Mott Problem: Formulation, Interpretation, and Implications

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September 14, 2012

0.1 Introduction

The Mott Problem was first set out in a 1929 paper by Sir Neville Mott [3], and is still highly relevant to modern interpretations of quantum mechanics. The problem was originally formulated in terms of a radioactive nucleus in a Wilson cloud chamber. The radioactive decay process is represented as an α particle slowly leaking out of the nucleus, where the α wavefunction is spherical. Experimentally we observe that the α produces a straight track of ionized atoms in the cloud chamber. So: how does a spherical wavefunction lead to a straight track?

Mott's original paper focuses on a couple particular aspects of the issue: namely, what exactly constitutes the quantum system under consideration, and when exactly is an observation made? The paper then proceeds to go through how the wave mechanics actually do predict the emergence of a linear track, in a "shut-up-and-calculate" spirit. Various subsequent papers by various authors set out extensions to the original problem, and use such extensions to probe other questions in quantum foundations.

Some key issues we can probe via the Mott Problem and its extensions:

- **Emergence of classical trajectories, which are radial.** The problem is much more general than a radioactive atom in such a chamber. It's great to work out (as in Mott's original paper) the details of the α+gas system, but we could just as easily have an [other s-wave particle]+[other particle detector]+[other surrounding environment] system where radial trajectories would still be found.

- **QM $\rightarrow$ classical statmech.** In general, what's going on at this limit?

- **Emergence of time, causality, and the choice of only outgoing solutions.** We have a timeless formalism:

$$H\psi(x) = \omega\psi(x)$$

$$H = \frac{-1}{2Mr^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{L^2}{2Mr^2} + W(r)$$

  And yet, time is clearly necessary to describe classical radial motion. Is time something we have to just "add in" by hand, or is time somehow emergent? Furthermore, how does time end up with an "arrow", with only outgoing particle solutions (not incoming particle solutions) being "chosen"?

- **What constitutes a measurement, and what constitutes a measuring apparatus.** It's obvious that the ionization of an atom constitutes a measurement, but what about the failure of an atom to be ionized? In general, what if a null result provides some new knowledge that affects the probability distribution corresponding to an observable of the particle? (This would seem to imply a change to the particle's wavefunction, without any apparent interaction.)

This talk will examine how all of these questions can be addressed – some in the original Mott formulation, and some in view of key modern concepts in quantum foundations. The resulting discussions enter a wide range of fields, from statistical mechanics to quantum cosmology.

0.2 Original Formulation

- Naive intuition: because of the spherical wavefunction, the α should ionize atoms in a spherically symmetric random distribution throughout the space of the cloud chamber. Clearly wrong... but why?

- Naive explanation: the spherical wavefunction is just for predicting the probability of disintegration; the α has wave-like properties only while it is still in the nucleus. As soon as the particle leaves the nucleus, an observation is made, via interaction with the gas of the cloud chamber. Then the α takes on particle-like properties, i.e. it should be represented by a wave packet moving in a definite direction, so as to produce the straight track. This assumes that the α alone constitutes the entire quantum system under consideration, such that the gas constitutes a measurement apparatus external to the system.

- Rebuttal of the naive explanation: Actually, we must consider the α and the gas all together as one system. "... Then it is ionized atoms we observe; interpreting the wavefunction should give us simply the probability that such and such an atom is ionized. Until this final interpretation is made, no mention should be made of the α-ray being a particle at all. The difficulty that we have in picturing how it is that a spherical wave can produce a straight track arises from our tendency to picture the wave as existing in ordinary 3-dimensional space, whereas we are really dealing with wavefunctions in the multispace formed by the co-ordinates both of the α-particle and of every atom in the Wilson chamber." [3]

- Better explanation: When we properly consider the entire system and crunch through the calculations, we find that the probability of any two atoms both being ionized is essentially zero unless they form a straight line with the nucleus. So overall, we end up with a linear track. But any direction for the linear track is equally probable (hence the role of the spherical symmetry.)

The procedure for the calculations in Mott's paper:

- Consider spherical coordinates, with the radioactive nucleus at the origin, one hydrogen atom at position $\vec{a_1}$, and the other at $\vec{a_2}$ (with $a_2 > a_1$. Construct a periodic wavefunction $\Psi(\vec{R}, \vec{r_1}, \vec{r_2})e^{iEt/\hbar}$ for the α and the two atomic electrons, all together. Also construct a wavefunction for each of the two hydrogen atoms, yielding $\Phi^1_J(\vec{r})$ and $\Phi^2_J(\vec{r})$ where the subscript J indicates the state of the atom (ground or excited).

