A.2. ELEMENTARY QUANTUM THEORY

An acquaintance with elementary quantum mechanics is assumed here - the purpose of this sub-section is to briefly review the results. We begin by recalling the standard formulation of QM in terms of state vectors (the "wave-function"), along with operators, etc., and the Schrödinger eqn. This is done both in abstract Hilbert space and in ordinary real space, for 1-particle systems. Then a more general formulation is given in terms of density matrices - it is really only a historical accident that Q.M. is usually presented in terms of pure state wave functions, & so I will stress the importance of the density matrix formulation.

A.2.1. WAVE-FUNCTIONS & Q.M.

The original formulation of Q.M. in terms of either a wave-function (Schrödinger, 1925-26) or in matrix algebraic terms (Heisenberg, 1925) was fairly quickly superseded by a more mathematical formulation in terms of state vectors in Hilbert space (von Neumann, 1935, building on the earlier work of Dirac). All of these are equivalent, and they all deal with pure states (as opposed to the density matrix formulation). Because they are all equivalent, I will simply present them all together, with no regard for historical distinctions.

A.2.1 (a) STATES & OPERATORS IN HILBERT SPACE : We begin with the most abstract

formulation, but without any mathematical sophistication. Recall that in classical mechanics, the theory begins with the fundamental entity of the "classical state", defined by either a point in $6N$-dimensional configuration space or $6N$-dimensional phase space.

In Q.M. we can define a Hilbert space $\mathcal{H}$, which is spanned by a set of N_H complex "ray" vectors. We use the Dirac notation, and write

$$\{|\alpha\rangle\} = |\alpha_1\rangle, |\alpha_2\rangle, |\alpha_3\rangle, \ldots |\alpha_{N_H}\rangle \quad \in \mathcal{H} \tag{75}$$
$$\mathcal{D}[\mathcal{H}] = N_H$$

where $\mathcal{D}[\mathcal{H}]$ is the (complex) dimension of the Hilbert space $\mathcal{H}$ (so that N_H complex numbers are required to specify the state). We will assume orthonormality:

$$\langle \alpha_k | \alpha_{k'} \rangle = \delta_{kk'} \tag{76}$$

and define the projection operator $\hat{P}_\alpha$:

$$\sum_\alpha \hat{P}_\alpha \equiv \sum_\alpha |\alpha\rangle\langle\alpha| = 1 \tag{77}$$

from which

$$\sum_\alpha \langle \beta | \alpha \rangle \langle \alpha | \gamma \rangle \equiv \langle \beta | \alpha \rangle \langle \alpha | \gamma \rangle = \delta_{\beta\gamma} \tag{78}$$

where we use the summation convention in which repeated indices are summed over. We can expand any state vector in terms of the complete orthonormal set $\{|\alpha\rangle\}$, as

$$|\psi\rangle = \sum_\alpha c_\alpha |\alpha\rangle \qquad \text{with} \quad \sum_\alpha |c_\alpha|^2 = 1 \tag{79}$$

where $\quad c_\alpha = \langle \alpha | \psi \rangle \qquad c_\alpha^* = \langle \psi | \alpha \rangle$

Transformations on the vectors in the Hilbert space are effected by operators $\hat{A}, \hat{B}, ..$ and one has

$$\hat{A}|\alpha\rangle = |\beta\rangle = \sum_{\alpha} A_{\alpha\beta}|\alpha\rangle \qquad \Big\} \quad (80)$$

with $\qquad A_{\alpha\beta} = \langle\alpha|\hat{A}|\beta\rangle$

If the state $|\alpha\rangle$ is an eigenstate of the operator $\hat{A}$, then

$$\hat{A}|\alpha\rangle = a_{\alpha}|\alpha\rangle \qquad \Big\} \quad (81)$$

$$\langle\beta|\hat{A}|\alpha\rangle = a_{\alpha}\delta_{\alpha\beta}$$

A change of basis from states like $|\alpha\rangle, |\beta\rangle$, etc., to states like $|\mu\rangle, |\nu\rangle$, etc., is effected by a rotation in Hilbert space:

$$|\mu\rangle = \hat{R}_{\alpha\mu}|\alpha\rangle \qquad\qquad R_{\alpha\mu} = \langle\alpha|\hat{R}|\mu\rangle = \langle\alpha|\mu\rangle \qquad (82)$$

and we can in the same way change the basis for operator expressions:

$$A_{\mu\nu} = \langle\mu|A|\nu\rangle = \langle\mu|\alpha\rangle\langle\alpha|A|\beta\rangle\langle\beta|\nu\rangle \qquad \Big\} \quad (83)$$

$$= \langle\mu|\alpha\rangle A_{\alpha\beta}\langle\beta|\nu\rangle$$

or in a mixed representation

$$A_{\mu\beta} = \langle\mu|A|\beta\rangle = \langle\mu|\alpha\rangle\langle\alpha|A|\beta\rangle \qquad \Big\} \quad (84)$$

$$= \langle\mu|\alpha\rangle A_{\alpha\beta}$$

Consider now some of the operators and sets of eigenfunctions we are likely to meet. The first two are the position and momentum operators $\hat{P}$ and $\hat{r}$, for which we have

$$\hat{P}|\underline{k}\rangle = \hbar\underline{k}|\underline{k}\rangle \qquad\qquad \langle\underline{k}|\hat{P}|\underline{k}'\rangle = \hbar\underline{k}\,\delta_{k-k'} \qquad \Big\} \quad (85)$$

$$\hat{r}|\underline{r}\rangle = \underline{r}|\underline{r}\rangle \qquad\qquad \langle\underline{r}|\hat{r}|\underline{r}'\rangle = \underline{r}\,\delta(r-r')$$

and $\qquad \boxed{\begin{array}{l}\langle\underline{r}|\underline{k}\rangle = e^{i\underline{k}\cdot\underline{r}} \\ \langle\underline{k}|\underline{r}\rangle = e^{-i\underline{k}\cdot\underline{r}}\end{array}} \qquad \Big\} \quad (86)$

from which we see that for any operator $\hat{f}_x$ which has as eigenstates some function of $\underline{r}$, i.e.,

$$\hat{f}_x|\underline{r}\rangle = f_x(\underline{r})|\underline{r}\rangle \qquad (87)$$

then $\qquad \langle\underline{k}|\hat{f}_x|\underline{k}'\rangle = \langle\underline{k}|\underline{r}\rangle\langle\underline{r}|\hat{X}|\underline{r}'\rangle\langle\underline{r}'|\underline{k}'\rangle$

$$\equiv \int d^3r \int d^3r'\, e^{i\underline{k}\cdot\underline{r}} e^{-i\underline{k}'\cdot\underline{r}'} f_x(\underline{r})\,\delta(r-r') \qquad \Big\} \quad (88)$$

$$= \int d^3r\, f_x(\underline{r})\, e^{i(\underline{k}-\underline{k}')\cdot\underline{r}}$$

and in the same way, if we define an operator $\hat{g}_P$ which has as eigenstates some

function $g_p(\ )$ of $\underline{k}$, then we have

$$\hat{g}_p |k\rangle = g_p(\hbar k) |k\rangle \tag{89}$$

and

$$\langle \underline{r} | \hat{g}_p | \underline{r}' \rangle = \sum_k g_p(\hbar k) e^{i\underline{k} \cdot (\underline{r}' - \underline{r})} \tag{90}$$

