Quantum Jamming: Critical Properties of a Quantum Mechanical Perceptron

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In this paper we analyze the quantum dynamics of the perceptron model, where a particle is constrained on a \((N - 1)-\)dimensional sphere, subjected to a set of \(M = \alpha N\) randomly placed hard-wall potentials. This model has several applications, ranging from learning protocols to the effective description of the dynamics of an ensemble of hard spheres in Euclidean space in \(d \to \infty\) dimensions. We find that the quantum critical point at \(\alpha = 2\) does not show the mean-field exponents of the classical model, which points to a non-trivial critical quantum theory. We also find that the physics of such a quantum critical point is not confined to the low-temperature region. Our findings have implications for the theory of glasses at ultra-low temperatures and for the study of quantum machine-learning algorithms.

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Constraint satisfaction problems (CSP), which arise naturally in computer science, have taken up a prominent role in statistical mechanics in the last 20 years, as it has been shown that methods and ideas from the theory of disordered systems can shed light on the possible origin of their computational difficulty \([1–3]\) and even inspire efficient algorithms and valuable heuristics \([4, 5]\) to solve them. While problems defined in terms of discrete phase variables (i.e. bits) map naturally to Ising spin glasses (the disorder arising due to the sampling of instances from a large ensemble), CSP defined in terms of continuous variables \([6, 7]\) have shown several similarities and a deep connection with the sphere-packing problem and their jamming transition (i.e. configurational glasses) \([8–14]\). In both problems, substituting a classical spin-flip dynamics with a transverse field or the free particle kinetic term with its quantized counterpart can have profound consequences, both at the theoretical and the practical level. In the spin-glass/discrete variable case, a large literature has investigated the impact of quantum dynamics on the spin glass transition \([15,17]\). Recently, partly motivated by the technological progress on the way to build a universal quantum computer \([18]\), many authors have been looking at ways to use quantum dynamics to speed up the solution of the classical problems. It has been found that the presence of both disorder and quantum mechanical interference produces a plethora of new phenomena which are not present in the classical spin-flip dynamics, and highlights profound connection with, for example, Anderson and Many-Body Localization Physics \([19–22]\). The continuous variable case endowed with quantum dynamics, instead, has not received the same kind of attention so far. This is surprising, in light of the connection with the jamming transition, and the fact that the observation of anomalous (i.e. non-Debye) behavior of thermodynamic quantities of configurational glasses at ultra-low temperature \([23,24]\) (such as \(C_V(T) \sim T\)) has a natural explanation in terms of quantum mechanical tunneling \([32,33]\). So, quantum mechanical effects are definitely important in configurational glasses but no firm results or solvable toy models exist (see, for example, \([34]\) for criticism to \([32,33]\)). The purpose of this paper is precisely to show that, in a model that describes the limit \(d \to \infty\) of the jamming transition, quantum mechanical effects change the nature of the critical phase radically. This paper complements the semiclassical analysis of \([14]\), in which the corrections to the classical quantities were computed at \(O(h)\), and a linear specific heat \(C_V(T)\) was found. In this paper we show that the limits \(h \to 0\) and \(T \to 0\) do not commute at the jamming point, and that for non-zero \(h\) one gets different critical exponents, independent of the temperature, and that \(C_V(T) \sim e^{-\Delta/T}\). One recovers the semiclassical result by looking at the high-frequency behavior of the correlation function, and we therefore elucidate in which region of parameters a semi-classical dressing of the classical model captures the Physics. We end this Introduction noticing that the name quantum perceptron has been already defined in the past, as a learning problem for quantum states \([35]\): Our problem is different as we have implemented a quantum dynamics on a classical classification problem.

