State-dependent forces in cold quantum gases

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of the degree of Doctor of Philosophy

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Chapter 8

Hidden variables for semiclassical models with state-dependent forces

Hidden variable theories [CITE, CITE] are interpretations of quantum mechanics which posit that there are definite states underlying quantum wavefunctions, such that quantum indeterminacy is an illusion—an emergent phenomenon rather than a fundamental fact. The Bell inequality [CITE] proves that any such theory must be *nonlocal* in order to explain all the predictions of quantum mechanics, and perhaps in light of this, most physicists surveyed [CITE] do not believe that hidden variables underlie physical reality.

However, by framing quantum systems in classical terms, hidden variable theories can provide an excellent computational tool for *approximate* models of quantum systems, when it is reasonable to approximate some degrees of freedom as classical, yet other degrees of freedom need to be modelled quantum mechanically. Just as hidden variable theories have framed the quantum world in terms that are agreeable to the classical view of the world in the minds of some interpreters of quantum mechanics, so can they bridge the gap between a *simulated* quantum world and a *simulated* classical world coexisting in the same computer simulation.

In this chapter I describe what I call the 'hidden variables semiclassical' method: a method of combining quantum simulations with classical simulations, with hidden variables bridging the gap between the classical and quantum degrees of freedom. I describe existing semiclassical methods and posit that they are already using hidden variables, but with a poor choice of hidden variable theory. Knowing this, we can choose a better hidden variable theory to make these models agree more closely with the underlying model they are approximating, and ultimately, with experiment.

8.1 Semiclassical models

A semiclassical model is any model in which some degrees of freedom are treated quantum mechanically, and others classically. The most common combination is that of treating an atom's internal electronic state quantum mechanically and its motional degree of freedom classically. This is useful whenever the quantum effects of the atom's motion are not of interest, for example if temperatures are high and thus atomic wavelengths are short—such that quantum effects simply aren't visible in the motion of the particles and so they can accurately be modelled as classical billiard balls. The energy gaps between different electronic states are so large however that only at very high temperatures (at which atoms ionise anyway) do they start to appear as a continuum compared to thermal energy scales, and the interaction of different spin states of the atom with different optical and magnetic fields does not make them appear as classical continua either. Thus, quantum effects can

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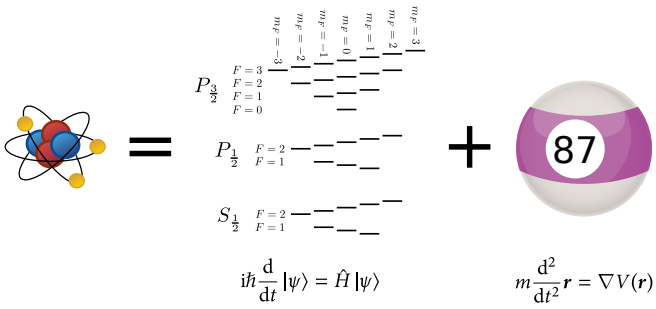

Figure 8.1: Artist's depiction of a semiclassical atom.

be ignored for centre of mass motion of the atom, but not for the relative motion of its electrons with respect to the nucleus, or for the nuclear and electronic spin degrees of freedom.

In this regime, atoms are often modelled semiclassically, with these internal degrees of freedom modelled using a state vector evolving according to a Hamiltonian via the Schrödinger equation, and the centre of mass motion modelled as a position $\boldsymbol{r}$ and velocity $\boldsymbol{v}$ evolving according to Newton's second law (Figure 8.1).

Once one has defined a potential function $V(\boldsymbol{r})$ and a Hamiltonian (also possibly varying with space) $H(\boldsymbol{r})$, and other possible additions[I], ones job is done and the rest can be left to numerical differential equation solvers to evolve some concrete vector representation $\boldsymbol{\psi}$ of $|\psi\rangle$ as well as the state variables for motional degree of freedom $\boldsymbol{r}$ and $\boldsymbol{v}$ in time.