Another important operator is the Hamiltonian $\hat{\mathcal{H}}$, which in ordinary 1-particle quantum theory is just

$$\hat{\mathcal{H}} = \frac{1}{2m} \hat{P}^2 + V(\hat{r}) \tag{91}$$

with matrix elements

$$\mathcal{H}_{kk'} = \langle k | \hat{\mathcal{H}} | k' \rangle = \frac{P^2}{2m} + V_{kk'} \tag{92}$$

$$\mathcal{H}_{rr'} = \frac{1}{2m} P^2_{rr'} + V(r)$$

where

$$V_{kk'} \equiv \langle \underline{k} | \hat{V}(r) | \underline{k}' \rangle = \int d^3r \, V(r) e^{i(\underline{k}' - \underline{k}) \cdot \underline{r}} \tag{93}$$

$$P^2_{rr'} \equiv \langle \underline{r} | \hat{P}^2 | \underline{r}' \rangle = \sum_k \hbar^2 k^2 e^{i\underline{k} \cdot (\underline{r} - \underline{r}')}$$

The eigenstates of $\hat{\mathcal{H}}$ are energy eigenstates:

$$\hat{\mathcal{H}} | \psi_n \rangle \equiv \mathcal{H} | n \rangle = \epsilon_n | n \rangle \tag{94}$$

and the crucial time evolution of the state vectors is given by the time-dependent Schrödinger eqn:

$$\boxed{\hat{\mathcal{H}} = i\hbar \partial_t} \tag{95}$$

Now let's pause a moment and look at the logical development. Equation (86) is important, and we can treat it here as a postulate about the inner product of 2 different vectors in Hilbert space, from which we will then derive the form of $\hat{P}$ in r-space, as well as commutation relations.

Thus consider the "wave-function" ψ_k, ie the inner product of a state vector $|\psi\rangle$ with the momentum eigenstate $\underline{k}$:

$$\psi_k = \langle k | \psi \rangle \qquad \text{ie,} \qquad |\psi\rangle = \sum_k \langle k | \psi \rangle | k \rangle \tag{95}$$

ie we can think of the quantities $\langle k | \psi \rangle = \psi_k$ as expansion coefficients in the representation of $|\psi\rangle$ in momentum eigenfunctions, viz.,

$$|\psi\rangle = \sum_k C_k | k \rangle \qquad \text{with} \qquad C_k \equiv \langle k | \psi \rangle. \tag{96}$$

• Now consider the quantity

$$\langle k | \hat{P} | \psi \rangle = \langle k | \hat{P} | k' \rangle \langle k' | \psi \rangle$$
$$= \sum_{k'} \delta_{kk'} \hbar k' C_{k'} = \hbar k C_k \tag{97}$$

We note that the "expectation value" $\langle p \rangle$ is given by the weighted sum

$$\langle p \rangle = \langle \psi | \hat{P} | \psi \rangle = \langle \psi | k \rangle \langle k | \hat{P} | k' \rangle \langle k' | \psi \rangle$$
$$= \sum_k \hbar k \, |C_k|^2 \tag{98}$$

and indeed the expectation value of any operator is given by

$$\langle \hat{A} \rangle \; = \; \langle \psi | \hat{A} | \psi \rangle \tag{99}$$

But now suppose we try to redo (94) in real space — then we must compute

$$\langle k | \hat{p} | \psi \rangle \; = \; \langle k | \hat{p} | k' \rangle \langle k' | r \rangle \langle r | \psi \rangle$$
$$= \; \hbar k \int d^3 r \, e^{-ik \cdot r} \, \psi(r) \Bigg\} \tag{100}$$

But now notice that $\hbar k e^{-ik \cdot r} = i \hbar \partial_r e^{-ik \cdot r}$; and if we do the integral in (100) by parts, we get

$$\langle k | \hat{p} | \psi \rangle \; = \; -i\hbar \int d^3 r \, e^{-ik \cdot r} \, \nabla_r \, \psi(r) \tag{101}$$

where the term $\left[i\hbar \, e^{-ik \cdot r} \, \psi(r) \right]_{-\infty}^{\infty}$ is assumed to vanish (ie, the function $\psi(r)$ falls off at $\pm \infty$).

But this simply means that

$$\boxed{\hat{p} \; \equiv \; -i\hbar \, \hat{\nabla}_r} \tag{102}$$

and we can similarly show that

$$\boxed{\hat{r} \; = \; i \, \partial_k} \tag{103}$$

From this it is easy to demonstrate the standard commutation relations for the momentum & position operators; writing $p = (p_x, p_y, p_z) = p_j$, and likewise $r = (x_1, x_2, x_3) = x_j$, we have

$$\boxed{[\, \hat{p}_i, \hat{x}_j \,] \; \equiv \; \hat{p}_i \hat{x}_j - \hat{x}_j \hat{p}_i \; = \; -i\hbar \, \hat{\delta}_{ij}} \tag{104}$$

Notice that this means that $\hat{p}$ is the generator of transformations in the position (and vice-versa). We can write

$$\psi(r + \delta r) \; \equiv \; \langle r + \delta r | \psi \rangle \; = \; e^{\frac{i}{\hbar} \delta r \cdot \hat{p}} \, \langle r | \psi \rangle \tag{105}$$

where we use $e^{\frac{i}{\hbar} \delta r \cdot p} = (1 + \delta r \cdot \hat{p}) = (1 + \delta r \cdot \nabla_r)$. In the same way we can show that if make an infinitesimal rotation in space, by an angle $\delta \phi$ or (oriented along the direction of $\delta \phi$, ie about an axis along this direction), then

$$\psi(r + \delta \phi \times r) \; = \; \exp \left\{ \frac{i}{\hbar} \delta \phi \cdot \hat{L} \right\} \psi(r) \tag{106}$$

where the operator

$$\boxed{\hat{L} \; = \; \hat{r} \times \hat{p}} \tag{107}$$

and the components $\hat{L}_i$ satisfy

$$\boxed{[\, \hat{L}_i, \hat{L}_j \,] \; = \; i\hbar \, \epsilon_{ijk} \, \hat{L}_k} \tag{108}$$

ie., we are dealing with the standard Q.M. angular momentum operator.

As you doubtless know (and as we recall in the next subsection), results such

as the commutation relations (104) and (105), and Hilbert space scalar product (86), are conventionally defined by starting from a wave-function $\psi(\xi)$, and a definition like (102) of the momentum operator, derived using a semi-classical correspondence (ie., the Schrödinger method). However in starting from a Hilbert space formulation, we have inverted the logical order of derivation.

Finally let's look at the time-dependence of physical quantities. We note that from Schrödinger's eqtn (95) we can write

$$| \psi(t) \rangle_s = e^{-\frac{i}{\hbar}\hat{H}t} | \psi(0) \rangle = U_H(t) | \psi(0) \rangle \tag{109}$$

where the subscript "S" indicates the "Schrödinger picture", in which all the time dependence is put into the wave function. Note that (109) implies that $\hat{H}$ is the generator of time translations, in the same way that $\hat{p}$ is the generator of space translations.