The Hamiltonian of the system is

\[
\hat{H} = \frac{\hat{P}^2}{2m} + \sum_{\mu=1}^{M} v(h_{\mu}(\hat{X})),
\]

with canonical commutation relations

\[
[\hat{X}_i, \hat{P}_j] = i\hbar \delta_{ij},
\]
and the constraint $X^2 = N$; the hard-wall potential is defined as $v(r) = 0$ if $r > 0$, $v(r) = \infty$ for $r < 0$;

$$h_\mu(X) = \frac{1}{\sqrt{N}} \xi^\mu \cdot X - \sigma,$$

(3)

and $\xi^\mu$ are $M$ random, $N$-dimensional vectors. The limit $N \to \infty$ is taken, eventually, with only surviving parameters being $\sigma, \alpha \equiv M/N$, and the inverse temperature $\beta$. The classical system (when $m \to \infty$ or $h \to 0$) is independent of the temperature and has two thermodynamic phases, essentially determined by the geometric problem of whether there is or there is not any volume left by the intersection of the $M$ constraints: $\bigcup_n^M \{X \in \mathbb{R}^N : X^2 = N, h_\mu(X) > 0\}$. The result is that, for $N, M \to \infty$, for $\alpha < \alpha_c(\sigma)$ the volume is non-zero (the so-called SAT phase), while for $\alpha \geq \alpha_c(\sigma)$ it is zero (the UNSAT phase). Going deeper into the details of the phases, one observes that for $\sigma < 0$ the phase transition is preceded by a de Almeida-Thouless line (replica-symmetry-breaking (RSB) phase) at $\alpha_{dAT} < \alpha_c$, while for $\sigma \geq 0$ the replica-symmetric (RS) solution is everywhere stable [13]. For our purposes we will concentrate on the value $\sigma = 0$, for which it is known that $\alpha_c(0) = 2$, that is at the border of the RS stable region.

We want to compute the partition function $Z = \text{Tr}(e^{-\beta H})$, the free energy $F = -\beta^{-1} \ln Z$, and then take a quenched disorder average. After following the procedure in [14 36], the quenched free energy is expressed in terms of the autocorrelation function $G(t-s) \equiv \langle r(t)r(s) \rangle_r$, $r(t)$ being a one-dimensional, $\beta\hbar$-periodic auxiliary process and

$$\langle \bullet \rangle_r = \frac{1}{Z_0} \int D r e^{-\frac{1}{4} \int_0^{\beta\hbar} dt \langle r(t)G^{-1}(t-s)r(s) \rangle_r} \bullet,$$

(4)

with $Z_0$ a suitable normalization. Specifically, the RS free energy per dimension (and per replica) reads [39]

$$-\beta f \equiv -\frac{\beta F}{nN} = \frac{1}{2} \sum_{n \in \mathbb{Z}} \ln G_n + \frac{q}{2G_0} - \frac{\beta m}{2} \sum_{n \in \mathbb{Z}} \omega_n^2 G_n +$$

$$-\frac{\beta \mu}{2} \left[ \sum_{n \in \mathbb{Z}} G_n - (1-q) \right] +$$

$$+ \alpha \gamma_q \star \ln \langle e^{-\beta \int_0^{\beta\hbar} dt \pi \cdot \pi v(r(t)+h)} \rangle_r,$$

(5)

where $\bullet_n \equiv \hat{\bullet}(\omega_n)$ is the Fourier transform of $\bullet(t)$, $\omega_n \equiv 2\pi n/\beta\hbar$ are the Matsubara frequencies, $q$ is the Edwards-Anderson order parameter (overlap between different replicas) [36], and $\gamma_q \star (h) \equiv \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi \beta \hbar}} e^{-\beta t^2/2q} \bullet(h)$. The dynamics of the random process is defined self-consistently by the saddle-point equations for the parameters $G_n$, $\mu$ and $q$:

$$G_n^{-1} = \beta m \omega_n^2 + \beta \mu + \beta \Sigma_n$$

(6)

$$\sum_n G_n = 1 - q$$

(7)

$$q = \alpha \gamma \star \langle r_0 \rangle_v^2$$

(8)

where

$$\beta \Sigma_n \equiv \alpha \left( G_n^{-1} - G_n^{-2} \gamma_q \star \left( \langle r_n^2 \rangle_v - \delta_{n0} \langle r_0 \rangle_v^2 \right) \right)$$

(9)

and

$$\langle \bullet \rangle_v = \frac{\langle e^{-\beta \int_0^{\beta\hbar} dt \pi \cdot \pi v(r(t)+h)} \rangle_r}{\langle e^{-\beta \int_0^{\beta\hbar} dt \pi \cdot \pi v(r(t))+h)} \rangle_r}$$. (10)

In our conventions, however, we will shift $\Sigma \to \Sigma_n + \Sigma_0$ and reabsorb $\Sigma_0$ into $\mu$, so that $\Sigma(\omega)$ starts from 0 at $\omega = 0$ remaining continuous as a function of $\omega$.