[I] Such using a Monte-Carlo wave-function method [CITE, SE-CREF?] to model the effect of spontaneous emission on $|\psi\rangle$, and modifying $\boldsymbol{v}$ instantaneously by a random-direction recoil velocity upon each photon emission

8.2 The problem: Stern–Gerlach separation and evaporative cooling

In the Stern–Gerlach experiment [CITE], particles with quantum spin and a magnetic moment, atoms for example, are fired as a beam through a region of space with a magnetic field gradient. The well known result is that two clusters of positions (if the atoms are spin $\frac{1}{2}$) are observed once the beam emerges, rather than a continuous smear of positions, indicating that angular momentum—like many quantities in quantum mechanics—is quantised.

One can go further and intentionally spin-polarise the particles before they are passed through the magnetic field gradient, say putting them in an eigenstate of the $\hat{F}_x$ operator. Then, if the magnetic field is along the z direction, and the gradient is also in the z direction, then two clusters of positions are also observed, even though all particles were in the same state when they entered the region in which there was a magnetic field gradient. This is a display of the indeterminacy of quantum mechanics: even though all particles had the same initial state, there were nonetheless different outcomes for each particle.

The Stern–Gerlach effect is a consequence of quantum mechanics, to be sure, but it has little to do with the wave nature of the atoms. If we introduced some double slits for the atoms to pass through in addition to the magnetic field gradient, then we would be seeing the wave nature of the atoms as interference patterns at the detection screen at the end of the experiment. But if we do not, and if the particles have short de-Broglie wavelengths, then quantum mechanics is not apparent in the motion of the particles through space—except via the influence of spin on seemingly choosing one trajectory or the other. How are we to model this effect quantum mechanically?

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A similar situation exists in RF evaporative cooling (Section **??**) of cold atoms en-route to BEC. Atoms are trapped in a magnetic trap, and are spin polarised so as to be fully spin down (for ^{87}Rb this is the trapped state) with respect to the local magnetic field at the position of each atom. The magnetic field's direction—not just its magnitude—varies in space, and so different atoms have different spins, but they are all spin down with respect to the quantisation axis of the local magnetic field.[2]. As the atoms move through space, they move in orbits—punctuated by collisions—about the magnetic field zero at the centre of the trap, since they feel a force $F \propto -\nabla|\boldsymbol{B}|$ due to the gradient of the Zeeman potential. Provided they are moving slowly (specifically, provided their Larmor precession period is short compared to the time the magnetic field as seen by the atom takes to change by a non-negligible fraction of its current value), the atoms' spins adiabatically follow the local field and remain spin-down, even as the field as seen by each atom fully reverses its direction every half orbital period.

[2] Out of habit we are already speaking semiclassically—to talk about the atoms' position is to assume they have one—and yet we're describing their spin quantum mechanically

Near the centre of the trap where the atoms are moving faster, the fields are small and therefore have large fractional derivatives and lead to large Larmor periods, adiabaticity no longer holds and the atoms may make spin transitions with respect to their local magnetic field.

TODO:

- Define/describe what a hidden variable theory is, drawing heavily on Aaronson's [**?**] explanations. Give examples, argue why the Schrodinger theory is appealing.
- Motivate with Stern-Gerlach experiment, and derive the method, show what sorts of problems it solves and where it disagrees with other models, provide simulation results. Limitations: no time dependent potentials, no 3D.
- Possibly include speculation about these:
- Maybe include a test to see whether it actually does work in 3D as-is, since we haven't actually checked, we just haven't been able to show on paper that current behavior is correct in 3D (also haven't shown it's incorrect).
- Time dependent potentials could potentially be handled by approximating unitary as product of part due to spatial variation in H, and part due to time variation in H. compute transition probs for both such that a transition can be attributed to one or the other - only do velocity jumps to conserve potential if due to spatial motion, as time dependent potential can exchange energy with particle.
- Matrix scaling for Schrodinger theory, discuss methods: Sinkhorn-Knopp, Lineal, and my one. Compare time complexity of algorithms so as to define the computational complexity of the hidden variables semiclassical method. Method is of course parallelisable on GPU or similar so is fast on parallel machines even if matrix scaling is slow.
- Discuss how it would make sense for the systems to behave in the presence of collisions w.r.t collapse of state vectors.
- Be sure to include picture from KOALA talk of atoms going in multiple directions