From (109) we can immediately compute the time-dependence of matrix elements:

$$\frac{d}{dt} \hat{A}^s_{\alpha\beta} \equiv \frac{d}{dt} {}_s\langle \alpha | \hat{A} | \beta \rangle_s = \partial_t \hat{A}^s_{\alpha\beta} + \frac{1}{i\hbar} [\hat{A}, \hat{H}]^s_{\alpha\beta} \tag{110}$$

where we have

$$\left. \begin{array}{l} \partial_t A^s_{\alpha\beta} \equiv {}_s\langle \alpha | \frac{\partial \hat{A}}{\partial t} | \beta \rangle_s \\[2mm] [A, \mathcal{H}]^s_{\alpha\beta} \equiv {}_s\langle \alpha | [A, \mathcal{H}] | \beta \rangle_s \end{array} \right\} \tag{111}$$

Alternatively, we can use the "Heisenberg picture", ie., put the time-dependence all into the operators. This means that we write

$$\left. \begin{array}{l} {}_s\langle \alpha | \hat{A} | \beta \rangle_s = \langle \psi_\alpha(0) | U_H^{-1}(t) \hat{A} U_H(t) | \psi_\beta(0) \rangle \\[2mm] = \langle \psi_\alpha(0) | A_H(t) | \psi_\beta(0) \rangle \end{array} \right\} \tag{112}$$

with the Heisenberg picture operator defined as

$$\hat{A}_H(t) = e^{\frac{i}{\hbar}\hat{H}t} \hat{A}_s e^{-\frac{i\hat{H}}{\hbar}t} \tag{113}$$

using (109). One then easily finds that

$$\langle \psi_\alpha(0) | \frac{d}{dt} \hat{A}^H(t) | \psi_\beta(0) \rangle = \dot{A}^H_{\alpha\beta} = \partial_t A^H_{\alpha\beta} + \frac{1}{i\hbar} [A^H, \mathcal{H}]_{\alpha\beta} \tag{114}$$

which is the operator eqtn. of motion in the Heisenberg picture.

This summarizes the abstract Hilbert space presentation of the structure of non-relativistic 1-particle Q.M. Notice that the classical structure begins to appear in it once we assume certain things, notably that the inner product of states corresponding to "momentum" operators and "position" operators is given by a function in real space of the form (86). One then immediately sees the analogy between commutation relations and Poisson brackets, and the equation of motion (compare (47) and (114)), the definition of momenta in terms of a spatial gradient, etc. In the Hilbert space formulation this all appears by magic, and one wonders where it comes from. The answer of course is to be found in the Schrödinger formulation of wave mechanics, to which we now turn.

A.2.1.(b). SCHRÖDINGER FORMULATION OF Q.M.:

Now let us go back to the problem faced by Schrödinger in 1925, which was to derive Q.M. from what was known about the correspondence between classical & quantum phenomena – embodied at that time in the correspondence principle and in physical notions of wave-particle duality.

Schrödinger, once things became clear to him, began by considering the remarkable "ray" picture that emerges from the Hamilton-Jacobi eqtn. in the form (73) for a single particle. Guided by the need (evident from de Broglie's work in 1924) that one needed some sort of wave equation* to deal with quantum phenomena, Schrödinger made the ansatz :

$$ S = \kappa \ln \psi \qquad \psi = e^{S/\kappa} \tag{115} $$

where S was the action – which we recall represents surfaces of constant phase (this substitution is natural – cf. the analogy with the "stream function" in fluid dynamics and/or complex variable theory). Substituting in the H-J eqtn. (73) gives

$$ \frac{\kappa^2}{2m}(\nabla\psi)^2 + (V-E)\psi^2 = 0 \tag{116} $$

and, to abbreviate the subsequent development here, we will note that $\boxed{\kappa = -i\hbar}$ (117) which Schrödinger later realised by comparing with, e.g., the de Broglie work.

Now (116) implies the variational result

$$ \delta \int d^3r \, (\mathcal{H}-E) = \delta \int d^3r \left[-\frac{\hbar^2}{2m}(\nabla\psi)^2 + (V-E)\psi^2 \right] = 0 \tag{118} $$

which leads immediately to 2 equations:

$$ \boxed{\begin{aligned} \left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) \right] \psi(r) &= E\,\psi(r) \\ \oint_S d\underline{S} \cdot \frac{\partial \psi}{\partial \underline{n}} \, \delta\psi &= 0 \end{aligned}} \tag{119} $$

The first of these is the famous time-independent Schrödinger equation, and the second is a boundary condition on some surface S which encloses the system (with $\underline{n}$ a normal to the surface).

This result was obtained by going from classical mechanics to Q.M.; but nowadays one is more interested in the reverse. Suppose we assume the Schrödinger eqtn, now in its time-dependent form

$$ \boxed{ \hat{\mathcal{H}}\,\psi(r,t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) \right]\psi(r,t) = i\hbar\partial_t \psi(r,t) } \tag{120} $$

which can be obtained in exactly the same way as above, but now using the full H-J eqtn in the form (51) (ie., assuming $\mathcal{H} = -\partial S/\partial t$). Now, lets make the ansatz for $\psi(r,t)$ in the form

$$ \boxed{ \psi(r,t) = A(r,t)\, e^{iS/\hbar} } \qquad \text{(SEMICLASSICAL)} \tag{121} $$

where we assume that $A(r,t)$ is a slowly varying function of its variables compared to the exponential phase $\phi(r,t) = S(r,t)/\hbar$. This is the "semiclassical approximation" which we will discuss at length later on.

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* APPARENTLY SCHRÖDINGER WAS STIMULATED BY A RATHER SARCASTIC REMARK MADE BY DEBYE DURING A SEMINAR GIVEN BY SCHRÖDINGER IN ZURICH; HIS COLLEAGUE REMARKED THAT INSTEAD OF PLAYING WITH "CHILDISH" NOTIONS OF PHASES & WAVE FRONTS, ONE SHOULD FIND A WAVE EQUATION. A FEW WEEKS LATER SCHRÖDINGER GAVE ANOTHER SEMINAR WHICH HE BEGAN BY ANNOUNCING HE HAD FOUND ONE!

Substitution of (121) into (120) gives

$$A\partial_t S - i\hbar\partial_t A - \frac{\hbar^2}{2m}\nabla^2 A - \frac{i\hbar}{2m}\left(A\nabla^2 S + 2\nabla A.\nabla S\right) + \frac{A}{2m}\left(\nabla S\right)^2 + V(r)A = 0 \qquad (122)$$

which separates into 2 eqtns (one real & one imaginary); dropping the term $\sim O(\hbar^2)$, we get

$$\frac{1}{2m}\left(\nabla S\right)^2 + V(r) = -\partial_t S \qquad (123)$$

and

$$\partial_t A^2(r,t) + \nabla.\left(A^2(r,t)\frac{\nabla S}{m}\right) = 0 \qquad (124)$$

The first is the time-dependent H-J eqtn, as expected since it was used to get the time-dep. Schrödinger eqtn (120) in the first place. The second is just the eqtn of continuity for $A^2 = |\psi|^2$; this becomes the equation of conservation in the standard interpretation of Q.M. (see later).