To solve these equations we have used an iterative method, together with a Montecarlo sampling for the $\langle \bullet \rangle_{r,v}$, (for an analog calculation in the SK model see [37 38]). As a result, we obtain the value of the order parameter $q$ as a function of $\alpha, \beta$, which is plotted in Fig. 1 against the classical result.

The classical value of $q$, $q_{cl}(\alpha)$, unlike the quantum case, is independent of the temperature and, for $\alpha \to 2$, goes to 1 with the mean-field critical exponent value $\kappa_{cl} = 1$: $(1 - q_{cl}(\alpha)) \approx 1/4(2 - \alpha)$. The value of $q$ for the quantum dynamics is always larger than the classical one, and this can be understood easily: The ground state of a particle in a billiard is more concentrated than a flat distribution on the billiard table (because of the Dirichlet boundary conditions on the walls), which is the classical case. Moreover, it becomes more concentrated the larger the aspect ratio of the billiard, namely if one of the sides is larger than the others. Quantitatively, already at lowest order in $\alpha$, one has $q = \alpha \langle r_0 \rangle_v^2(h=0) + \mathcal{O}(\alpha^2)$, and the propagator $G_n = \beta m \omega_n^2 + \beta \mu + \mathcal{O}(\alpha)$ is that of a harmonic oscillator, with $\mu$ fixed in such a way that $\langle r^2 \rangle_r = 1$. So, for $\beta \to \infty$ the average over $v$ with $h = 0$
is the ground state of a harmonic oscillator with a wall in the origin. This problem is easily solved and one finds $q = \frac{5}{2} \alpha + O(\alpha^2)$ to be compared with $q_{cl} = \frac{2}{\pi} \alpha + O(\alpha^2)$.

Finally, the quantum dynamics depends on the temperature $T = 1/\beta$, and it reduces to the classical dynamics only when the de Broglie wavelength $\lambda_T = \frac{\hbar}{\sqrt{mT}}$ is much smaller than the typical linear size $\ell$ of the cage. However, as estimated by the classical calculation, $\ell \sim \sqrt{1 - q_{cl}} \sim \sqrt{2 - \alpha}$, so the quantum dynamics is effectively at zero temperature as soon as the energy gap to the first excited state becomes larger than the temperature, i.e. when $\frac{\hbar^2}{2m(1 - q_{cl})} \sim \frac{\hbar^2}{m(2 - \alpha)} > T$. For any $T, h, m$ as $\alpha \to 0$ one eventually enters a quantum critical regime, where quantum mechanics dominates the dynamics and defines, among other things, novel critical exponents.

The value of the critical exponent $\kappa$ regulating the relation $(1 - q) \sim (2 - \alpha)\kappa$ can be extracted by looking at the low-temperature, large-$\alpha$ data. As usual, a sufficiently large number of Trotter slices must be taken, and it increases as $\alpha \to 2$, so the calculations become more demanding. However, fortunately, the asymptotic region is reached already at $\alpha > 1$. The data in Fig. 2 clearly show that the critical exponent of the quantum theory is not the mean-field one, $\kappa_{cl} = 1$ (which is the value valid at $\sigma \geq 0$, while for $\sigma < 0$ one has $\kappa_{cl} = 1.41574\ldots$ [13]), and it departs more and more from it as the number of Trotter slices is increased. In Fig. 2 the data for variable number of Trotter slices $N$ are shown, together with the log-log fit to extract a critical exponent, in a region of $\alpha \in [1, 1.7]$. Extrapolating as $N \to \infty$, we get $\kappa = 2.0 \pm 0.1$.

