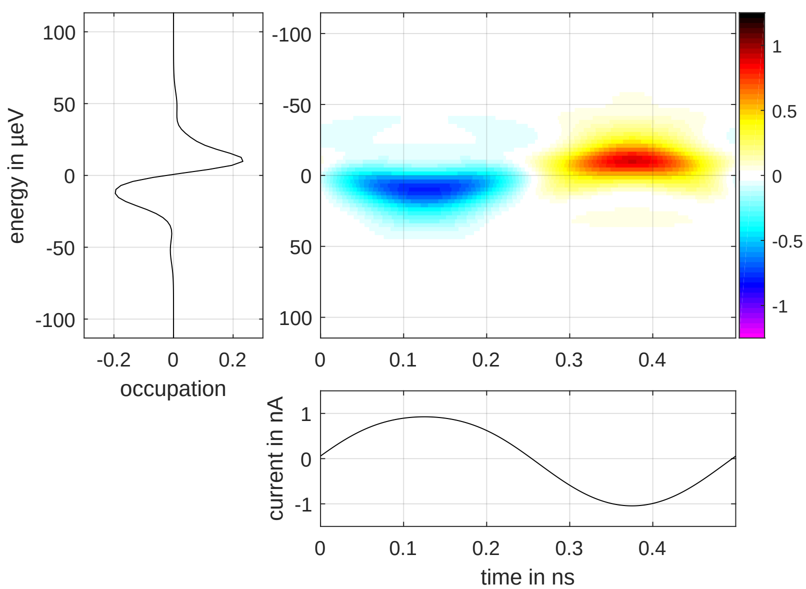

Figure 2: Wigner function extracted thanks to JMAP algorithm from same sinus drive measurement.

4 Gradient projection for box-constraint

JMAP algorithm is already a big improvement of the inverse problem solving method. Still its estimated Wigner function does not verify the Cauchy-Schwartz inequality. Verifying this inequality is important for the wigner to represent a physical state. This inequality is expressed for the G_n by

$$|G_n(\epsilon)|^2 \leq |G_0(\epsilon - n\frac{\hbar\Omega}{2})G_0(\epsilon + n\frac{\hbar\Omega}{2})| \tag{17}$$

Since this inequality does not give any prior knowledge for G_0, this case is solved using JMAP algorithm. Whereas for $n \neq 0$ this inequality define a box-constraint for G_n. The implemented method is then to keep the

Bayesian point of view by minimizing the criteria $||\Delta\tilde{S}_n - H_n G_n||^2_{V_e} + ||G_n||^2_{V_f}$, but looking for a minimum inside the box-constraint. The implemented minimum search algorithm is a Gradient Projected method. It consists of first initializing the solution inside the allowed solution ensemble. And than descent along the least gradient direction. While performing descent gradient steps, we enforce the solution to stay in the box by projecting the gradient. The detailed algorithm is presented in the following.

Algorithm *Gradient Projected method*

1. compute Cauchy-Schwartz bounds $\mathrm{MAX}G_n(\epsilon) = \sqrt{|G_0(\epsilon - n\frac{\hbar\Omega}{2})G_0(\epsilon + n\frac{\hbar\Omega}{2})|}$

2. choose amplitude v_f and width w of $V_f(\epsilon)$ envelope.

3. compute $\tilde{G}_n = (H'V_e^{-1}H + V_f^{-1})^{-1}H'V_e^{-1}\Delta\tilde{S}_n$

4. project under Cauchy-Schwartz bounds $\tilde{G}_n(\epsilon) := \min(\tilde{G}_n(\epsilon), \mathrm{MAX}G_n(\epsilon))$ and $\tilde{G}_n(\epsilon) := \max(\tilde{G}_n(\epsilon), -\mathrm{MAX}G_n(\epsilon))$

5. **repeat**

5.1. compute gradient $\nabla\tilde{G}_n = -H'V_e^{-1}(\Delta\tilde{S}_n - H\tilde{G}_n) + V_f^{-1}\tilde{G}_n$

5.2. project gradient $\mathrm{P}\nabla\tilde{G}_n(\epsilon)$

if $|\tilde{G}_n(\epsilon)| \geq \mathrm{MAX}G_n(\epsilon)$ and $\tilde{G}_n(\epsilon) * \nabla\tilde{G}_n \leq 0$

than $\mathrm{P}\nabla\tilde{G}_n(\epsilon) = 0$

else $\mathrm{P}\nabla\tilde{G}_n(\epsilon) = \nabla\tilde{G}_n(\epsilon)$

5.3. compute furthest accessible displacement d_∞ along $\mathrm{P}\nabla\tilde{G}_n$ direction

for all $\mathrm{P}\nabla\tilde{G}_n(\epsilon) \neq 0$, $d_\infty = \min\left(\frac{\mathrm{MAX}G_n(\epsilon) - G_n(\epsilon)}{\mathrm{P}\nabla\tilde{G}_n(\epsilon)}\right)$

5.4. compute the optimum displacement d_0 along $\mathrm{P}\nabla\tilde{G}_n$ direction

$d_0 = (\mathrm{P}\nabla\tilde{G}'_n\mathrm{P}\nabla\tilde{G}_n)^{-1}\left(\mathrm{P}\nabla\tilde{G}'_n H'V_e^{-1}H\mathrm{P}\nabla\tilde{G}_n + \mathrm{P}\nabla\tilde{G}'_n V_f^{-1}\mathrm{P}\nabla\tilde{G}_n\right)$

5.5. compute the descent gradient $\tilde{G}_n(\epsilon) := \tilde{G}_n(\epsilon) + \min(d_0, d_\infty)\mathrm{P}\nabla\tilde{G}_n(\epsilon)$

5.6. **until** criteria is minimized

In our case this algorithm converges towards a solution plotted in figure 3. There are very few differences with the solution given by JMAP algorithm. The major interest of this method is to give a useful state representation for other quantity calculation like entropy of the state. Nevertheless one can notice that the secondary yellow spot at negative energy and secondary blue spot at positive energy are reduced compared to figure 2.

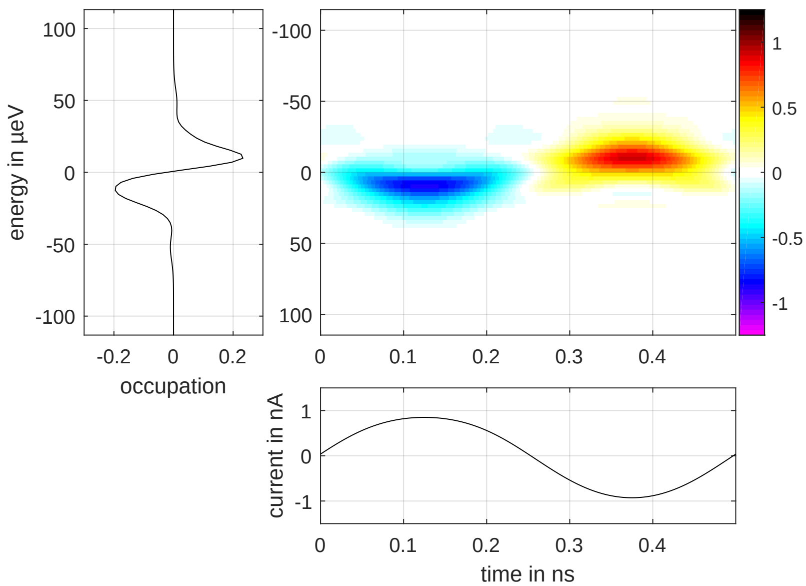

Figure 3: Wigner function extracted thanks to Gradient Projected algorithm from same sinus drive measurement.