This summarizes the derivation of the "wave mechanics" picture of Q.M. We see immediately now why one has the correspondence between classical and quantum aspects in the formalism, such as

CLASSICAL		QUANTUM

Poisson brackets $\{A,B\}$ $\longleftrightarrow$ Commutators $[\hat{A},\hat{B}]$

Eqtns of Motion $\frac{df}{dt} = \partial_t f + \{H, f\}$ $\longleftrightarrow$ $\frac{d\hat{A}}{dt} = \partial_t \hat{A} + \frac{i}{\hbar}[\hat{H},\hat{A}]$

Physical Quantities Position $r = -\partial S/\partial p$ $\longleftrightarrow$ $\hat{r} = i\hbar\,\partial/\partial\hat{p}$

Momentum $p = \nabla_r S$ $\longleftrightarrow$ $\hat{p} = -i\hbar\nabla_r$

Hamiltonian $H = -\partial_t S$ $\longleftrightarrow$ $\hat{H} = i\hbar\partial_t$

Angular Momentum $\underline{L} = \underline{r}\times\underline{p}$ $\longleftrightarrow$ $\hat{L} = \hat{r}\times\hat{p} \equiv -i\hbar\left(\hat{r}\times\nabla_r\right)$
$$\equiv i\hbar\left(\nabla_p\times\hat{p}\right)$$

$$(125)$$

and so on. The advantages of Q.M. as formulated in this language are of course well-known — it allows one to deal with physical problems using the language of differential equations, and to visualise quantum states not in Hilbert space but as ordinary functions in, eg., real space. Thus one can think in terms of "wave-packets" $\psi(r,t)$ in real space, or alternatively in momentum space in the form

$$\psi(p) = \int d^3r\, e^{ip/\hbar \cdot r}\,\psi(r) \qquad (126)$$

which is just the result $\langle p|\psi\rangle = \langle p|r\rangle\langle r|\psi\rangle$ written as a Fourier transform. In this language, statements such as the famous HEISENBERG UNCERTAINTY PRINCIPLE, in the form

$$\Delta r\,\Delta p \geq \hbar/2 \qquad (127)$$

where $(\Delta r)^2 = \langle r^2\rangle - \langle r\rangle^2$
$(\Delta p)^2 = \langle p^2\rangle - \langle p\rangle^2$ $\qquad\qquad (128)$

become a straightforward theorem about Fourier transforms.

A.2.2. DENSITY MATRICES & ENTANGLEMENT

The formulation of Q.M. in terms of pure states, as outlined in A.2.1., is the result of a historical accident. The more general formulation is that in terms of the density matrix. In the vast majority of physical situations, the system, whether closed or not, cannot be described as a pure state, but must be described as a statistical mixture.

Suppose we have a system in a mixture of states $|\psi_\alpha\rangle$, with probabilities p_α. Then the density matrix for the system is

$$\hat{\rho} = |\alpha\rangle p_\alpha \langle\alpha| \tag{129}$$

This operator has matrix elements

$$\rho_{ij} = \langle i|\hat{\rho}|j\rangle$$
$$= \langle i|\alpha\rangle p_\alpha \langle\alpha|j\rangle \tag{130}$$

in a basis of functions $\{|i\rangle\} \equiv \{|\phi_i\rangle\}$, which are in general quite different from the $\{|\alpha\rangle\}$. Thus, in the α-representation in which $\hat{\rho}$ is diagonal, we have

$$\rho_{\alpha\beta} = p_\alpha \delta_{\alpha\beta} \equiv \begin{pmatrix} p_1 & & & \\ & p_2 & & 0 \\ & & \ddots & \\ 0 & & & p_{N_\alpha} \end{pmatrix} \tag{131}$$

For a pure state $|\psi\rangle = \sum_j c_j |\phi_j\rangle$, the density matrix is just

$$\hat{\rho} = |\psi\rangle\langle\psi| = \sum_g |i\rangle \rho_{ij} \langle j| \tag{132}$$
$$\rho_{ij} = c_i c_j^* \qquad \text{(PURE)}$$

and if the density matrix is diagonal in the same basis that $|\psi\rangle$ is diagonal in, the density matrix reduces to a single diagonal entry.

The expectation value of operators is easily deduced from the fact that in a basis in which ρ is diagonal, we must have

$$\langle\hat{A}\rangle = \sum_\alpha p_\alpha \langle\alpha|A|\alpha\rangle = \text{Tr}[\hat{\rho}\hat{A}] \tag{133}$$

However it is clear that since $\text{Tr}[\hat{\rho}\hat{A}]$ is invariant under Hilbert space rotation, we must have quite generally that

$$\langle\hat{A}\rangle = \text{Tr}[\hat{\rho}\hat{A}] = \text{Tr}[\hat{A}\hat{\rho}] \tag{134}$$

The simplest way to distinguish a pure state density matrix from a mixture is via the simple inequality

$$\text{Tr}[\hat{\rho}^2] < \text{Tr}\,\hat{\rho} = 1 \quad \text{(MIXTURE)}$$
$$\hat{\rho}^2 = \rho \; ; \quad \text{and so} \quad \text{Tr}[\rho^2] = \text{Tr}\,\hat{\rho} = 1 \quad \text{(PURE STATE)} \tag{135}$$

This is obvious in the representation where $\hat{\rho}$ is diagonal, and is true in any representation because $\text{Tr}[\rho^n]$ is invariant under Hilbert space rotations.

Notice that any operator which commutes with ρ will not differentiate between a pure state and a mixture.

<u>Simple example : a TLS</u> : Consider a Two-Level System (TLS) or spin-½ system, and write the density matrix in the $|\uparrow\rangle, |\downarrow\rangle$ representation, ie., in eigenfunctions of $\hat{\tau}_z$. Then 2 examples of pure states are

(a) $|\psi\rangle = |\uparrow\rangle$ $\qquad \rho_{ij} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$

(b) $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$

$\qquad \equiv |\rightarrow\rangle$ $\qquad \rho_{ij} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$

$\left. \begin{array}{c} \\ \\ \end{array} \right\}$ PURE $\qquad (136)$

On the other hand a mixed state, in which ½ the spins are in state $|\uparrow\rangle$ and the other half in state down, is given by

$$\rho_{ij} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad (MIXED) \qquad (137)$$

Notice that this state is quite different from the pure state $\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$; however, an operator like $\hat{\tau}_z$ will not differentiate between the two, since $Tr[\rho\hat{\tau}_z]$ will look the same for both. However consider the effect of a measurement of τ_x; then we have

$$Tr\,\hat{\rho}\,\hat{\tau}_x = \frac{1}{2} Tr\left[\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right] = 1 \qquad (for\ |\rightarrow\rangle)$$

$$Tr\,\hat{\rho}\,\hat{\tau}_x = \frac{1}{2} Tr\left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right] = 0 \qquad (for\ mixed\ state)$$

$\left. \begin{array}{c} \\ \\ \end{array} \right\} (138)$
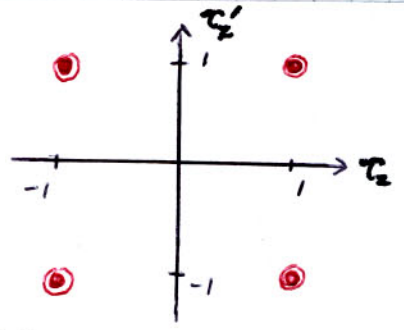
(a) PLOT OF DENSITY MATRIX FOR A SYSTEM IN STATE (134)
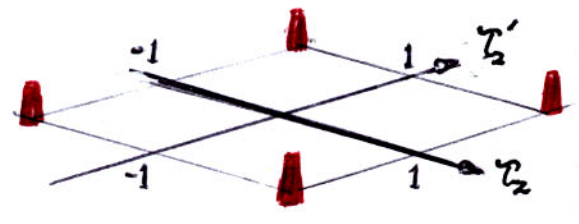
(b) SAME PLOT FOR THE SAME SYSTEM, A COMPLETELY MIXED 2-LEVEL SYSTEM. τ_z and τ_z' ARE THE DENSITY MATRIX ARGUMENTS, WITH $\tau_z, \tau_z' = \pm 1$.