- Expand Ψ in a series of wavefunctions of Φ_1 and Φ_2:

$$\Psi(\vec{R}, \vec{r_1}, \vec{r_2}) = \sum_{J_1 J_2} f_{J_1 J_2}(\vec{R}) \Phi^1_{J_1}(\vec{r_1}) \Phi^2_{J_2}(\vec{r_2})$$

so that $|f_{J_1 J_2}(\vec{R})|^2 dV$ is the probability of finding the α in the volume element dV at the same time as the first atom is in the state J_1 and the second is in J_2.

- Treat the interaction of the atoms and the α as a perturbation, and employ a Born-style method of successive approximations:

$$\Psi = \Psi_{(0)} + \Psi_{(1)} + \Psi_{(2)} + ...$$

- Non-zero possibility of both atoms being excited doesn't show up in the expansion until $\Psi(2)$. Solving for this term, we obtain a term we'll call $\varphi(\vec{r})$ (the term from $\Psi_{(1)}$ corresponding to one atom excited and one in ground state) multiplied by a term we'll call $\xi(\vec{r} - \vec{a_2})$. The $\varphi(\vec{r})$ term vanishes except in the neighbourhood of a narrow cone with its vertex at $\vec{a_1}$, pointed directly away from the origin. The $\xi(\vec{r} - \vec{a_2})$ vanishes except in the neighbourhood of $\vec{a_2}$. To have a significantly non-zero probability of both atoms being excited, there must exist some $\vec{r}$ that lies near $\vec{a_2}$ and that lies in the narrow cone. This is only possible if the origin, $\vec{a_1}$ and $\vec{a_2}$ form a straight line. Hence, the radial track of excited atoms.

0.3 A Modern View: Decoherence

Here it is useful to employ density matrices ρ rather than wavefunctions Ψ. To compute the mean value of some observable O for a quantum system with density matrix ρ, we use

$$\langle O \rangle_\rho = Tr(\rho O).$$

The off-diagonal terms of ρ represent quantum interference terms. If these terms go to 0, calculations of quantum-mechanical probabilities (via amplitudes and norms) reduce to classical-style calculations where probabilities can simply be added together. In decoherence, ρ becomes diagonalized so that quantum-mechanical predictions go over to classical statmech predictions.

In the Lippmann-Schwinger basis $\{|\omega+\rangle\}$, we can diagonalize the Hamiltonian as

$$H = \int_\infty^0 \omega |\omega+\rangle\langle\omega + | d\omega.$$

We can express any observable O as

$$O = \int_\infty^0 O_\omega |\omega+\rangle\langle\omega + | d\omega + \int_\infty^0 \int_\infty^0 O_{\omega\omega'} |\omega+\rangle\langle\omega' + | d\omega d\omega'$$

where the functions $O_\omega, O_{\omega\omega'}$ are regular, and $O \in \mathcal{O} \subset \mathcal{H} \oplus (\mathcal{H} \otimes \mathcal{H})$.

We can now consider $\langle O \rangle_\rho$ as a linear functional ρ on the vectors O, where $\rho \in \mathcal{O}'$. The basis of $\mathcal{O}$ is $\{|\omega), |\omega, \omega')\}$ where

$$|\omega) = |\omega+\rangle\langle\omega+|, |\omega, \omega') = |\omega+\rangle\langle\omega'+|.$$

The basis of $\mathcal{O}'$ is $\{(\omega|, (\omega, \omega'|\}$. We have

$$(\omega|\omega') = \delta(\omega - \omega')$$

and

$$(\omega, \omega'|\omega', \omega''') = \delta(\omega - \omega')\delta(\omega'' - \omega''').$$

A generic quantum state now reads

$$\rho = \int_\infty^0 \rho_\omega (\omega| d\omega + \int_\infty^0 \int_\infty^0 \rho_{\omega\omega'} (\omega, \omega'| d\omega d\omega' \tag{1}$$

or, with time evolution (more on the time situation later):

$$\rho(t) = \int_\infty^0 \rho_\omega (\omega| d\omega + \int_\infty^0 \int_\infty^0 \rho_{\omega\omega'} e^{i(\omega - \omega' t)} (\omega, \omega'| d\omega d\omega'. \tag{2}$$

When we consider the mean values of observables in quantum states, we obtain:

$$\begin{aligned} \langle O \rangle_{\rho(t)} &= (\rho(t)|O) \\ &= \int_\infty^0 \rho_\omega Q_\omega d\omega + \int_\infty^0 \int_\infty^0 \rho_{\omega\omega'} O_{\omega\omega'} e^{-i(\omega - \omega' t)} d\omega d\omega' \end{aligned} \tag{3}$$

It turns out [1] that, where ρ' is a diagonal equilibrium state $\rho' = \int_0^\infty \rho_\omega (\omega| d\omega$:

$$\lim_{t \to \infty} \langle O \rangle_{\rho(t)} = \langle O \rangle_{\rho'}$$

The off-diagonal terms here don't vanish, they just oscillate such that the mean value of any observable is the same as it would be if the terms were zero. This reads as, "any quantum state goes to an equilibrium diagonal state weakly, if we observe and measure the system evolution with any possible observation of space" [1], and it can be considered as decoherence in energy. Note, we are focusing on $\langle O \rangle_{\rho(t)}$, i.e. on the mean value of an observable, because we are trying to bring QM to classical statmech (where the mean values are what really matters). We're not trying to bring QM to classical mechanics of a single particle here.

