Failure of Effective Potential Approach: Nucleus-Electron Entanglement in the \( \text{He}^+ \)-Ion.

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Entanglement may be considered a resource for quantum
terrestial, information processing, as the origin of robust and universal
equilibrium behaviour, but also as a limit to the validity of an
effective potential approach, in which the influence of certain
interacting subsystems is treated as a potential. Here we show
that a closed three particle (two protons, one electron) model
of a \( \text{He}^+ \)-ion featuring realistic size, interactions and energy
scales of electron and nucleus, respectively, exhibits different
types of dynamics depending on the initial state: For some
cases the traditional approach, in which the nucleus only ap-
ppears as the center of a Coulomb potential, is valid, in others
this approach fails due to entanglement arising on a short
time-scale. Eventually the system can even show signatures
of thermodynamical behaviour, i.e. the electron may relax
to a maximum local entropy state which is, to some extent,
independent of the details of the initial state.

During the last decades entanglement has attracted
considerable interest in a lot of fields of quantum me-
chanical research. In the beginning, after the publication
of the famous EPR-paradox [1], it was mostly considered
a philosophical puzzle, challenging the basic principles of
quantum physics itself.

Later on, methods to deliberately produce and detect
entanglement were developed, originally in the field of
quantum optics [2,3].
After that, the idea of exploiting entanglement in a tech-
nical sense became popular and a number of so-called
quantum algorithms have been suggested, that could out-
perform corresponding classical algorithms [4–6]. Those
algorithms require the controlled manipulation of many
entangled subsystems. Although there is presently much
research directed towards those ends, no large scale quan-
tum computers are in sight so far; obviously, the engi-
neering of entanglement is a very hard problem [7].

Probably because entanglement is so difficult to control
and its consequences may seem puzzling, it has rarely
been discussed in the context of “effective potentials”.
However, taking a closer look one has to admit that there
are very few true “single system” scenarios. Even the
historical double slit or the famous “particle-in-a-box”
problem are, in fact, compound systems, if one starts
from first principles, for the wall with the slits or the box
are systems consisting of many particles themselves, that
should be described by wavefunctions. Almost all po-
tentials (even so-called “classical” ones, underlying, e.g.,
mesoscopic or microscopic structure models) are due to
interacting subsystems. So, the question arises, why the
standard effective potential approach seems to be succes-
ful in so many cases, despite entanglement being fairly
generic, whenever systems interact [8,9].

On the other hand, this generic nature, together with
the fact that entanglement leads to increased entropy for
the entangled subsystems, has even led to the idea that
entanglement with the surrounding could be responsible
also for the validity of the second law for thermodynam-
ical systems [10]. It is, therefore, tempting to look for
possible transitions between thermodynamic and micro-
scopic behaviour, i.e. between macro- and micro-control
[16].

For this purpose we are going to study a closed bi-partite
quantum system hierarchically grouped into a tightly
bound pair, which approximately generates an effective
potential for the third, weakly bound particle. Thus we
want to present here a concrete example for a system
showing entanglement for certain initial states, after the
classical effective potential has been replaced by a sub-
system with internal degrees of freedom. This example is
the \( \text{He}^+ \)-ion and the subsystem the nucleus itself. This
object has been chosen for two reasons: Firstly, one can
come up with a fairly simple model, which does not re-
quire complicated numerical analysis, and is nevertheless
reasonably close to reality. Secondly, the nuclear and
electronic excitations represent so different energy scales
that entanglement appears to be beyond reasonable ex-
pectation. While this is, indeed, correct from an experi-
mental point of view, it may, nevertheless, come as a
surprise that mathematically “typical” initial states will,
indeed, lead to entanglement.