8.3 Approximate Markovian decoherence rate for separating wavepackets

Positional separation of two different internal states of an atom leads to decoherence of those states, with a decoherence factor $r_{ij}(t)$ equal to the overlap of the spatial wavefunctions of the two components in question a time t after they began separating. Approximating both wavepackets as initially overlapping Gaussians of width σ, ignoring dispersion,

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and assuming they separate with constant relative acceleration a_{ij}, the decoherence factor is

$$r_{ij}(t) = \langle \psi_i(t) | \psi_j(t) \rangle \tag{8.1}$$

$$= C \int_{-\infty}^{\infty} e^{-\frac{x^2}{4\sigma^2}} e^{-\frac{(x-x_{\text{rel}})^2}{4\sigma^2} + ik_{\text{rel}}x} \, \mathrm{d}x, \tag{8.2}$$

where

$$x_{\text{rel}}(t) = \frac{1}{2} a_{ij} t^2 \tag{8.3}$$

and

$$k_{\text{rel}}(t) = \frac{m}{\hbar} a_{ij} t \tag{8.4}$$

are the wavepackets' relative[3] position and wavenumber due to acceleration for a time t starting from zero relative velocity, and

$$C^{-1} = \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma^2}} \, \mathrm{d}x \tag{8.5}$$

is a normalisation constant [TODO CHECK IF NEEDS TO BE SQUARED]. Note that this expression holds for any number of dimensions—relative motion is only along one axis so the integrals in all other directions equal one.

Evaluating the Gaussian integral (8.2) gives the following expression for the decoherence factor $r_{ij}(t)$:

$$r_{ij}(t) = e^{-\left[\frac{1}{8\sigma^2} x_{\text{rel}}^2 + \frac{i}{2} x_{\text{rel}} k_{\text{rel}} + \frac{\sigma^2}{2} k_{\text{rel}}^2\right]}. \tag{8.6}$$

This is a decoherence *factor*; it is the factor by which the (i, j) off-diagonal of the reduced density matrix for the atom's internal state will be reduced at time t. The corresponding decoherence *rate* is given by the logarithmic derivative of (8.6):

$$\Gamma_{ij}(t) = -\frac{1}{r_{ij}(t)} \frac{\mathrm{d}}{\mathrm{d}t} r_{ij}(t). \tag{8.7}$$

The fact that (8.6) does not describe a constant decoherence rate (i.e., it does not have the functional form of exponential decay) means that the back-action on the atom's internal state caused by measurements of its motional state will be different depending on the interval of time between measurements.

For example, the logarithmic derivative of (8.6) approaches zero as t goes to zero. This means that in the limit of infinitely frequent measurements, no decoherence occurs at all in between measurements, and the motional state is reset after each measurement such that the wavepackets never separate at all. This is the quantum Zeno effect, and its appearance in models of open quantum systems is usually treated as a reminder that the assumption of infinitely frequent strong measurements is unphysical [CITE].

Since experimentally we are not measuring atoms' motional states so frequently, we ought to wait until the wavepackets are completely separated before performing a projective measurement. As in quantum optics models of open quantum systems, in which the measurement interval "should be large enough to allow the photons to get away from the atom" [CITE The Quantum Jump Approach and Quantum Trajectories

[3] a_{ij}, x_{rel} and k_{rel} are the acceleration, position, and wavenumber of the j^{th} component with respect to the i^{th} component, that is, $a_{ij} = a_j - a_i$, etc.

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Gerhard C. Hegerfeldt], ours should be large enough for the atomic states to get away from each other.

If at large enough times, a decoherence rate is independent of time, that decoherence is called Markovian at that timescale. A Markovian environment is one that has no memory of the decoherence process—it "forgets" any information caused by past interaction with the system. Even though at short times, all decoherence rates in quantum mechanics tend to zero [CITE], if they become Markovian on a timescale shorter than other timescales of interest, the Markov approximation can be used and a constant decoherence rate used at all times. In quantum optics, the decoherence factor for the internal state of an atom due to photon emission indeed tends to exponential decay on timescales that are still much shorter than that of the system evolution, and thus the Markov approximation is accurate.

