Journal Club for Condensed Matter Physics
https://www.condmatjclub.org
DOI:10.36471/JCCM_October_2020_01

A New Approach to the Classical-Quantum Correspondence

Quantum eigenstates from classical Gibbs distributions
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arXiv:2007.07264

Recommended with a Commentary by Daniel Arovas, University of California, San Diego

As students we all learn of the beautiful path integral formulation of quantum mechanics, in which the real time propagator $\langle\, x(t_2)\,|\,x(t_1)\,\rangle$ may be written as the functional integral, with respect to the so-called Wiener measure, over all paths $x(t)$ connecting the endpoints $x(t_1) = x_1$ and $x(t_2) = x_2$, weighed by the phase $e^{iS/\hbar}$, where $S\big[x(t)\big] = \int_{t_1}^{t_2} dt\,\big\{\frac{1}{2}m\dot{x}^2 - V(x)\big\}$ is the action functional. In the semiclassical limit, one regards $\hbar$ as a small parameter, and the stationary phase approximation $\delta S[x(t)] = 0$ yields the classical Euler-Lagrange equations of motion $m\ddot{x} = -V'(x)$. As $\hbar \to 0$, quantum uncertainties become negligible and one recovers classical mechanics†. It might at first seem that inverting this procedure, *i.e.* deriving quantum mechanics, the Schrödinger equation, state vectors and Hermitian operators from classical mechanics, is an impossible task. However, it turns out that a program of this sort is indeed possible, as elucidated by Claeys and Polkovnikov, clarifying and extending earlier work of Hayakawa and others [3].

Given any stationary classical probability distribution $P(x,p)$ and a free parameter ϵ with dimensions of $\hbar$, one can define a *quasi-density matrix* $\mathcal{W}_\epsilon(x_1,x_2)$ according to

$$\mathcal{W}_\epsilon(x+\tfrac{1}{2}\xi, x-\tfrac{1}{2}\xi) = \int\limits_{-\infty}^{\infty} dp\, P(x,p)\, e^{-ip\xi/\epsilon} \quad , \tag{1}$$

where $x_{1,2} = x \pm \frac{1}{2}\xi$. When $\epsilon = \hbar$ and $\mathcal{W}_\hbar = \varrho(x_1,x_2)$ is the density matrix, $P(x,p)$ is the usual Wigner function. More generally, since $P(x,p)$ is real, $\mathcal{W}_\epsilon(x_1,x_2) = \mathcal{W}^*_\epsilon(x_2,x_1)$ is Hermitian and may be expressed in an orthonormal basis of eigenfunctions: $\mathcal{W}_\epsilon(x_1,x_2) = \sum_\alpha w_\alpha\, \psi^*_\alpha(x_1)\, \psi_\alpha(x_2)$, with $\mathsf{Tr}\,\mathcal{W}_\epsilon = \int\limits_{-\infty}^{\infty} dx\, \mathcal{W}_\epsilon(x,x) = \int\limits_{-\infty}^{\infty} dx \int\limits_{-\infty}^{\infty} dp\, P(x,p) = \sum_\alpha w_\alpha$. The catch

†See [1]. The classical limit of the equations of motion can also be recovered via the use of coherent states, or through the Wigner-Weyl phase space formalism discussed, *e.g.*, in [2] is that the eigenvalues w_α are not necessarily confined to the unit interval $[0,1]$, which is always the case for a proper density matrix[†].

If $P(x,p,t)$ is time-dependent, satisfying the Liouville equation $\partial_t P = \big\{H,P\big\}$ with Poisson bracket dynamics, then $\mathcal{W}_\epsilon$ inherits a corresponding dynamics, $i\epsilon\,\partial_t\mathcal{W}_\epsilon = \widehat{\mathcal{L}}_\epsilon\,\mathcal{W}_\epsilon$, where $\widehat{\mathcal{L}}_\epsilon$ is a linear operator. For $H(x,p)=\frac{p^2}{2m}+V(x)$ and in the $\epsilon\to 0$ limit, one recovers the Schrödinger equation $i\epsilon\,\partial_t\psi_\alpha(x,t) = \big\{-\frac{\epsilon^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\big\}\,\psi_\alpha(x,t)$ for each eigenfunction ψ_α, along with the condition that the eigenvalues w_α are time-independent. Furthermore, and for arbitrary ϵ, averages with respect to the classical distribution $P(x,p)$ can be expressed as an expectation value of operators with respect to the quasi-density matrix $\mathcal{W}_\epsilon$ *viz.*

