Analysis of electron tunneling events with the hidden Markov model

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The charge fluctuations of a quantum dot defined by depletion gates in a semiconductor heterostructure can be observed using a charge sensor. The charge sensor can observe electrons transiting on and off of the quantum dot in real time. From such data information about the quantum states of electrons on the dot can be inferred. We present an approach to analyzing charge sensor data based on the hidden Markov model (HMM). HMM theory provides a mathematical approach for inferring the details of a stochastic process from indirect observations. We discuss how this applies to the problem of charge sensor data analysis. We apply HMMs to data from a previous quantum dot experiment and demonstrate its usefulness in extracting the electron transition rates. Further potential for the HMM in the context of quantum dot experiments is discussed.

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The conductance of a quantum point contact (QPC) (Refs. 1 and 2) or single electron transistor (SET) (Refs. 3 and 4) near to a quantum dot can be sensitive to the charge on the dot, with sufficient resolution to count individual electrons on the dot.[5,6] In a typical experiment a quantum dot is coupled by tunnel barriers to one or more leads, which are thermal reservoirs of electrons.[7] An electron can tunnel from a lead onto a quantum dot if it has the same energy as the quantum dot state it will occupy; likewise an electron on the quantum dot can tunnel off if there is an unoccupied state in the lead at the same energy. When the lead(s) are tuned so that there are both occupied and unoccupied states at the energy level of a quantum dot state, electrons transition on and off of the dot stochastically, a process which can be observed in real time by a QPC or SET acting as a charge sensor. The conductance of the charge sensor shows random transitions between two levels that are commonly referred to as a random telegraph signal (RTS). An example of RTS data is shown in Fig. 2.

From a sequence of observations of the transitions of electrons between the quantum dot and the lead(s), we would like to be able to determine what electron states are possible in the quantum dot and describe their dynamics quantitatively. This paper proposes an approach to analyzing charge sensor data in quantum dot experiments based on the hidden Markov model (HMM). A HMM is a statistical model, diagrammed in Fig. 1, in which the state of the system is a Markov process that cannot be observed directly; instead, at regular time steps the system produces an observation that depends probabilistically on the state the system is in at that time. Information about the sequence of states must be inferred indirectly from the observations. In our application, the Markov process models the electron state of the quantum dot and the observations are the charge sensor data. The state is "hidden" because the signal inevitably contains noise, and it represents only the charge state of the quantum dot and does not contain any information about other degrees of freedom such as spin or orbital quantum numbers. The HMM is well suited for dealing with both of these limitations. Using HMM analysis we can extract the transition rates between the various states of the system. HMM analysis also offers the possibility to infer the existence of multiple states with the same number of electrons, i.e., distinct orbital or spin states that cannot be distinguished directly by a charge sensor.

Hidden Markov modeling is a well-developed statistical field dating from the 1960s.[8] HMMs have been applied to data analysis problems in a variety of other fields, including automatic speech recognition,[9] financial modeling,[10] and a number of biological applications, but to our knowledge it has not been used in a quantum physics context. The type of model proposed here is closely related mathematically to HMMs developed in the study of biological ion channels.[11,12] A good introduction to HMMs is given by Rabiner;[9] a recent comprehensive text is by Cappe *et al.*[13]

In our approach the electron state of the quantum dot is modeled as a discrete first-order Markov process. At each discrete unit of time t the system is assumed to be in one of a finite number M of definite quantum states, denoted by $X_1, X_2, \ldots, X_M$. The system transitions randomly between states, with the probability of the system being in state X_j at time t depending only on the state of the system at time

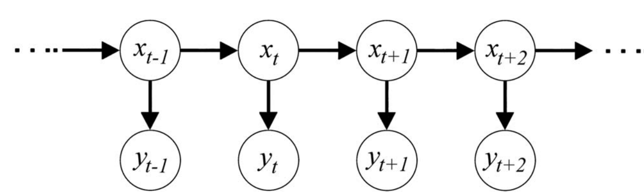

FIG. 1. Diagram of a general HMM, which consists of a Markov process $\boldsymbol{x}=\{x_1,x_2,\ldots,x_N\}$ and a sequence of observations $\boldsymbol{y}=\{y_1,y_2,\ldots,y_N\}$. Arrows indicate conditional dependence between variables. The state x_t depends only on the previous state x_{t-1} and the observation y_t depends only on the current state x_t. In our implementation the Markov process $\boldsymbol{x}$ represents the electron state of the quantum dot as it changes over time and the observations $\boldsymbol{y}$ represent charge sensor measurements.