That $\kappa > 1$ in the quantum case can be understood also from a simple variational calculation [39]. Using in the scaling region $\alpha \to 2$ the (uncontrolled) approximation $G^{-1}_n = \beta m(\omega_n^2 + \hbar^2/4m^2)/(1 - q)$, one is able to solve explicitly Eq. (5) when $\beta \to \infty$. Indeed, $\langle r_0 | r | r \rangle_v$ reduces to $\langle \psi_0^{(h)} | r | \psi_0^{(h)} \rangle$, $\psi_0^{(h)}$ being the ground state of a harmonic oscillator with infinite wall in $h$. Such wavefunction can be well approximated by a simple variational ansatz, or found numerically. In both cases we have observed that $\kappa = 3/2$. The value $\kappa \approx 2$ from the Montecarlo simulations presumably comes once the true behavior of $\Sigma(\omega)$ is considered.

The internal energy per degree of freedom $u$ (see [14]) is independent of $\beta$, like $q$, already at $\alpha \geq 1$, but it depends on the number of Trotter slices $N$. Extrapolating the data for $N \to \infty$ we obtain the result in Fig. 3, which show a divergence of the energy as $\alpha \to 2$. This is again interpreted in terms of reduced volume and uncertainty principle. In particular, we observe that $u \sim (1 - q)^{-1}$ with good accuracy for $\alpha \to 2$, in a region where the dependence on $\beta$ is lost.

At fixed temperature, we have just shown that the critical properties of the system are determined by the ground state, and the gap to the first excited state grows as $\Delta E \sim h^2/m(1 - q)$ for $\alpha \to 2$. If we focus on frequencies $\omega \ll \Delta E$, or times $t \gg 1/\Delta E$, there is no dynamics. In order to see some dynamical behavior one should scale $\omega \gtrsim \Delta E$ in $G(\omega)$. At these large frequencies the form of $\Sigma(\omega)$ changes significantly, as shown in Fig. 4. Indeed, at any $\alpha < 2$, the self-energy is an analytic function of $\omega^2$ in a neighborhood of the origin, $\omega = 0$. As $\alpha \to 2$ this behavior becomes extended to increasing values of $\omega$. Then, at larger frequencies, $\Sigma(\omega)$ develops a linear
part that is reminiscent of the semiclassical result \[14\]. Moreover, for any \( \alpha < 2 \), \( \lim_{\omega \to \infty} \Sigma(\omega) = 0 \), as can be seen from its definition.

Performing a log-log fit, we find that the constant contribution to the autocorrelation function scales as \( \beta \mu \sim (1 - q)\delta \) where \( \delta \approx -0.9 \). From a quadratic fit of \( \beta \Sigma(\omega) \) at small \( \omega \), we find that the coefficient of the quadratic term is instead almost independent of \( (1 - q) \), while the maximum of \( \Sigma \) is obtained for \( \omega \sim (1 - q)^{-1} \).

It is the behavior of \( \Sigma(\omega) \) which defines the effective dynamics of the theory. Moreover, the analytical properties of \( \Sigma(\omega) \) around the origin determine the low-temperature behavior of thermodynamic properties. Indeed, the analyticity of \( \Sigma(\omega) \) around \( \omega = 0 \) and the independence of \( \beta \) of all the observables, including the internal energy \( u \), show that the specific heat is non-analytic in \( T \), \( C_V(T) \sim e^{-\Delta/T} \) with \( \Delta \to \infty \) when \( \alpha \to 2 \). This is only apparently in contrast with the results of \[14\], where a semiclassical analysis gave \( C_V(T) \sim T \) at small \( T \) near the jamming point. In fact, the semiclassical analysis in \[14\] takes the limit \( \hbar \to 0 \) with \( \hbar/T \) kept fixed, while in our case we send \( T \to 0 \) keeping \( \hbar = 1 \). Different physical situations can fall in different regimes, deep quantum or semiclassical.

We have studied the quantum perceptron with hard-wall potentials in the RS ansatz as a model for jamming, at the jamming point. We have found that quantum mechanics dominates the dynamics sufficiently close to the critical point, irrespective of the temperature. The quantum critical point has critical exponents different from the classical, mean-field ones and an exponentially small \( C_V(T) \) for any finite \( \hbar \). The linear specific heat is recovered in a range of frequencies/temperatures which diverges at the critical point. A natural extension of this study is to soften the hard-wall potentials, having a finite \( \nu' \equiv \partial v/\partial r \big|_{r=0} \). We, of course, do expect the quantum jamming transition to go into a crossover (like the classical one does). The phenomenology outlined in this paper, including critical exponents, will however be observed until the energy \( u \sim \nu'\delta X \lesssim \nu'(1 - q)^{1/2} \). This means \( (1 - q) \lesssim (\nu')^{-2/5} \) or \( \alpha \lesssim 2 - c(\nu')^{-1/5} \). For \( \alpha \) closer to the transition than this value the effective dynamics changes and, as in the classical case, we expect the quantum jamming transition to be smoothened into a crossover. Finally, in the case of soft potentials it is possible to access the UNSAT phase and have insight into the physics of configurational glasses.