$$\langle\, O(x,p)\,\rangle = \int\limits_{-\infty}^{\infty}\!dx\int\limits_{-\infty}^{\infty}\!dp\; O(x,p)\,P(x,p) = \sum_\alpha w_\alpha\,\langle\,\psi_\alpha\,|\,\mathcal{O}(\hat{x},\hat{p})\,|\,\psi_\alpha\,\rangle \quad , \tag{2}$$

where to each function $O(x,p)$ corresponds a Hermitian operator $\mathcal{O}(\hat{x},\hat{p})$, expressed in terms of $\hat{x}=x$ and $\hat{p}=-i\epsilon\,\partial_x$.

It is instructive to consider the Gaussian distribution $P(x,p)=(\pi\epsilon)^{-1}\,e^{-x^2/2\sigma_x^2}\,e^{-p^2/2\sigma_p^2}$. Claeys and Polkovnikov show that when the uncertainty ratio $u\equiv\sigma_x\sigma_p/(\epsilon/2)=1$ the quasi-density matrix $\mathcal{W}_\epsilon(x_1,x_2)=\psi_0^*(x_1)\,\psi_0(x_2)$ is a pure state, where ψ_0 is the harmonic oscillator ground state wavefunction. When $u>1$, $\mathcal{W}_\epsilon$ corresponds to a Gibbs distribution with $w_n=e^{-n\gamma}/\mathcal{Z}$ and $\gamma=\ln\big[(u+1)/(u-1)\big]$. When $u<1$, the eigenvalues oscillate, with $w_n=(-1)^n\,e^{-n\widetilde{\gamma}}/\mathcal{Z}$ and $\widetilde{\gamma}=\ln\big[(1+u)/(1-u)\big]$. Thus, negative probabilities result when $P(x,p)$ violates the uncertainty relation $\sigma_x\sigma_p\ge\frac{\epsilon}{2}$.[‡]

Consider next the microcanonical distribution, $P(x,p;E)=\delta\Big(E-\frac{p^2}{2m}-V(x)\Big)\Big/D(E)$, where $D(E)$ is the density of states[‖]. For linear and quadratic potentials, the eigenstates of the quasi-density matrix correspond exactly to the quantum eigenstates, and their associated eigenvalues w_α can be obtained exactly. In the case of the linear potential $V(x)=\alpha x$, the spectrum $w_{\mathcal{E}}(E)$ of $\mathcal{W}_\epsilon$ is labeled by a continuous parameter $\mathcal{E}$ with dimensions of energy, and is proportional to an Airy function of the difference $E-\mathcal{E}$. When $\mathcal{E}\ll E$, the eigenvalues are exponentially small and positive, while for $\mathcal{E}\gg E$ the eigenvalues are highly oscillatory and negative over an infinite set of $\mathcal{E}$ intervals. For the harmonic potential $V(x)=\frac{1}{2}m\omega^2x^2$, the spectrum is discrete; with $w_n(E)$ exponentially small for $E_n\equiv(n+\frac{1}{2})\,\epsilon\omega<E$ and oscillating for $E_n>E$. By convolving the microcanonical distribution with a Gaussian energy uncertainty function of width σ_E, the oscillations can be completely suppressed provided $\Delta E\,\Delta t\gtrsim\epsilon$, where $\Delta E=\sigma_E$ and $\Delta t=(m\epsilon/\alpha^2)^{1/3}$ for the linear potential and $\Delta t=1/\omega$ for the harmonic potential are characteristic time scales.