$t-1$. Let x_t represent the state of the system at time t. We define the transition matrix of the system, A, whose elements are the probability of being in state X_j at time $t+1$, given that the system was in state X_i at time t,

$$A_{ij} = P(x_t = X_j | x_{t-1} = X_i). \tag{1}$$

The transition rate from state i to state j is $A_{ij}/\Delta t$, where Δt is the time between data points. Introducing a probability vector $\boldsymbol{p}(t)$ such that $p_i(t)$ is the probability that the system is in state X_i at time t, the evolution of the system is described by the Markov equation,

$$\boldsymbol{p}_{t+1} = A^T \boldsymbol{p}_t. \tag{2}$$

This equation is the discrete-time analog of the classical master equation (also known as the continuous-time Markov equation) commonly used to describe the dynamics of mesoscopic systems.

In the HMM paradigm the sequence of states $\boldsymbol{x}=x_1,x_2,\ldots x_N$ is not known. At each time t, the system produces a random output or observation, y_t, which depends only on the current state of the system x_t (not on any previous state or observation). In our models we assume that if the system is in state X_i the conductance through the charge sensor y_t is a value g_i, which is a function of the number of electrons in state X_i, plus Gaussian white noise with amplitude σ_i,

$$p(y_t = y | x_t = X_i) = \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left[-\frac{(y-g_i)^2}{2\sigma_i^2}\right]. \tag{3}$$

Together, Eqs. (2) and (3) constitute a HMM. The model is fully characterized by the set of parameters $\boldsymbol{\phi}=\{A, g_1, g_2, \ldots g_M, \sigma_1, \sigma_2, \ldots \sigma_M\}$. The parameters can be constrained as appropriate, for example if state i and state j have the same number of electrons we make the constraint $g_i = g_j$. We assume the noise amplitudes are equal for each state.

Existing HMM theory provides a number of useful analytical tools. From Eqs. (2) and (3) we can compute the likelihood $p(\boldsymbol{y}|\boldsymbol{\phi})$ of obtaining the sequence of observations $\boldsymbol{y}$ given a set of model parameters $\boldsymbol{\phi}$, which is useful for judging how well a model $\boldsymbol{\phi}$ fits the observed data $\boldsymbol{y}$. For practical details of computing the likelihood function, see Rabiner.[9] Given a model $\boldsymbol{\phi}$ and a sequence of observations $\boldsymbol{y}$, we can determine the most likely sequence of states the system was in at each time step using the Viterbi algorithm.[9,14] That is, we can find the sequence of states $\boldsymbol{x}$ which maximizes the likelihood $p(\boldsymbol{y}|\boldsymbol{x},\boldsymbol{\phi})$.