We can plot results like (137) in a simple way as shown at left, where we see plots of $|\rho(\tau_z, \tau_z')|$ for the TLS, where τ_z, τ_z' are the variables of the TLS, taking values $\tau_z, \tau_z' = \pm 1$ $(\equiv \uparrow, \downarrow)$.

Notice that in these plots we can't capture the full behaviour of ρ_{ij}, because in general the off-diagonal elements will be complex, with real and imaginary parts. Note that the most general form for the TLS density matrix is

$$\rho(\tau_z, \tau_z') = \begin{pmatrix} P_\uparrow & ae^{i\phi} \\ ae^{-i\phi} & P_\downarrow \end{pmatrix} \qquad (139)$$

with $P_\uparrow^2 + P_\downarrow^2 = 1$, ie., we need 3 numbers to specify it. To get a better feeling for the way in which density matrices work, it is useful to fool around with different possibilities, seeing how they transform under rotation. etc.

_____

It is also of interest to look at the time-dependence of $\hat{\rho}$. This is easy to determine from the def^n (129), and the time dependence of the Schrödinger wave-function — we have

$$\hat{\rho}(t) = \sum_\alpha p_\alpha |\alpha(t)\rangle\langle\alpha(t)|$$
$$= e^{-\frac{i}{\hbar}Ht}\,\rho(0)\,e^{\frac{i}{\hbar}Ht} \qquad\qquad (140)$$

and differentiating this we get

$$\boxed{\frac{d\hat{\rho}}{dt} = \frac{i}{\hbar}\left[\hat{\rho}(t),\hat{\mathcal{H}}\right]} \qquad\qquad (141)$$

It is important to notice the change of sign in this eqtn. compared to that in the usual operator eqtns of motion (110) and (114) (ie, $i/\hbar$ instead of $-i/\hbar$); thus the density matrix operator is a little different from others.

This summarizes some of the main properties of the density matrix. Let us now look at some more detail.

A.2.2 (a) $\rho(r, r'; t)$ FOR CONTINUOUS SYSTEMS : Suppose we are dealing with a

single particle moving in 3d space. It is useful to be a little more specific about how the density matrix works for such systems. We can rewrite some of the key formulae for such a system, as follows:

- The density matrix in position & momentum representations give expectation values for functions of position of the form

$$\langle A \rangle = \int dr \int dr'\, \rho(r, r'; t)\, A(r'; r; t) \qquad\qquad (142)$$

where
$$\rho(r, r'; t) = \langle r|\hat{\rho}(t)|r'\rangle$$
$$A(r, r'; t) = \langle r|\hat{A}(t)|r'\rangle \qquad\qquad (143)$$

and
$$\langle A \rangle = \sum_{p p'} \rho(p, p'; t)\, A(p'; p; t) \qquad\qquad (144)$$

in momentum space. For the case of a diagonal operator $A(r) = A(r)\delta(r-r')$, like eg. the potential energy or the position, this reduces to

$$\langle A \rangle = \int dr\, \rho(r, r; t)\, A(r, t) \qquad\qquad (145)$$

and likewise in momentum space. The probability of a system being in Hilbert space state $|\psi\rangle$ is

$$P_\psi = \langle\psi|\hat{\rho}|\psi\rangle \equiv \sum_\alpha p_\alpha |\langle\alpha|\psi\rangle|^2 \qquad\qquad (146)$$

which here becomes
$$P_\psi = \int dp \int dp'\, \rho(p, p'; t)\, \psi^*(p)\, \psi(p')$$
$$= \int dr \int dr'\, \rho(r, r'; t)\, \psi^*(r)\, \psi(r') \qquad\qquad (147)$$

- Note some special cases of all these general results. Thus, the probability of finding the system at position r is just

$$\rho(r) = \rho(r, r; t) \qquad\qquad (148)$$

and the expectation value of position is given by

$$\langle \underline{r} \rangle = \int d^3\underline{r}\ \underline{r}\ \rho(\underline{r},\underline{r};t) \tag{149}$$

Suppose now we want to know the expectation value of momentum $\underline{p}$. Clearly this is given by

$$\langle \underline{p} \rangle = \sum_p \underline{p}\ \rho(\underline{p},\underline{p};t) \tag{150}$$

but it is also useful to have it in a real space representation - we then need to have the form of the operator $\hat{p}$ in (142), and we have to be a little more careful then we have in writing the results in (125). We wish to know what is the correct form of $P_{rr'} \equiv \langle \underline{r}|\hat{p}|\underline{r}'\rangle$. One can do this directly from (90), viz,

$$\langle \underline{r}|\hat{\underline{p}}|\underline{r}'\rangle = \sum_k \hbar k\, e^{ik\cdot(\underline{r}-\underline{r}')} = -i\hbar \nabla_r\, \delta(r-r') \tag{151}$$

or simply note that eqtns (102) and (125) imply that if $\hat{p} \equiv -i\hbar \nabla_r$, then

$$\langle \underline{r}|\hat{p}|\psi\rangle = -i\hbar \nabla_r \langle r|\psi\rangle = -i\hbar \nabla_r \psi(r) \tag{152}$$

so $\quad \langle r|\hat{p}|r'\rangle\langle r'|\psi\rangle = -i\hbar \nabla_r \psi(r)$

ie we have

$$\langle \underline{r}|\hat{p}|r'\rangle = -i\hbar \nabla_r\, \delta(\underline{r}-\underline{r}') \tag{153}$$

It then follows that

$$\langle \underline{p} \rangle = \int d^3r\, d^3r'\ \langle \underline{r}|\hat{p}|\underline{r}'\rangle\ \rho(\underline{r}',\underline{r};t) \tag{154}$$

and integrating by parts gives

$$\langle \underline{p} \rangle = i\hbar \int d^3r \int d^3r'\ \delta(\underline{r}-\underline{r}')\nabla_r\, \rho(\underline{r}',\underline{r};t) \left.\begin{array}{c}\\\\\end{array}\right\}$$
$$= i\hbar \int d^3r\ \nabla_r\, \rho(r,r')\big|_{r=r'} \tag{155}$$

In applications it is often found to be useful to use a _mixed representation_ for the density matrix, in which we mix momentum and position. The idea for this comes from classical mechanics - recall (beginning of section A.1.2(b)) how we can in classical mechanics define a distribution function $\rho(P,Q;t)$ for an ensemble of classical systems in phase space. For a single particle in QM we define the analogous Wigner function as

$$\boxed{\begin{array}{l} f_w(\underline{p},\underline{r};t) = \int d^3x\, e^{-\frac{i}{\hbar}p\cdot x}\, \rho(\underline{r}+\tfrac{x}{2},\, r-\tfrac{x}{2};t) \\[2mm] \rho(\underline{r},\underline{r}';t) = \sum_p e^{\frac{i}{\hbar}p\cdot(\underline{r}-\underline{r}')}\, f_w(\underline{p},\tfrac{1}{2}(\underline{r}+\underline{r}'');t) \end{array}} \tag{156}$$

For an operator $\hat{A}(\underline{r})$ or $\hat{A}(\underline{p})$, we can write

$$\langle A \rangle = \int d^3r \sum_p A(r) f_w(\underline{p},r) \quad \text{or} \quad \int d^3r \sum_p A(\underline{p}) f_w(\underline{p},\underline{r}) \tag{157}$$

In particular
$$P(\underline{r}) \equiv \rho(\underline{r},\underline{r}) = \sum_p f_w(\underline{p},\underline{r}) \left.\begin{array}{c}\\\\\end{array}\right\}$$
$$P(\underline{p}) \equiv \rho(\underline{p},\underline{p}) = \int d^3r\, f_w(\underline{p},\underline{r}) \tag{158}$$

However we can't mix the two, ie.,

$$\langle A(r,p) \rangle \;\neq\; \sum_p \int d^3r \; f_w(p,r) \, A(r,p) \tag{159}$$

Thus in particular, we can't calculate the expectation value of the total energy just by integrating over the Wigner function, weighting with the Hamiltonian.