For the case of the canonical distribution $P(x,p)=\mathcal{Z}^{-1}\,e^{-\beta p^2/2m}\,e^{-\beta V(x)}$, the eigenvalue

[†]Similarly, the Wigner function $W(x,p,t)=(2\pi\hbar)^{-1}\!\int_{-\infty}^{\infty}d\xi\,\langle\,x+\frac{1}{2}\xi\,|\,\varrho\,|\,x-\frac{1}{2}\xi\,\rangle\,e^{ip\xi/\hbar}$ is real but in general not everywhere positive.

[‡]In both cases, $\mathcal{Z}=\sum_{n=0}^{\infty}w_n$ is the partition function.

[‖]Thus $\mathsf{Tr}_{x,p}\,P(x,p;E)=1$.

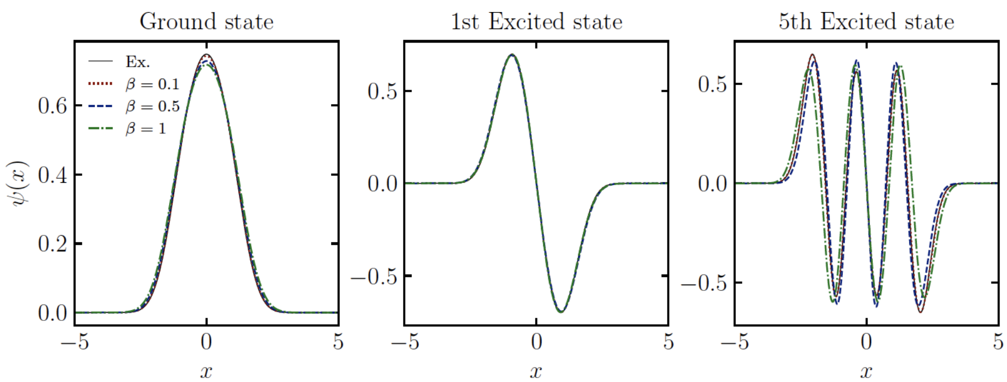

Figure 1: Comparison of classical eigenstates obtained from the Gibbs distribution with $\beta = 0.1$, 0.5, and 1 (broken lines) in comparison with the exact quantum stationary states for the quartic potential $V(x) = \frac{1}{4}\nu x^4$, with $m = \epsilon = \hbar = \nu = 1$.

equation may be written exactly as

$$w_n\, \psi_n(x) = \frac{1}{\mathcal{Z}_x} \int\limits_{-\infty}^{\infty} d\xi\ \exp\!\bigg[-\frac{m\xi^2}{2\beta\epsilon^2} - \beta V(x - \tfrac{1}{2}\xi)\bigg]\, \psi_n(x-\xi) \quad . \tag{3}$$

where $\mathcal{Z}_x = \int_{-\infty}^{\infty} dx\, e^{-\beta V(x)}$. The Schrödinger equation $-\frac{\epsilon^2}{2m}\,\psi_n''(x) + V(x)\,\psi_n(x) = E_n\,\psi_n(x)$ is then recovered both (i) when $\epsilon \to 0$ as well as (ii) when $\beta \to 0$, with $w_n = e^{-\beta E_n}/\mathcal{Z}$ with $\sum_{n=0}^{\infty} w_n = 1$. In the latter case, the correct quantum stationary states are recovered when we set $\epsilon = \hbar$, independent of the accuracy of the WKB approximation. In the opposite limit, when $\beta \to \infty$ and the classical distribution becomes narrow, the eigenspectrum of $\mathcal{W}_\epsilon$ features negative probabilities. The example of the quartic potential $V(x) = \frac{1}{4}\nu x^4$ is shown in Fig. 1. With $\beta = 0.1$, the classical eigenstates obtained from the Gibbs distribution reproduce the energies of the ten lowest eigenstates to better than 0.05%. Claeys and Polkovnikov find similarly good agreement for the case of the tunneling states in the one-dimensional double well potential $V(x) = \frac{1}{4}\nu(x^2-1)^2$. Their results for the two-dimensional system with

$$V_{\mathsf{A}}(x,y) = \tfrac{1}{2}m(\omega+\delta)^2x^2 + \tfrac{1}{2}m(\omega-\delta)^2y^2 + \tfrac{1}{4}\nu x^2y^2 \tag{4}$$

are shown in Fig. 2. The classical equations of motion are thus nonlinear and exhibit chaotic trajectories.