More interestingly, from a data set $\boldsymbol{y}$ we can find the set of model parameters $\hat{\boldsymbol{\phi}}$ which best fit the data, in the sense of maximizing $p(\boldsymbol{y}|\boldsymbol{\phi})$, using the Baum-Welch algorithm.[8,9] The physics of the system are encapsulated in the transition probabilities A_{ij}, so those parameters we are especially interested in estimating. The Baum-Welch algorithm is a hill-climbing algorithm: each iteration takes as input a set of observations $\boldsymbol{y}$ and a set of model parameters $\boldsymbol{\phi}$, and computes a set of model parameters $\boldsymbol{\phi}'$ such that $p(\boldsymbol{y}|\boldsymbol{\phi}') \geq p(\boldsymbol{y}|\boldsymbol{\phi})$. Thus, beginning with an initial guess for $\boldsymbol{\phi}$, repeated applications of the Baum-Welch algorithm converge to a maximum in the likelihood function. Finding the true maximum-likelihood estimator $\hat{\boldsymbol{\phi}}$ of the model parameters such that $p(\boldsymbol{y}|\hat{\boldsymbol{\phi}})$ is maximal depends on having a initial guess for the model parameters which leads to the global maximum and not a suboptimal local maximum. To obtain the initial guesses for signal means and standard deviations, we form a histogram of all the conductance data points and fit them to a mixture of Gaussian functions. The initial guess for the transition matrix is chosen arbitrarily. The Baum-Welch algorithm can be repeated with multiple initial guesses to increase the chance of finding the global maximum of the likelihood function; in our analyses so far this has not been necessary. The maximum-likelihood estimator $\hat{\boldsymbol{\phi}}$ has been shown to have advantageous properties such as strong consisistency[15] and asymptotic normality[16] for the type of model described here.

To illustrate the use of HMMs on charge sensor data we present analysis of data from a previous quantum dot experiment.[17] In this experiment a lateral quantum dot was defined by depletion gates in a two-dimensional electron gas in a GaAs/AlGaAs heterostructure, shown in Fig. 2. The dot was coupled to a single lead by a tunnel barrier. The Fermi level of the lead was tuned so that one electron remains fixed on the dot while a second electron may tunnel to and from the dot. The transitions are observed by measuring the current through a nearby QPC; an example of such a data set is shown in Fig. 2. The chemical potential of the quantum dot states can be changed relative to the Fermi level of the reservoir by changing the voltage on the plunger gate, V_P. As the chemical potential of the quantum dot state is increased, the occupancy of electron states in the reservoir that can couple to the quantum dot decreases, decreasing the rate of electron transitions onto the dot and increasing the transition rate off of the dot. Assuming the quantum dot transitions between just two states, state 1 having $n=1$ electrons and state 2 having $n=2$, the transition matrix can be written

$$A = \begin{pmatrix} 1-p_{ON} & p_{ON} \\ p_{OFF} & 1-p_{OFF} \end{pmatrix}, \tag{4}$$

where p_{ON} and p_{OFF} are the probability of an electron tunneling onto and off of the dot, respectively, at each time step. For each value of V_P, 50 s of QPC data were taken at a sampling rate of 4096 Hz and the Baum-Welch algorithm was used to estimate the transition rates $\Gamma_{ON/OFF} = 4096 \cdot p_{ON/OFF}$.

The transition rates extracted by fitting the two-state model to our data are shown in Fig. 3. These transition rates were determined by fitting the QPC data to the purely mathematical HMM; next we fit them to a physical model. Assuming electrons tunnel to and from the lead at a rate Γ_0 multiplied by the fraction of occupied (unoccupied) states in the lead for transitions on (off) the dot,

$$\Gamma_{ON/OFF} = \Gamma_0 f\left(\frac{\pm(\Delta\mu - \alpha e V_P)}{k_B T}\right), \tag{5}$$

where $\Delta\mu = \mu_L - \mu_D$ is the difference between the Fermi level of the lead and the chemical potential of the dot at $V_P=0$, and α is the relative capacitance between the dot and gate P,