The above applies only to energy – what about the other dynamical variables? It turns out, it is possible to define a basis, called the final pointer basis, where the off-diagonal terms for the other dynamical variables all vanish for $t \to \infty$. Then there is a "perfect and complete decoherence". For a system with spherical symmetry such as in the Mott Problem, the complete set of commuting observables corresponding to the final pointer basis is simply $\{H, L^2, L_z\}$. (The hand-waving explanation for this is, the spherical symmetry requires the CSCO to contain the generator of angular rotation.) So, the final pointer basis is just the familiar $\{|\omega, l, m\rangle\}$.

0.4 A Modern View: $\hbar \to 0$

In classical mechanics, position and momentum are of course treated as independent dynamical variables. At so-called macroscopic scales, we can under certain circumstances make the approximation $\hbar \to 0$, allowing for this independence.

Applying this approximation, we can then find the "Wigner function" (or Wigner quasi-probability distribution) of ρ'. Essentially, there is a map between Hermitian operators and real phase-space function, by which a quantum density matrix maps to a Wigner quasi-probability distribution. The Wigner $P(x,p)$ for wavefunction ψ and a pair of conjugate variables (x,p) is defined as:

$$P(x,p) = \frac{1}{\pi\hbar}\int_{-\infty}^{\infty} \psi^*(x+y)\psi(x-y)e^{2ipy/\hbar}dy.$$

Technically, the Wigner is the generating function for all spatial autocorrelation functions of a given QM wavefunction, and is the quantum moment-generating functional forming the basis of the phase space formulation of QM. In plainer language, it plays an analagous role to the classical phase-space Liouville density, but does not satisfy all properties of a conventional probability distribution. For quantum states that have no classical model (i.e. where is quantum interference), the Wigner distribution generally goes negative. Compact regions of negative value do not extend to regions larger than a few $\hbar$, and the Wigner can be smoothed through a filter larger than $\hbar$, i.e. convolved with a phase-space Gaussian, to make it positive-semidefinite and coarsen it to a semi-classical distribution. The point of all this is, where we have eliminated all the interference in ρ' and have taken $\hbar$ to zero, the Wigner transform $\rho'_{cl}([x],[k])$ of ρ' can be expressed as:

$$\rho^{cl'}([x],[k]) = \int p_{la}\rho^{cl}_{la_0}([x],[k])dlda$$

where $\rho^{cl}_{la_0}([x],[k])$ is a classical density, strongly peaked in a trajectory defined by the initial coordinates a and momenta l, and p_{la} is the probability of each trajectory. For each of the classical motions, $\{H, L^2, L_z\}$ are perfectly well-defined and are constants of the motion. The classical motions are functions only of $\{H, L^2, L_z\}$, not of their classically canonically conjugate variables (which are completely undefined.) The motions homogeneously fill the "surface" $\{H, L^2, L_z\} = const$, yielding the usual classical torus of phase space.

Note that if we take the classical analogue of the Hamiltonian, we obtain:

$$H = \frac{p_r^2}{2M} + \frac{L^2}{2Mr^2} + W(r)$$

In the limit $r \to \infty$, we can therefore consider $L^2 = 0$. So, classical motions far from the nucleus are indeed radial.

0.5 Time and Causality

Remember we simply jumped from Eqn 1 to Eqn 2 (first we had a timeless general expression for a quantum state, and then we stated an expression with time evolution)? How did the time get in there? Well, we can postulate that there is a symmetry in the system, with a symmetry group e^{-iHt}. Essentially, we add time in by hand, not because anything in the preceding math suggests we should do so, but simply because we know time is needed eventually. In fancier language, it's "a global fact imposed by the structure of the universe where we suppose the model is immersed" [1].