Unlike quantum optics models, our decoherence factor does not describe Markovian decoherence on any timescale. In the limit of large t, its functional form is e^{-t^4}, not the exponential decay required to treat the decoherence as Markovian [CITE] at that timescale. Nonetheless, if we wish to write a time-local differential equation for the internal state of the atom, Markovian decoherence is the only kind we can include [CITE].

To that end, we will now construct a "time ignorant" version of $r_{ij}(t)$ that answers the question "What is the expected decoherence factor at all future times, if you don't know how long it has been since the two wavepackets began separating?" In this way we can compute an *average* decoherence rate Γ_{ij} described by our decoherence factor, even though $r_{ij}(t)$ does not have a constant decoherence rate at large times. This essentially amounts to finding the best fitting exponential to $r_{ij}(t)$. Whilst this approximation is crude, it is nonetheless an improvement over the Ehrenfest model, which has no decoherence at all (i.e. it has a decoherence rate that is also constant like ours—but equal to zero).

We define the time-ignorant decoherence factor $\tilde{r}_{ij}(t)$ as the overlap of the wavefunction of the i^{th} internal state with a superposition of wavepackets of the j^{th} internal state, with the superposition being over all times in the past the wavepackets began separating:

$$\tilde{r}_{ij}(t) = \langle\psi_i(t)| A \int_{-\infty}^{0} |\psi_j(t-t')\rangle \, \mathrm{d}t', \tag{8.8}$$

where A is a normalisation constant such that $\tilde{r}_{ij}(0) = 1$. Since $|\psi_i(t)\rangle$ is time independent (rather, since we can perform our calculations in the frame of reference in which it is stationary), this is:

$$\tilde{r}_{ij}(t) = A \int_{-\infty}^{0} r_{ij}(t-t') \, \mathrm{d}t', \tag{8.9}$$

which is simply the convolution of our decoherence factor with a step function which is nonzero at all negative times. Our average decoherence rate Γ_{ij} is then given by the logarithmic derivative of $\tilde{r}_{ij}(t)$ at $t = 0$:

$$\Gamma_{ij} = -\frac{\tilde{r}'_{ij}(0)}{\tilde{r}_{ij}(0)} \tag{8.10}$$

$$= -\frac{\int_0^\infty \tilde{r}'_{ij}(t) \, \mathrm{d}t}{\int_0^\infty \tilde{r}_{ij}(t) \, \mathrm{d}t} \tag{8.11}$$

$$\Rightarrow \Gamma_{ij}^{-1} = \int_0^\infty e^{-\left[\frac{1}{8\sigma^2} x_{\text{rel}}^2 + \frac{i}{2} x_{\text{rel}} k_{\text{rel}} + \frac{\sigma^2}{2} k_{\text{rel}}^2\right]} \mathrm{d}t. \tag{8.12}$$

As mentioned, Γ_{ij} is the decay constant for the best fitting exponential to our decoherence factor (8.6). Although (8.6) looks nothing like a decaying exponential in time, an

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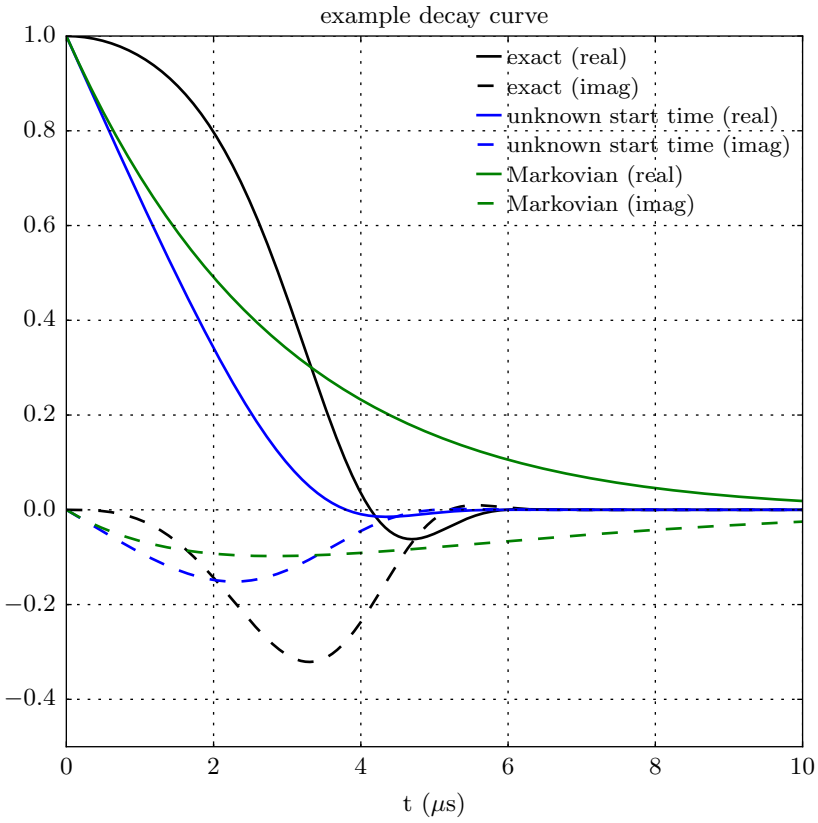