Once soft potentials are employed, it would also be interesting to move to the region \( \sigma < 0 \) and solve the self-consistent equations in the RSB framework. In this region, in fact, the allowed volume becomes clustered and quantum effects may play double role: For low disorder, tunneling may help the particle to explore many disconnected flat regions, and speed up the search of solutions (as it happens in the QREM model \[23\]–\[25\]); for high disorder Anderson Localization may take place, breaking ergodicity and changing significantly the classical phase diagram.

The interplay of these behaviors has implications for quantum machine learning algorithms based on continuous variables data, and for the theory of low-temperatures anomalies in configurational glasses.

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[35] This quantity, as it is written, is divergent, as discussed in [14], and in that paper it is shown how to properly regularize and renormalize it. In particular, the thermodynamic observables, like specific heat and order parameter, are divergence-free.

SUPPLEMENTARY MATERIAL
Derivation of the self-consistent equations

We need to compute the quenched disorder average of the free energy \( F = -β^{-1} \ln \text{Tr}(e^{-βH}) \), with \( H \) given by Eq. [1]. Introducing the imaginary time \( t \), the Lagrange multiplier \( λ \) associated to the constraint \( X^2 = N \) and \( n \) replicas, one can find \( F \) as a function of the overlap matrix

\[
Q_{ab}(t, s) = \frac{(X_a(t) \cdot X_b(s))}{N},
\]

where \( Q_{ab}(t, s) \) periodic in \( t \) and \( s \) with period \( β\hbar \) and \( a,b \) are replica indices. It reads, per dimension \( N \) and per replica \( n \):

\[
-βnf = \frac{1}{2} \ln \det \hat{Q}(t, s) + \frac{m}{2\hbar} \int_0^{β\hbar} dt \partial_s^2 Q_{aa}(t, s)|_{s=t} + \frac{m}{2\hbar} \int_0^{β\hbar} dt \partial_a \lambda_a(t)(Q_{aa}(t, t) - 1) + α \ln ζ, \tag{12}
\]

where

\[
ζ = \exp \left( \frac{1}{2} \sum_{a,b} \int_0^{β\hbar} dt ds \frac{β}{βh} Q_{ab}(t, s) \frac{δ^2}{δr_a(t) δr_b(s)} \right), \tag{13}
\]

The RS ansatz for the saddle point is:

\[
Q_{ab}^{\text{RS}}(t, s) ≡ \frac{R}{|qd(t-s)−q|d_αq + q} \tag{14}
\]

where \( q_d(t) \) is the autocorrelation function of a replica, while the off-diagonal order parameter \( q \) is the analog of the Edwards-Anderson order parameter: it is the overlap of two different replicas. As usual, one shall send \( n \to 0 \) after computing the quantities involving \( Q \).

We need to find the saddle point with respect to variations of \( Q \), namely of \( q_d(t) \) and \( q \). It is convenient to define

\[
G(t−s) ≡ q_d(t−s) − q. \tag{15}
\]

By considering the \( β\hbar \)-periodicity in imaginary time, we have as variables the countable set of Fourier components of \( G(t) \), i.e. \( \{G_n\}_{n∈Z} \), together with \( q \) and \( μ \equiv mλ \). The free energy is then the one displayed in Eq. [5], and the saddle-point equations are Eqs. [6], [7] and [8].

Exponent \( κ = 3/2 \) in the quadratic approximation

Setting \( G_n^{−1} = βm(ω_n^2 + h^2/4m^2)/(1 − q) \) as in the text, the spherical constraint, Eq. [7], is automatically satisfied up to exponentially small corrections, and the values of \( m \) and \( q \) can be fixed by Eqs. [6] and [8]. Note that there is an equation of the form [6] for every \( n ∈ Z \), yielding a deeply overcomplete set of constraints for our ansatz, but we restrict to the \( n = 0 \) case only.