The \( \text{He}^+ \)-ion consists, on the level of nucleons and elec-
trons, of five particles. Since the neutrons do not feel the
Coulomb force they are neglected here. The remaining
three particles, which are relevant for our model are de-
scribed by the following Jacobi-coordinates as sketched in
Fig.1:

\begin{align}
\vec{x}_c &= \vec{S} + \frac{2M}{2M+m} \vec{R} \\
\vec{x}_{p_1} &= \vec{S} - \frac{m}{2M+m} \vec{R} + \frac{1}{2} \vec{K} \\
\vec{x}_{p_2} &= \vec{S} - \frac{m}{2M+m} \vec{R} - \frac{1}{2} \vec{K}.
\end{align}
Here $M$ is the proton-mass and $m$ the electron-mass. These coordinates are chosen to decouple the center of mass degree of freedom from the others. The Hamiltonian reads:

$$\hat{H} = -\frac{\hbar^2}{2(2M+m)} \nabla^2 \vec{R} - \frac{\hbar^2}{M} \nabla^2 \vec{K} + V(\vec{K}) - \frac{\hbar^2(2M+m)}{4Mm} \nabla^2 \vec{r} - \alpha \frac{\hbar c}{\vec{R}} \left( \frac{1}{|\vec{R} - \frac{1}{2}\vec{K}|} + 1 \right) \left( \frac{1}{|\vec{R} + \frac{1}{2}\vec{K}|} \right) \tag{2}$$

where $\alpha$ is the fine structure constant and $V(\vec{K})$ describing the internuclear force is chosen to be:

$$V(\vec{K}) := \begin{cases} 0 & : |\vec{K}| \leq 2r_0 \\ \infty & : |\vec{K}| > 2r_0 \end{cases}, \tag{3}$$

with $r_0 \approx 2 \cdot 10^{-15} m$ [11] taken as the radius of alpha-particles obtained from scattering experiments. After the center of mass degree of freedom has been separated, there is, obviously, no way of decoupling the Hamiltonian in terms of $\vec{R}$ and $\vec{K}$ by means of any further transformation (non-separability).

In a classical analysis one would always argue that $|\vec{K}| \ll |\vec{R}|$ and therefore expand the last part of the Hamiltonian neglecting all higher order terms and thus decouple the Hamiltonian completely. We will eventually do something similar, but boldly applying the same argument in quantum mechanics would miss the crucial point, as will be seen below.

The idea now is to analyze this model using perturbation theory. Therefore we have to divide the Hamiltonian into a main ($\hat{H}_0$) and a perturbative ($\hat{H}_1$) part. Simply taking the last term in (2) as the perturbation would definitely not be good enough, for the electron would be free according to $\hat{H}_0$, and one could not expect the perturbation series to converge. It seems more promising to introduce an effective potential, which models the mean effect of the nucleus on the electron in $\hat{H}_0$, and take the deviation of the “real” interaction from this effective potential as the perturbation. Following these ideas and putting aside the center of mass degree of freedom, we get:

$$\hat{H}_0 = -\frac{\hbar^2}{M} \nabla^2 \vec{K} + V(\vec{K}) - \frac{\hbar^2(2M+m)}{4Mm} \nabla^2 \vec{r} - \frac{2\alpha \hbar c}{\vec{R}}$$

$$\hat{H}_1 = -\alpha \frac{\hbar c}{\vec{R}} \left( \frac{1}{|\vec{R} - \frac{1}{2}\vec{K}|} + 1 \right) \left( \frac{1}{|\vec{R} + \frac{1}{2}\vec{K}|} \right) - \frac{2}{\vec{R}} \tag{4}$$

Obviously, the full Hamiltonian has not changed, but $\hat{H}_0$ describes now two decoupled systems, the nucleus, $c$, and the electron, $e$, like it is usually treated, bound by a potential that would arise if the nucleus was a pointlike object without any substructure. Taking into account that the ratio of the radius of the nucleus to a typical distance of the electron from the nucleus (say, the Bohr radius) is smaller than $10^{-4}$ [11,12] one would expect that $\hat{H}_0$ should already give a pretty good picture of the real system, so that the effect of $\hat{H}_1$ should be comparatively small. To verify this, one needs to calculate the perturbation matrix. This analysis, which is straightforward, but too long to be presented here, shows, that all its entries are much smaller than the corresponding energy differences of the electron system (roughly by a factor of $10^{-10}$) and that it is almost diagonal within the degenerate eigenspaces of $\hat{H}_0$. This means that the (product)energy eigenstates of the unperturbed problem remain practically unchanged, what matters are the corrections to the energy eigenvalues, induced by the effective coupling.