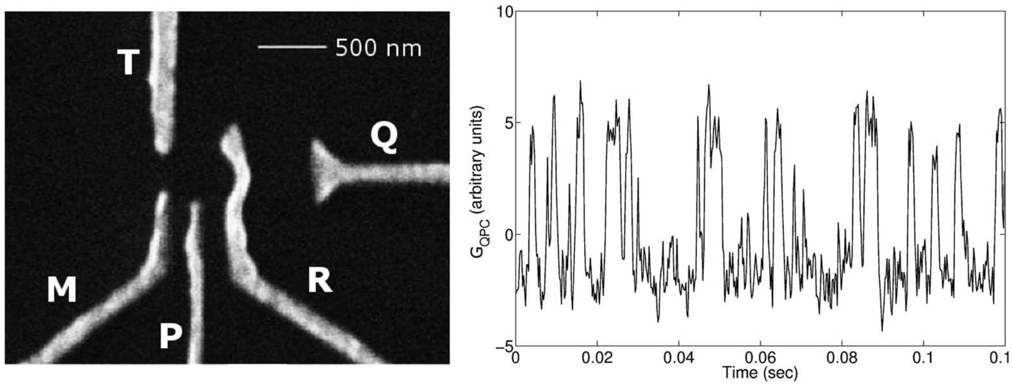

FIG. 2. (Left) SEM image of the quantum dot structure used in the experiment described. Negative voltages on the metal gates deplete the 2DEG (dark areas, below the gates), forming a quantum dot in the center of gates M, P, R, and T. A tunnel barrier is formed between gates M and T so that electrons can tunnel to/from the lead (dark area to the left). A QPC is formed between gates R and Q so that the current passing between them is sensitive to the presence of electrons on the dot. (Right) Example of charge sensor data set taken from the experiment described in the text. The QPC conductance alternates between two distinct levels as electrons enter and leave the quantum dot. In this case the upper level corresponds to $n=1$ electron on the quantum dot and the lower level corresponds to $n=2$.

which was determined from Coulomb diamond measurements to be $\alpha=0.011$ for this device. The electron temperature was $T=0.5$ K. f is the Fermi distribution function, which represents the occupation of electron states in the lead. The results of fitting the transition rates to this model are shown in Fig. 3. The transition rates fit the thermal reservoir model well except for the tail of the Γ_{OFF} rates, which do not go to zero as expected but level off at about 15–20 Hz. It appears that there is an unexpected slow process by which electrons leave the quantum dot that is independent of V_P.

In this experiment it is not clear *a priori* that only two

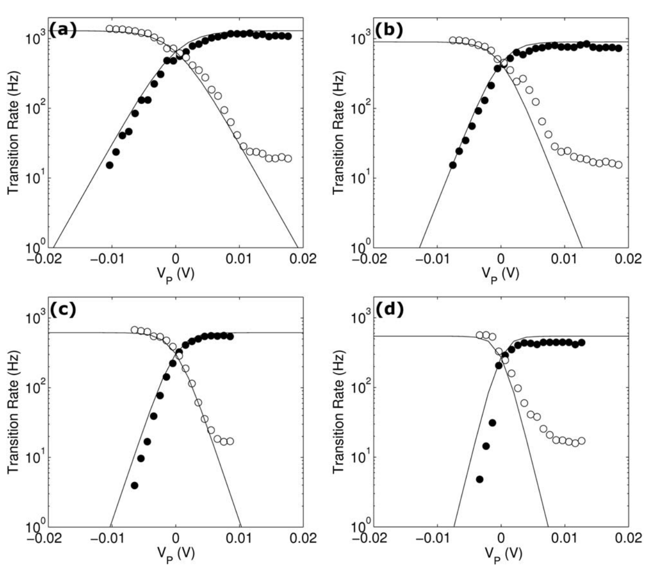

FIG. 3. Electron transition rates Γ_{ON} (closed circles) and Γ_{OFF} (open circles) determined from HMM analysis. The voltage V_P is varied in each plot, which changes the chemical potential for the electron to tunnel onto the dot relative to the Fermi level of the lead. Four different values of the voltage on gate M are shown: (a) $V_M=-775$ meV. (b) $V_M=-800$ meV. (c) $V_M=-825$ meV. (d) $V_M=-850$ meV. Lowering the voltage on gate M raises the tunnel barrier to the lead and lowers the tunnel rate. Solid lines show fits to a Fermi distribution as described in the text.