Claeys and Polkovnikov [4] have also investigated their pseudo-density matrix in the context of the Bohigas-Giannoni-Schmidt conjecture [5], which says that the spectra of chaotic quantum systems exhibit random matrix statistics associated only with certain global symmetries. They construct a two-dimensional potential $V_{\mathsf{B}}(x,y)$ corresponding to a Sinai billiard system from a sequence of smoothed step functions, depicted in Fig. 3. From the canonical distribution $P(x,y,p_x,p_y) = Z^{-1}e^{-\beta H(\boldsymbol{x},\boldsymbol{p})}$ they once again derive $\mathcal{W}_\epsilon(\boldsymbol{x}_1,\boldsymbol{x}_2)$ and analyze the eigenvalue spacings distribution

$$r_n = \frac{\lambda_{n+1}-\lambda_n}{\lambda_{n+2}-\lambda_{n+1}} \equiv \frac{\log(w_n/w_{n+1})}{\log(w_{n+1}/w_{n+2})} \quad . \tag{5}$$

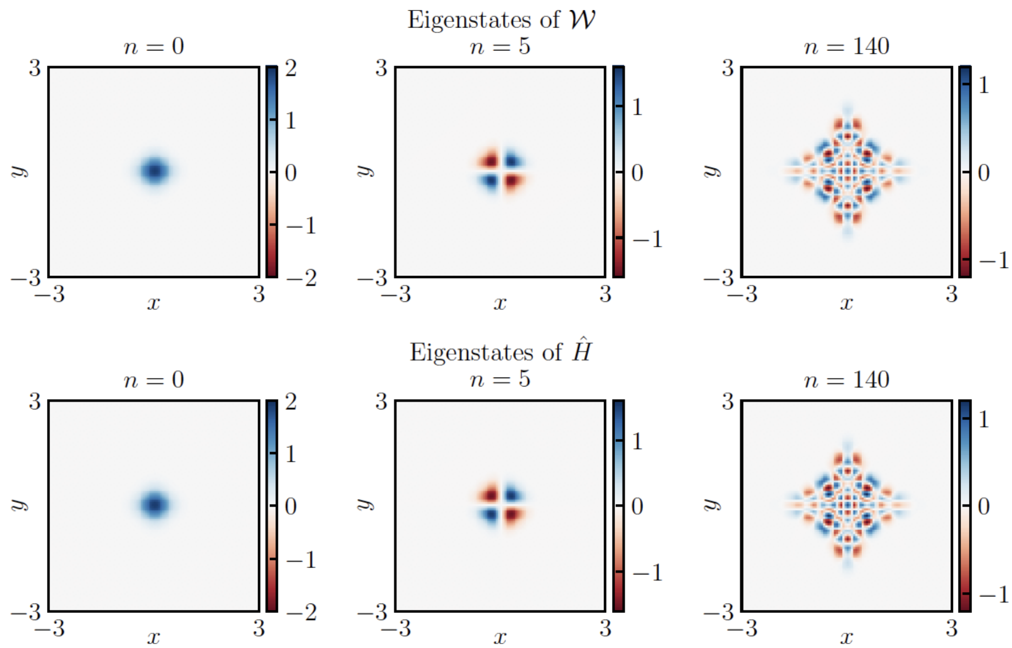

Figure 2: Top: classical eigenstates obtained from the Gibbs distribution with $\beta = 1$. Bottom: quantum eigenstates of the Hamiltonian $\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + V(\hat{x}, \hat{y})$ where the potential $V_{\mathsf{A}}(x, y)$ is given in the text. The parameters are $m = \omega = \epsilon = \hbar = 1$, $\delta = 0.1$, and $\nu = 20$.