For states with vanishing orbital angular momentum of the electron system as well as of the nucleus system, those corrections can be calculated analytically to first order:

$$E_{nN}^1 = \frac{\alpha \hbar c^2}{6 \alpha n^3} \left( 1 - \frac{1}{2\pi^2 N^2} \right) \tag{5}$$

Here, $a$ is the Bohr radius, $n$ is the principal quantum number of the electron, $N$ that of the nucleus. These corrections are at most on the order of $10^{-10}$eV which is extremely small compared to the energy-scale of the uncoupled system. Nevertheless, they are nonadditive (which could not happen if the perturbation was local) and can, though being very small, cause entanglement. Entanglement measures for general multi-partite systems are still under dispute [13]. However, if the state of the whole system is a pure state, and the full system is being regarded as divided into two subsystems, a convenient entanglement measure is $1 - P_e$, with

$$P_e(t) = Tr \left\{ \hat{\rho}_e(t) \right\} = Tr_e \left\{ \left( Tr_c \left\{ |\psi(t)\rangle \langle \psi(t)| \right\} \right)^2 \right\} \tag{6}$$

where $\hat{\rho}_e$ is the reduced density operator of subsystem $e$ and $|\psi(t)\rangle$ is the wave function of the total system. Under these conditions this quantity yields the same value, no matter for which subsystem it is calculated, i. e.,

$$P_e = P_e =: P.$$ 

$P$ is called the purity since it takes on its maximum value 1 if the subsystem is in a pure state. Furthermore, $P$ can be used as a criteria for a subsystem to act as an effective potential for the other subsystem: $P$ would have to be 1 for all times. The more $P$ deviates from 1 the larger is the error that would occur if a Hartree-type description was used to calculate the evolution.

The Figs. 2-3 display the time evolution of the purity $P(t)$ for some specific initial product states of vanishing orbital angular momentum. In the following the numbers in the “ket” symbols give the principal quantum numbers of the electron ($n$) and the nucleus ($N$). The purity-evolution we find for the initial state $|\psi(0)\rangle = \frac{1}{\sqrt{2}} (|1\rangle + |2\rangle)^e \otimes (|1\rangle + |2\rangle)^n$ is displayed in Fig.2. Obviously, considerable entanglement is being built up on the $10^{-5}$ second timescale! The fact that the mean distance between the particles making up the nucleus is much
smaller than the mean distance of the electron from the nucleus does not mean that the nucleus may necessarily be treated as an effective potential. What really matters is whether or not the electron “feels” the different potentials the nucleus creates in its different energy eigenstates. And, obviously, already a slight difference destroys local coherence quite rapidly. Since the energy-transfer from the electron to the nucleus (or vice versa) can be neglected in this model, the dynamics are effectively restricted to the space of the four states occupied in the initial state. Within this effective two-level-two-system-subspace a maximum entangled state, an EPR-state, is implemented at the minima of the purity.

In the initial state $|\psi(0)\rangle = \frac{1}{2}(|1\rangle + |2\rangle)^c \otimes (|14\rangle + |15\rangle)^e$ the electron system is now in a superposition of states with higher principal quantum numbers (14,15 instead of 1,2) which reduces the probability to find the electron in the direct vicinity of the nucleus drastically. This difference shows in the purity-evolution: In principle it looks the same as the one in Fig.2, but instead of a timescale of $10^{-5}$ s, the purity reaches now values that differ significantly from $P = 1$ on a timescale of $10^{19}$ s (about the age of the universe!). Hence for all practical purposes an effective potential approach will yield excellent results in this case.