states are participating in electron transitions. It is also possible that more than one quantum state with the same number of electrons has a chemical potential level within the thermal broadening of the lead and electrons can tunnel into any of these states. If the transition rates of these states are significantly different from one another HMM analysis should be able to distinguish the states and determine the transition rates. For the data sets presented here we applied different HMMs containing an extra 1-electron state, an extra 2-electron state, and a four state model that had both. The HMMs were constrained so that states with the same number of electrons had the same average conductance measurement ($g_i=g_j$ if X_i and X_j have the same number of electrons). In all of these cases the results of such models did not fit the data significantly better (as judged by the maximum likelihood) than the simple two-state model. We conclude that there is not sufficient evidence in these data to justify a model with more than two states. Detection of "hidden" states may be a useful application of HMMs; we hope to demonstrate this in a future experiment.

Robustness against noise is a major advantage of the HMM approach relative to previous analyses of charge sensor data. Most previous studies applied a thresholding or change-detection[18] procedure to the signal to determine when it transitioned from one conductance level to the next; the timing of these events was then analyzed. In another approach, Yuzhelevski *et al.*[19] proposed a method for estimating transition rates that is substantially similar to the one presented here for the case of a system with two states and two conductance levels, except that at each step of their algorithm a definite state of the system is assigned to each data point. The HMM performs better in the presence of noise because it never assigns a definite state to the system. Instead, for each data point it computes a probability of the system being in each state. The final transition rate estimates are weighted averages over every available data point, instead of being unweighted averages over a relatively smaller number of transition events. To illustrate how errors in removing noise can bias estimates of the transition rates, we made several simulations of a Markov process and compared

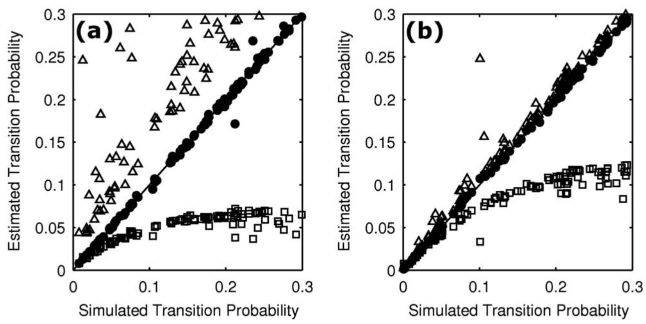

FIG. 4. Results of applying various data analysis techniques to 100 simulated RTSs. The transition rates estimated by three different analysis techniques are plotted against the true transition rate that was used in the simulation. The analysis techniques are HMM (closed circles), digitization by a change-detection algorithm (Ref. 18) (open squares), and digitization by a threshold determined from a two-Gaussian fit to the data (open triangles). The signal-to-noise ratio is: (a) SNR=3. (b) SNR=5.

the HMM estimates of the transition rates to two other techniques, the results of which are shown in Fig. 4. Each simulation is a two-state Markov process, with a noisy conductance measurement generated for each data point. The transition probabilities were then estimated from the simulated data using three different approaches: fitting to a HMM, digitization by a change-detection algorithm,[18] and digitization by a threshold determined from a two-Gaussian fit to the data. The transition rate estimated by each method is plotted against the true transition rate used in the simulation. The change-detection method underestimates transition rates because it tends to fail to detect transition events. The threshold method tends to overestimate transition rates because it counts spurious transitions. The HMM approach can estimate transition rates with a signal-to-noise ratio as low as 3, and could do better if longer data sets were used.

In conclusion, we believe that the approach to analysis of charge sensor data described in this article will prove useful in understanding the results of future quantum dot experiments. It has already demonstrated superior robustness with respect to noise than our previous data analysis techniques, and holds the possibility of distinguishing multiple states with the same number of electrons. We applied the technique to experimental data and extracted the transition rates for electrons to tunnel on and off the quantum dot. We tried fitting the data to models with additional quantum states and did not find compelling evidence for such states in this experiment, but we believe such models will find use in the future. It may be possible in future work to extend the technique to model the system using a quantum master equation, allowing estimation of the density matrix of the system and of coherent processes.

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