Figure 8.2: Caption.

exponential approximation to it nonetheless ought to decay to zero on the same timescale. An example of this is shown in Figure 8.2

In order to obtain an approximate analytic expression for this integral, we consider two limiting cases and then stitch them together in the intermediate regime. In the limit of small wavepackets, σ is small and thus the first term in the exponent in (8.12) is largest, and the third term is smallest. In this regime, which describes when positional separation (as opposed to separation in k-space) dominates the decoherence, we'll neglect the third term in the exponent and treat the second term as small relative to the first. This gives us:

$$\Gamma_{ij\,(\mathrm{pos})}^{-1} \approx \int_0^\infty e^{-\left[\frac{1}{8\sigma^2}x_{\mathrm{rel}}^2 + \frac{i}{2}x_{\mathrm{rel}}k_{\mathrm{rel}}\right]}\,\mathrm{d}t. \tag{8.13}$$

$$\approx \int_0^\infty e^{-\frac{1}{8\sigma^2}x_{\mathrm{rel}}^2}\left(1 - \frac{i}{2}x_{\mathrm{rel}}k_{\mathrm{rel}}\right)\,\mathrm{d}t. \tag{8.14}$$

$$= 2^{\frac{5}{4}}\Gamma(\tfrac{5}{4})\sqrt{\frac{\sigma}{a_{ij}}} - 2i\frac{m\sigma^2}{\hbar}, \tag{8.15}$$

where we used a first-order Taylor expansion of an exponential in (8.14). We similarly use a first order expansion to take the reciprocal of (8.15) (since the second term is much smaller than the first[4]), and arrive at:

$$\Gamma_{ij\,(\mathrm{pos})} \approx \frac{1}{2^{\frac{5}{4}}\Gamma(\frac{5}{4})}\sqrt{\frac{a_{ij}}{\sigma}} + \frac{i}{2\sqrt{2}\Gamma(\frac{5}{4})^2}\frac{m\sigma a_{ij}}{\hbar} \tag{8.16}$$

[4] This isn't necessary in order to obtain a simple expression for $\Gamma_{ij\,(\mathrm{pos})}$—the reciprocal without this approximation is equally simple—but it leaves us with power laws for the real and imaginary parts of $\Gamma_{ij\,(\mathrm{pos})}$, which are easier to stitch together with those from the large σ regime.

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Similarly for the large σ regime, we neglect the first term in the exponent of (8.12) and consider the second term small relative to the third. This is the regime in which the decrease in overlap of the two wavepackets is dominated by their separation in velocity space. Following the same process as above gives:

$$\Gamma^{-1}_{ij\,(\mathrm{vel})} \approx \int_0^\infty e^{-\left[\frac{i}{2}x_{\mathrm{rel}}k_{\mathrm{rel}}+\frac{\sigma^2}{2}k^2_{\mathrm{rel}}\right]}\,\mathrm{d}t. \tag{8.17}$$