The Wigner function is crucially different from any classical distribution $\rho(P,Q)$ since it is complex (it is after all the density matrix, Fourier transformed!), and so we can't think of it as a probability distribution.

Simple Example: a Wave-Packet in 1-dimension

It is interesting to look at an example in which we have 2 simple wave-packets which interfere with each other. We consider first a pure state wave-function, and then look to see what happens when "decoherence" sets in, ie., we start to get a mixture component in the density matrix.
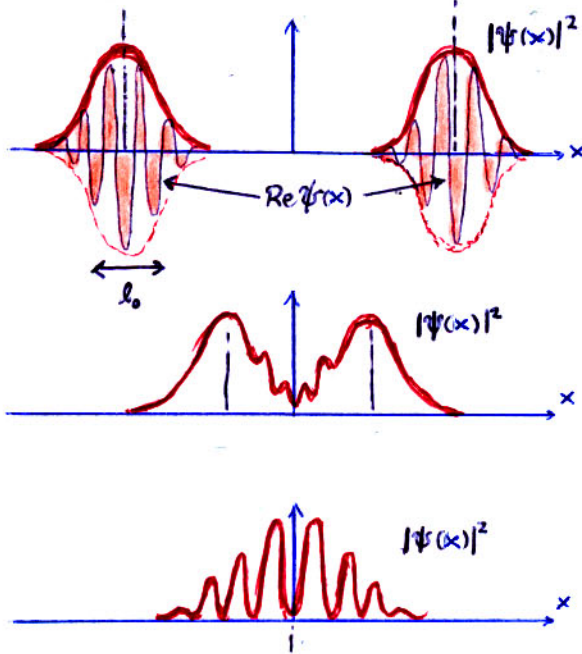
Suppose we have a pure state wave-function of form

$$\psi(x) = \tfrac{1}{2}\left[g(x-q_1) e^{ik_1 x} + g(x-q_2) e^{ik_2 x} \right] \tag{160}$$

which is a superposition of 2 wave-packets, each having the Gaussian normalised form factor

$$g(x) = \frac{1}{\pi^{1/2} \ell_0} e^{-(x/\ell_0)^2} \tag{161}$$

and with mean momentum k_1 and k_2 respectively.

If $|q_1 - q_2| \gg \ell_0$, so the wave-packets are widely separated, then there is little interference between them. We can write everything in terms of the centre of mass momentum K_0 and relative momentum K, with

$$\left. \begin{aligned} K_0 &= \tfrac{1}{2}(k_1 + k_2) \\ K &= \tfrac{1}{2}(k_1 - k_2) \end{aligned} \right\} \tag{162}$$

so that

$$\psi(x) = \tfrac{1}{2} e^{iK_0 x}\left[g(x-q_0) e^{iKx} + g(x+q_0) e^{-iKx} \right] \tag{163}$$

where we have also gone to the centre of mass frame with difference coordinate

$$\left. \begin{aligned} Q_0 &= \tfrac{1}{2}(q_1(t) + q_2(t)) \\ q_0(t) &= \tfrac{1}{2}(q_1(t) - q_2(t)) \end{aligned} \right\} \tag{164}$$

Without loss of generality we can also now assume that

$$K_0 = 0, \quad Q_0(t) = 0 \tag{165}$$

We then have

$$\left. \begin{aligned} \rho(x,x') = \tfrac{1}{4}\Big[& g(x-q_0)g(x'-q_0) e^{iK(x-x')} + g(x+q_0)g(x'+q_0) e^{-iK(x-x')} \\ + & g(x-q_0)g(x'+q_0) e^{iK(x+x')} + g(x+q_0)g(x'-q_0) e^{-iK(x+x')} \Big] \end{aligned} \right\} \tag{166}$$

in which we can pick out terms that involve the sum $x+x'$, and the difference $x-x'$.

Let us now look at different special cases of this, corresponding to what we see in the

wave-functions, and ask what happens when we start "decohering" them, ie., adding in an impure or mixture component. Consider first the case of widely separated wave-packets.

If we plot (166), then we get a rather illuminating result. The plot at left shows
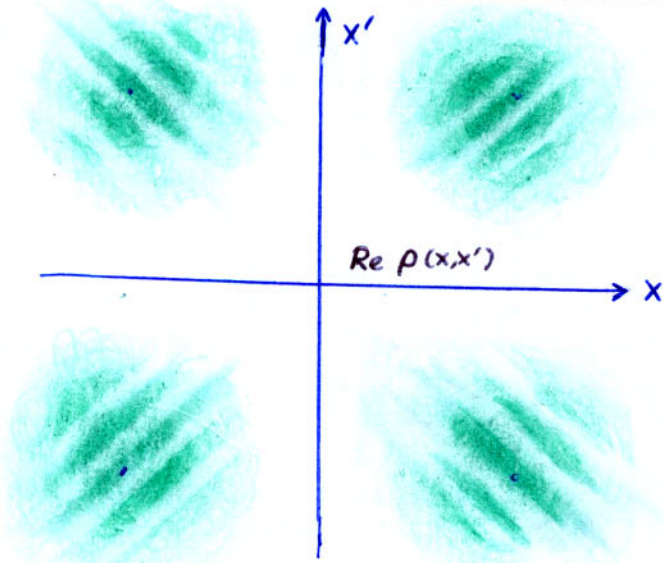
Re $\rho(x,x')$

$$Re\,\rho(x,x') =$$

$$\tfrac{1}{4}\left\{\,[g(x-q_0)g(x'-q_0) + g(x+q_0)g(x'+q_0)]\cos k(x-x')\right.$$
$$\left. + [g(x-q_0)g(x'+q_0) + g(x+q_0)g(x'-q_0)]\cos k(x+x')\right\} \quad (167)$$

and we see how the pair of Gaussians is multiplied by interference fringes referring to the sum and difference coordinates. However there is no interference in the wave-function itself between the 2 wave-packets — the diagonal part of ρ is given by

$$|\psi(x)|^2 \equiv \rho(x,x) \quad (168)$$

which for the general density matrix is just

$$\rho(x,x) = \tfrac{1}{4}\left[g^2(x-q_0) + g^2(x+q_0) + 2g(x-q_0)g(x+q_0)\cos 2kx\right] \quad (168)$$

and when $q_0 \gg \ell_0$, we have

$$\rho(x,x) \xrightarrow[q_0 \gg \ell_0]{} \tfrac{1}{4}\left[g^2(x-q_0) + g^2(x+q_0)\right] \quad (169)$$

However, as the wave-packets approach each other, things get more interesting. The 3rd interference term in (168) shows up along the diagonal ($x=x'$) in the plot of $\rho(x,x')$, and the 2 kinds of interference in (167) now appear together where there is overlap between the wave-packets. This we can see in the figure (a) at left. Finally, as the 2 wave-packets overlap completely, we go to figure (b) below left, for which we have

(a)
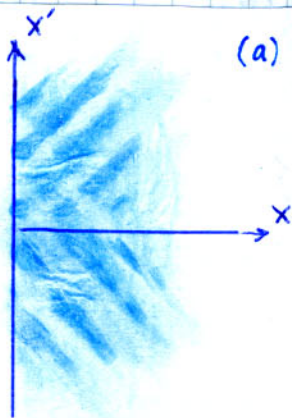
$$\rho(x,x') \xrightarrow[q_0 \to 0]{} g(x)g(x')\cos kx \cos kx'$$

$$\rho(x,x) = |\psi(x)|^2 \xrightarrow[q_0 \to 0]{} g^2(x)\cos^2 kx \quad \Biggr\} \quad (170)$$

and we see that interference fringes as functions of x and x' completely overlap.