The results match extremely well with those expected from the Gaussian orthogonal ensemble (GOE) of random matrix theory.

To summarize, the Wigner transform which maps a quantum mechanical density matrix $\varrho(x_1, x_2)$ to a classical phase space distribution $W(x, p)$ can be inverted, mapping a classical phase space distribution $P(x, p)$ to a (quasi-)density matrix $\mathcal{W}_\epsilon(x_1, x_2)$, where ϵ is a free parameter which plays the role of $\hbar$. Moreover, $\mathcal{W}_\epsilon(x_1, x_2, t)$ inherits dynamics from the Liouville dynamics of $P(x, p, t)$. One can expand $\mathcal{W}_\epsilon(x_1, x_2) = \sum_\alpha w_\alpha\, \psi_\alpha^*(x_1)\, \psi_\alpha(x_2)$ in terms of its orthonormal eigenfunctions $\psi_\alpha(x)$ and their corresponding eigenvalues w_α, normalized according to $\sum_\alpha w_\alpha = 1$. However, the condition $w_\alpha \in [0, 1]$ is in general violated whenever the classical distribution violates the uncertainty relation $\Delta x\, \Delta p \gtrsim \epsilon$, similar to what happens with the Wigner function itself, which can take negative values and is thus a quasi-distribution on phase space. For the Gibbs distribution $P(x, p) = Z^{-1}\, e^{-\beta H(x,p)}$, the "classical eigenstates" of $\mathcal{W}_\epsilon$ precisely agree with their quantum counterparts in the high temperature ($\beta \to 0$) limit. Finally, the level spacings distribution obtained from a potential corresponding to a Sinai billiard, but smoothed at the spatial boundaries, reproduces extremely well the predictions of the GOE from random matrix theory. Further connections of this work to issues of thermalization and classical *vs.* quantum chaos, such as the phenomenon of quantum scars [6], should be interesting to pursue.

I am grateful to Pieter Claeys and Anatoli Polkovnikov for sharing the results depicted in Fig. 3 prior to distribution, and for helpful comments.

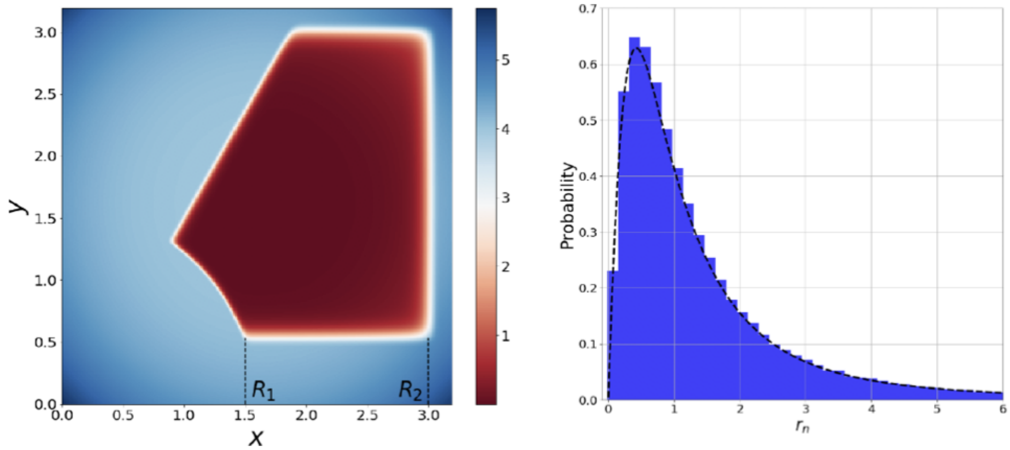

Figure 3: Left: Spatial probability distribution for a chaos-producing two-dimensional potential corresponding to a Sinai billiard system with smoothed spatial edges. Right: Histogram of the consecutive level spacings ratio r_n derived from the Gibbs ensemble with $m = 1$, $\beta = 0.3$ and $\epsilon = 0.2$. The dashed black curve shows the results of the Gaussian orthogonal ensemble (GOE).

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