$$\approx \int_0^\infty \left(1-\frac{i}{2}x_{\mathrm{rel}}k_{\mathrm{rel}}\right)e^{-\frac{\sigma^2}{2}k^2_{\mathrm{rel}}}\,\mathrm{d}t \tag{8.18}$$

$$= \sqrt{\frac{\pi}{2}}\frac{\hbar}{m\sigma a_{ij}} - i\frac{\hbar^3}{2m^3\sigma^4 a_{ij}^2} \tag{8.19}$$

$$\Rightarrow \Gamma_{ij\,(\mathrm{vel})} \approx \sqrt{\frac{2}{\pi}}\frac{m\sigma a_{ij}}{\hbar} + \frac{i}{\pi}\frac{\hbar}{m\sigma^2} \tag{8.20}$$

Equations (8.16) and (8.20) are our final expressions for the docoherence rate in the limit of small and large wavepackets respectively. Adding their real parts in quadrature and adding the reciprocals of their imaginary parts then provides a reasonable approximation for Γ_{ij} over all wavepacket sizes:

$$\Gamma_{ij} \approx \left[\mathrm{Re}(\Gamma_{ij\,(\mathrm{pos})})^2 + \mathrm{Re}(\Gamma_{ij\,(\mathrm{vel})})^2\right]^{\frac{1}{2}} + i\left[\mathrm{Im}(\Gamma_{ij\,(\mathrm{pos})})^{-1} + \mathrm{Im}(\Gamma_{ij\,(\mathrm{vel})})^{-1}\right]^{-1}. \tag{8.21}$$

We now have an approximate analytic expression that is computationally inexpensive to evaluate for each atom in an ensemble at every timestep of a differential equation. An example showing the accuracy of (8.21), compared to the exact expression (8.12) for Γ_{ij} over a range of wavepacket sizes is shown in Figure 8.3.

8.4 Choice of wavepacket size

How big is a wavepacket?

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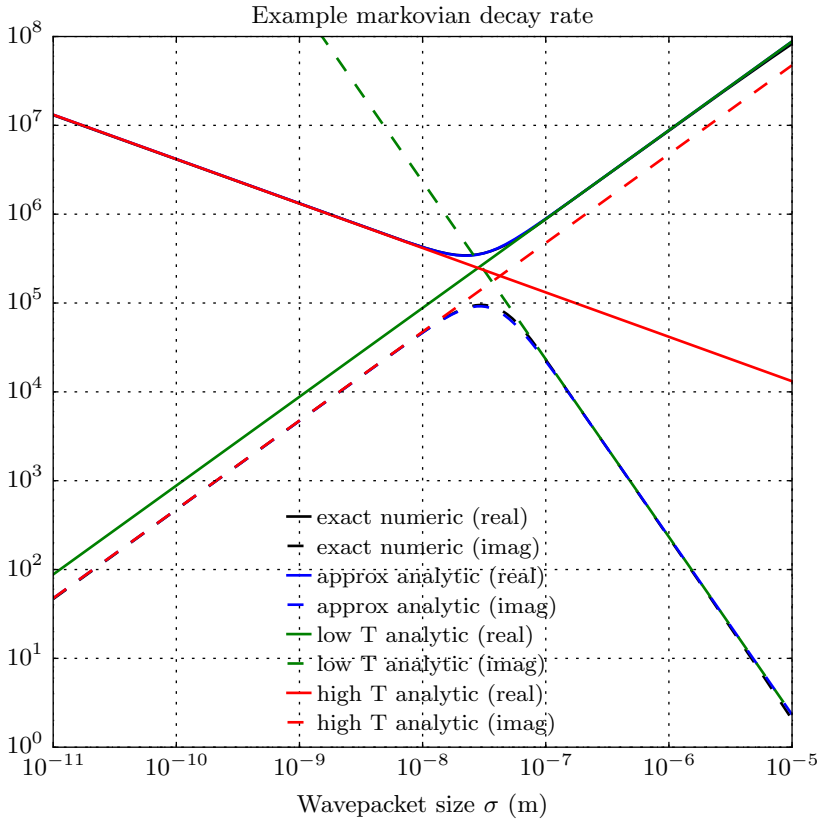

Figure 8.3: Caption.

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Words outside text (captions, etc.): 6094
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