Note that we could have also worked in momentum space. In this representation

(b)
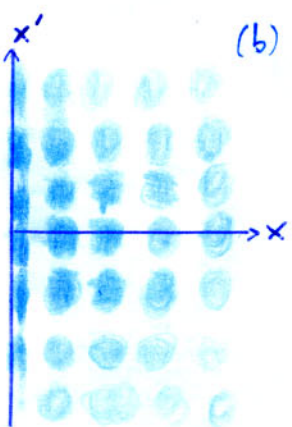
$$\psi(p) = \langle p|\psi\rangle$$

$$= \int dx\, e^{-ipx}\,\tfrac{1}{2}\left[g(x-q_1)e^{ik_1 x} + g(x-q_2)e^{ik_2 x}\right] \quad \Biggr\} \quad (171)$$

$$= \tfrac{1}{2}\left\{\bar{g}(p-k_1)e^{-i(p-k_1)q_1} + \bar{g}(p-k_2)e^{-i(p-k_2)q_2}\right\}$$

where $\quad \bar{g}(p) = \dfrac{\ell}{\pi^{1/2}}\,e^{-p^2 \ell_0^2} \quad (172)$

ie., we now have Gaussian wave-packets centred around k_1 and k_2 in momentum space, but having width $\Delta k \sim 1/\ell_0$.

Consider now the effect of decoherence. We will study this in more detail later, but here we can just note that by adding into $\rho(x, x')$ a mixture, we must be adding a function of x and x' which does not have any trace of interference in it. To see how this works, suppose instead of the wave-function in (160), we assume a mixture of the 2 wave-packets. This would imply a density matrix

$$\hat{\rho} = |\phi_1\rangle p_1 \langle \phi_1| + |\phi_2\rangle p_2 \langle \phi_2| \tag{173}$$

with components

$$\left. \begin{array}{l} \phi_1(x) = g(x-q_1) e^{ik_1 x} \\[6pt] \phi_2(x) = g(x-q_2) e^{ik_2 x} \end{array} \right\} \tag{174}$$

so that $\rho(x, x')$ is

$$\rho(x, x') = \tfrac{1}{2}\left[g(x-q_1)\, g(x'-q_1)\, e^{ik_1(x-x')} + g(x-q_2)\, g(x'-q_2)\, e^{ik_2(x-x')} \right] \tag{175}$$

We note immediately the difference (compare (166); the off-diagonal parts of the density matrix have gone. As an exercise you can redraw the plots for $\mathrm{Re}\,\rho(x, x')$, given on the last page, for this case.

In reality of course a density matrix will have both "coherent" (ie., corresponding to a pure state) & "incoherent" (ie., corresponding to a mixture) parts. Moreover, in any real physical situation, pure states tend to evolve towards mixed ones, so we will now see.

A.2.2(b) REDUCED DENSITY MATRICES; ENTANGLEMENT

Suppose we now extend the analysis here to 2 coupled systems (where the coupling is in general time-dependent, and can be zero). This then is the quantum version of the classical pair of systems considered in section A.1.1 (cf. eqtn. (23)). However the behaviour is very different. We assume a Hilbert space $\mathscr{H}(1,2) = \mathscr{H}_1 \otimes \mathscr{H}_2$, a product of the Hilbert spaces of each system. We assume that a general pure state $|\Psi\rangle$ for the combined system can be written in the form

$$|\Psi(1,2)\rangle = \sum_j \sum_\alpha c_{j\alpha} |\phi_j\rangle |\chi_\alpha\rangle \equiv \sum_{j\alpha} c_{j\alpha} |j\alpha\rangle \tag{176}$$

where the $\{|\phi_j(1)\rangle\}$ span $\mathscr{H}_1(1)$, and the $\{|\chi_\alpha(2)\rangle\}$ span $\mathscr{H}_2(2)$. Any operator $\hat{F}(1,2)$ acting on the combined system has expectation value

$$\langle \hat{F}(1,2)\rangle = \langle \Psi(1,2)| \hat{F}(1,2) |\Psi(1,2)\rangle \tag{177}$$

which in terms of the density matrix $\hat{\rho}(1,2) = |\Psi\rangle\langle\Psi| \tag{178}$

is just $\langle \hat{F}(1,2)\rangle = \mathrm{Tr}[\rho F] = \sum_{i\alpha}\sum_{j\beta} c_{i\alpha} c_{j\beta}^{\dagger} F_{j\beta, i\alpha} \tag{179}$

where $\hat{\rho}$ has matrix elements $\rho_{i\alpha, k\beta} = \langle i\alpha|\hat{\rho}|k\beta\rangle = c_{i\alpha} c_{k\beta}^{\dagger} \Big\}$

and $\hat{F}(1,2)$ has analogous matrix elements $F_{i\alpha, j\beta} = \langle i\alpha|A|j\beta\rangle \tag{180}$

So far so good. Now suppose we assume that the combined system is isolated, and has never ever correlated with any other system, so that it always remains in a pure state. Nevertheless there will still be internal correlations between the 2 systems, which

will show up in the density matrix, as off-diagonal matrix elements. These correlations go under the general name of _entanglement_ ; the details of this were first studied by Schrödinger in 1935, in the context of the famous EPR (Einstein-Podolsky-Rosen) paradox.

Simple Example : The TLS again

: Suppose we now consider a PAIR of TLSs. The density matrix is now a (4×4) matrix ; the general pure state has the form

$$|\Psi(1,2)\rangle = a_{11}|\uparrow\uparrow\rangle e^{i\phi_{11}} + a_{12}|\uparrow\downarrow\rangle e^{i\phi_{12}} + a_{21}|\downarrow\uparrow\rangle e^{i\phi_{21}} + a_{22}|\downarrow\downarrow\rangle e^{i\phi_{22}} \qquad (181)$$

so that $\hat{\rho}(1,2)$ is a complicated object. However let's compute 2 simple special cases of this:

(i) Suppose
$$|\Psi(1,2)\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow\uparrow\rangle + |\downarrow\uparrow\rangle e^{i\phi}\right]$$
$$\equiv \frac{1}{\sqrt{2}}(|\uparrow\rangle + e^{i\phi}|\downarrow\rangle)_1 \otimes |\uparrow\rangle_2 \qquad \Bigg\} \qquad (182)$$

so that
$$\langle \tau_z \delta_z | \hat{\rho} | \tau_z' \delta_z' \rangle = \frac{1}{2}\begin{pmatrix} 1 & 0 & e^{-i\phi} & 0 \\ 0 & 0 & 0 & 0 \\ e^{i\phi} & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad (183)$$

where we have written $\hat{\rho}$ in the basis of the z-components of the 2 spins τ and δ, ordered as $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle,$ and $|\downarrow\downarrow\rangle$.