Dissatisfied? Then, we can take an alternative view, by turning the traditional concept of time completely on its head. In our previous considerations, we first postulated the existence of time, and then the time evolution served as the origin of the decoherence in energy. And, in the decoherence of the other variables, the preservation of spherical symmetry by the time evolution was implied. But, what if we go the other way around? Namely, postulate decoherence first, by stating that there must exist "some kind of evolution with a final diagonal state that corresponds to the fact that the universe really ends in a classical state... the quantum physics of the universe is such that it has a tendency toward the classical regime (decoherence + elimination of the uncertainty relations). This tendency would be the primitive concept in this case and time would be a derived concept" [1]. In technical language, we can postulate the existence of a parameter η such that $|\eta\rangle = e^{-iHt}|0\rangle$. This parameter would then decohere to become a classical one that plays the role of time. Classical time in the Mott Problem would simply be the variable t for which, over the classical trajectory labelled by ω and l,

$$M\frac{dr}{dt} = \sqrt{2M\left[\omega - \frac{l(l+1)}{2Mr^2} - W(r)\right]}.$$

A related issue is that of causality. In the Mott formulation, why do we accept only outgoing-particle solutions, and not incoming-particle solutions? More generally, why is the universe apparently time-asymmetric even though its evolution laws are time-symmetric? Or, while the laws of physics yield two t-symmetric solutions to a given problem, why does the universe correspond to only one of these solutions? In more poetic terms, why does time have an arrow? Comments that are frequently made regarding the arrow of time in QM include:

- Outgoing scattering states behave spontaneously; incoming scattering states must be produced by a source of energy. In the case of a nucleus, incoming states transform the stable nucleus into an unstable one, while outgoing states radiate the energy produced when the unstable nucleus evolves to an equilibrium state.

- The space of admissible solutions in QM is not the whole Hilbert space, but a subspace of it. We can relate causality to the analytic properties of wavefunctions: promoting energy ω to a complex variable z, admissible solutions can be defined as those that are analytic and bounded in the lower complex half-plane of z rather than in the upper complex half-plane.

- The choice to keep one solution and throw away the other must be global (i.e. must be consistently carried out in the whole universe.)

0.6 What Constitutes a Measurement?

Instead of putting the radioactive atom in an old-fashioned cloud chamber, we could put a hemispherical particle detector in the vicinity of the atom (say, above the atom). Obviously, if the detector fires, we gain information about the path of the α (i.e. the atom travelled upward not downward), and ψ_α changes to take into account this new information. We can say that ψ_α was altered because of the interaction with the detector. But, if the detector fails to fire, we also gain information about the path – we know the α did not go upward (assuming perfect detector efficiency) or is very unlikely to have gone upward (assuming a slightly imperfect detector). So, a "null result" can still constitute a measurement! Just because the detector did not fire, does not mean the α did not "perceive" the detector's presence. This may remind you of the idea of a quantum particle probing all possible paths simultaneously.

An interesting modern thought experiment [2] involved an ion in a uniform magnetic field, trapped in a quadratic electrostatic potential such that it oscillates along the magnetic axis with a given frequency. An intense pulse of energetic photons then illuminates part of the trap, such that $\int_{illuminatedarea} |\psi|^2 = 0.5$. If the ion is found inside the illuminated area, it is multiply ionized and hence destroyed, yielding photoelectrons that we detect. If the photoelectrons are not detected, the ion survives, and is presumably located outside the illuminated area. So, the failure to detect photoelectrons alters ψ such that $\int_{illuminatedarea} |\psi|^2 = 0$. But now, with this altered ψ, the expectation value of the energy is higher! So, an energy change of the particle apparently occurred without any obvious interaction with the illuminating radiation.

One interpretation is that "the apparent lack of interaction between the atom and the EM field is only illusionary. In lowest order the perturbation calculation shows that the change in the atomic center-of-mass wave function is associated with the absorption of a photon from the incident wave packet and the subsequent return of the photon to the packet. If the absorbed photon could have been assumed to have had a well-defined momentum and energy... this type of photon absorption and re-emission would not result in the transfer of either momentum or energy to the atom. But... the observation requires the photons to be initially in a state for which neither the momentum nor the energy of the photon is well defined. Consequently, the photon exchange can result in a momentum or energy transfer." [2]

0.7 Applicability to Quantum Cosmology

Regarding the questions raised by the Mott Problem: "At this stage we must observe that this set of problems is very similar to those of quantum cosmology, where, in fact, we must explain the outcome of the classical regime, the appearance of time, the nature of the classical trajectories in superspace, and the direction of the corresponding motion, i.e., the arrow of time. Then several of the most important quantum universe problems... are already contained in our humble Mott model." [1]

Note, in particular, that when we are considering quantum cosmology we cannot treat time as "a global fact imposed by the structure of the universe where we suppose the model is immersed". The model isn't immersed in anything; the model is the entire universe! So, we cannot just add time in by hand – the alternative views of time become very important.

Bibliography

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