Yet a different situation arises if the initial state consists of superpositions of somewhat more than two energy eigenstates. Fig.3 shows the purity-evolution of the initial state $|\psi(0)\rangle = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} |n\rangle^c \otimes (|1\rangle + |2\rangle)^e$. In this case, the purity no longer oscillates but decays on an intermediate time-scale of 1 sec. to reach a final value of $\bar{P} \approx 0.19$. Note that this behaviour occurs even though the dynamics of the whole system is perfectly unitary. It is also “universal” in the sense that it appears independently of the phases of the amplitudes of the initial state. Since small purity values correspond to large von Neumann entropies, this behaviour is very much like the thermodynamical limit ($d \gg 1$). Nevertheless, the model clearly shows signatures of thermodynamical (statistical) behaviour for a large class of initial states. These features would become more and more significant as more and more energy eigenstates were superimposed in the initial state.

Thus, as already found by R. Jensen and R. Shankar [14], it is not necessary for a system to have many classical degrees of freedom in order to exhibit statistical behaviour. What does seem to be necessary is the coupling of the system to another system, such that a sizable part of the Hilbert space of the coupled system is accessible, even though the coupling might be weak and without energy-exchange.

A class of initial states for which practically no entanglement will ever arise is the set of product states without any superposition of energy-eigenstates in the nucleus. Although this class might not be large from a theoretical point of view, it contains the most common states realizable in the laboratory, namely the case of the nucleus being in the ground state. Since excitations of the nucleus are usually in the MeV regime, the nucleus will decay into the ground state due to the coupling to the electromagnetic field, on a timescale much shorter than the one on which entanglement arises. This coupling is completely absent in our present model. It would thus be extremely difficult to detect the predicted behaviour directly, even if one was able to put the nucleus into the required superposition.

Alternatively, one might look for spectroscopic features resulting from the energy-corrections given by eq.(5). To enhance the effect under consideration larger nuclei or muonic atoms might be of help. Of course, other three-particle models could be selected for much easier experimental access [17] but also for less “surprise”. Basically, though, our model represents a Gedanken-experiment, designed to show that entanglement can indeed appear “almost everywhere”.

In conclusion, we have shown, based on a hierarchical bi-partite quantum network, that there is a time period for which, starting from locally pure states, the effective potential approach works for all practical purposes. The length of this period depends sensitively on the initial state and might very well approach infinity for typical states accessible to experimentation. But there are also initial states for which this period is short enough for the entanglement to built up on a relevant timescale. For some initial states this entanglement will even lead to locally irreversible equilibrium behaviour, controlled by thermodynamical laws. Thus the standard Schrödinger equation can lead to both, unitary microscopic and ther-
modynamic behaviour, depending on the experimental setup.

Our findings thus question a rather common view for modelling quantum systems: That there are effective potentials for (quantum-) control and, independently, a bath to account for decoherence. Though the latter may, indeed, be present, typically, those two functions cannot be separated, control itself already implies “de-control”: If even a nucleus can cause decoherence with respect to an electron, then hardly anything needs to be save in this respect! We thank A. Otte, I. Kim, F. Tonner M. Stollsteimer, T. Wahl, T. Haury, M. Michel, P. Borowski and H. Schmidt for fruitful discussions. Financial support by the Deutsche Forschungsgemeinschaft is gratefully acknowledged.

![FIG. 1. Coordinates of the model: \( \vec{S} \) denotes the center-of-mass of the total system. Note: \(| \vec{K} | : | \vec{R} | \approx 10^{-4}\)](image)

![FIG. 2. Oscillating purity. Initial product state containing the two lowest subsystem-states each, see text.](image)

![FIG. 3. Decaying purity. Initial product state containing the ten lowest subsystem-states each, see text.](image)

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