It is convenient to set \( x ≡ r/\sqrt{1−q} \), \( H ≡ h/\sqrt{1−q} \), so that Eq. [8] becomes

\[
\frac{q}{(1−q)^{3/2}} = \alpha \int \frac{dH}{2\sqrt{πq}} e^{-\frac{(1−q)^2}{4q}} (ψ_0(H)|x|ψ_0(H))^2, \tag{16}
\]
where the reduced Schrödinger problem to solve is
\[ -\frac{1}{2} \frac{d^2}{dx^2} \psi_k^{(H)} + \frac{1}{8} x^2 \psi_k^{(H)} = E_k^{(H)} \psi_k^{(H)}, \quad \psi_k^{(H)}(H) = 0. \tag{17} \]

Self-consistently we will show that only the ground-state contribution matters (i.e. \( k = 0 \)). With this in mind we have employed the one-parameter variational wavefunction
\[ \psi^{(H)}(x; L) = \frac{1}{\sqrt{Z}} (x - H) \theta(x - H) e^{-x^2/4L^2}. \tag{18} \]

with an appropriate normalization \( Z \), for which the energy reads
\[ E^{(H)}(L) = \frac{1 + L^4 \phi(H/\sqrt{2}L)(H^2 + 3L^2) - 2HL}{8L^2} \frac{\phi(H/\sqrt{2}L)(H^2 + L^2) - 2HL}{\phi(H/\sqrt{2}L)(H^2 + L^2) - 2HL}, \tag{19} \]

where \( \phi(y) \equiv \sqrt{2\pi} e^{y^2} \text{Erfc}(y) \), and Erfc is the complementary error function. The equation \( dE^{(H)}(L)/dL = 0 \) can be solved separately in the regions \( H \gg L, \ |H/L| \ll 1 \) and \( H \ll L \) by using suitable expansions. Remembering that \( q \to 1 \) and therefore the range of \( H \sim \sqrt{q/(1-q)} \to \infty \) we see that the important region is \( H \gg 1 \), and self-consistently we obtain \( H/L \gg 1 \). Therefore we find \( \langle \psi_0^{(H)} | x^2 | \psi_0^{(H)} \rangle \simeq H + 3^{2/3}H^{-1/3} + O(H^{-5/3}) \) and by inserting it in Eq. (16) one arrives at
\[ q = \alpha \left[ (1 - q) \xi \left( \frac{q}{1 - q} \right) + \frac{q}{2} \right] \tag{20} \]

with
\[ \xi(\lambda) = \int_0^\infty \frac{dH}{\sqrt{2\pi} \lambda} e^{-H^2/2\lambda} \left[ \frac{(6H)^{2/3}}{2^{1/3}} + \cdots \right] \tag{21} \]
\[ = \frac{3^{2/3} \Gamma(5/6)}{\sqrt{2\pi} 2^{1/3} \lambda^{1/3}} + \cdots. \tag{22} \]

Eq. (20) can now be solved for \( q \), yielding \( \kappa = 3/2 \):
\[ q = 1 - \frac{\sqrt{2} \pi^{3/4} (2 - \alpha)^{3/2}}{24 \Gamma(5/6)^{3/2}}. \tag{23} \]

The same scaling has been observed by solving the Schrödinger equation (17) numerically, discretizing the \( x \)-axis and employing imaginary-time evolution to find the ground state.

Knowing \( q \) as a function of \( \alpha \), we can now solve the \( n = 0 \) case of Eq. (6) with the same technique. It reads
\[ m = \beta \gamma_{q/(1-q)} \star \langle \psi_0^{(H)} | x^2 | \psi_0^{(H)} \rangle \text{conn}. \tag{24} \]

By means of the same variational ansatz one finds that the connected average is \( 3^{1/3}H^{-2/3} \theta(H) + \cdots \) and finally
\[ m = \beta \frac{3^{1/3} \Gamma(1/6)}{2^{5/6}} \left( \frac{1 - q}{q} \right)^{1/3}. \tag{25} \]

Thus we see that, as \( q \to 1 \), \( \beta/m \to \infty \) and our approximation to take only the ground state becomes more and more reliable.