(ii) Now suppose that
$$|\Psi(1,2)\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle e^{i\phi}\right] \qquad (184)$$

so that
$$\langle \tau_z \delta_z | \hat{\rho} | \tau_z' \delta_z' \rangle = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & e^{-i\phi} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ e^{i\phi} & 0 & 0 & 1 \end{pmatrix} \qquad (185)$$

At first glance there is no obvious difference between the 2 states. However there is a fundamental difference — the state (182) can be _factorized_ into a product state as shown, whereas (184) can not — the 2 systems in (184) are _entangled_.

How can we tell if a state is entangled or not? It is not obvious from inspection - however let us now look at one very clear way.

REDUCED DENSITY MATRIX $\bar{\rho}(1)$

: Suppose we are only interested in one of the two systems, and so we simply trace out (i.e., average over) the information about the other. Thus we define the reduced density matrix

$$\boxed{\bar{\rho}(1) = \mathrm{Tr}_2\left[\rho(1,2)\right]} \qquad (186)$$

where the trace is over all the variables/states in system 2. The reduced density matrix elements are then

$$\bar{\rho}_{ij} = \langle i | \bar{\rho}(1) | j \rangle = \sum_{\alpha} c_{i\alpha} c_{j\alpha}^* \qquad (187)$$

and $\bar{\rho}$ has form
$$\hat{\rho}(1) = \sum_{\alpha} \langle \alpha | \left\{ \sum_i \sum_{j\beta} |i\alpha\rangle c_{i\alpha} c_{j\beta}^* \langle j\beta| \right\} |\alpha\rangle = \sum_{\alpha} \sum_{ij} |i\rangle c_{i\alpha} c_{j\alpha}^* \langle j| \qquad (188)$$

Notice that this simple average gives equal weight to all the different states of the 2nd system - clearly this can be generalized.

Now notice that for any operator $\hat{A}(1)$ acting on system 1 alone, nothing changes; we have

$$\langle A(1) \rangle = \mathrm{Tr}\,[\bar{\rho}, A(1)].$$
$$\equiv \mathrm{Tr}\,[\rho(1,2)\, A(1)] \qquad\qquad\qquad (189)$$

However this is not the case for an operator $\hat{F}(1,2)$ acting on both systems. Then we would write

$$\langle A(1,2) \rangle \equiv \mathrm{Tr}_2 \langle A(1,2) \rangle \equiv \mathrm{Tr}\,[\rho(1)\, \mathrm{Tr}_2\, \hat{F}(1,2)]$$
$$\equiv \sum_{\alpha}\sum_{ij} \langle i|\bar{\rho}(1)|j\rangle \langle j\alpha|F(1,2)|i\alpha\rangle \qquad (190)$$
$$= \sum_{\alpha}\sum_{ij} c_{i\alpha}\, c_{j\alpha}^{*}\, F_{j\alpha, i\alpha}$$

The point is that all information about the correlations between systems 1 and 2 (i.e., about the entanglement between them) is lost once we go to $\bar{\rho}(1)$. Indeed we can see quite dramatically the difference between the reduced density matrices, depending on whether the initial combined state $\Psi(1,2)$ is entangled or not. Compare two diametrically opposed cases:

(i) <u>Unentangled product state</u>: Then $|\bar{\Psi}\rangle = \sum_{j\alpha} c_{j\alpha}|j\alpha\rangle = \sum_{j\alpha} a_j\, b_\alpha\, |j\rangle|\alpha\rangle$ $\quad$ (191)

and the full density matrix is $\quad \rho_{i\alpha j\beta} = a_i\, a_j^{*}\, b_\alpha\, b_\beta^{*}$ $\qquad\qquad$ (192)

with reduced density matrix $\quad \bar{\rho}_{ij} = a_i\, a_j^{*}$

(ii) <u>Fully entangled state</u>: Here we assume $|\Psi\rangle = \sum_{j} c_{j\alpha}|j\alpha\rangle = \sum_J c_J|\psi_J \chi_J\rangle$ $\quad$ (193)

i.e., every state of system 1 is uniquely correlated with a single state of system 2; it then follows that

$$\rho_{i\alpha, j\beta} = c_i\, c_j^{\dagger}\, \delta_{i\alpha}\, \delta_{j\beta} \qquad\qquad (194)$$
$$\bar{\rho}_{ij} = |c_j|^2\, \delta_{ij} = p_J\, \delta_{ij}$$

using (187) or (188). In other words, if we have 2 systems that are in a completely entangled pure state, averaging over one of them gives a completely incoherent mixture for the reduced density matrix of the other system. On the other hand if they are not entangled, then averaging over one has no effect on the other - it leaves it in a pure state.

However, we do not measure density matrices - they are not observables - but instead we measure operator expectation values. So the following result is then quite illuminating. Suppose we do in fact have an entangled state $|\Psi(1,2)\rangle$; which operators, acting on both system 1 and system 2, will reveal the entanglement? The answer is simple; for any such operator, the expectation value is

$$\langle \hat{F}(1,2) \rangle = \mathrm{Tr}_{1,2}\,[\hat{\rho}(1,2)\, \hat{F}(1,2)] = \sum_{i\alpha}\sum_{j\beta} c_{i\alpha}\, c_{j\beta}^{*}\, F_{j\beta, i\alpha} \qquad (195)$$

from (179), and this is indistinguishable from the result expected from a mixture, with a diagonal density matrix $|i\alpha\rangle c_{i\alpha} c_{i\alpha}^{*} \langle i\alpha|$, and expectation

$$\langle \hat{F}(1,2) \rangle_{\text{MIXTURE}} = c_{i\alpha}\, c_{j\alpha}^{*}\, F_{j\alpha, j\alpha} \qquad\qquad (196)$$

unless there are off-diagonal matrix elements $F_{i\alpha, j\beta}$ with $i \neq j$ and/or $\alpha \neq \beta$ in the

operator elements $F_{(\alpha,\beta)}$. Thus even the completely entangled state (193) cannot be distinguished from the entangled state (191) by an operator with only diagonal elements. Note we have already seen this result in the context of a single TLS (cf discussion between eqtns (137) and (138)).

We will return to a more detailed analysis of this when discussing measurement theory in section A.4. Let us briefly return to our example of two TLS's:

(i) If we take the factorized state $|\Psi(1,2)\rangle = \frac{1}{\sqrt{2}}[|\uparrow\uparrow\rangle + |\downarrow\uparrow\rangle e^{2i\phi}]$ in (182), we easily compute the reduced density matrix to be

$$\bar{\rho}_{ij}(1) = \frac{1}{2}\begin{pmatrix} 1 & e^{-i\phi} \\ e^{i\phi} & 1 \end{pmatrix} \tag{197}$$

which we notice is a pure state density matrix. As discussed after eqtn. (137), we cannot tell the difference between this state and a simple mixture of states $|\uparrow\rangle$ and $|\downarrow\rangle$, with density matrix

$$\bar{\rho}_{ij}^{MIXED} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{198}$$

except using operators like $\hat{\tau}_x$ or $\hat{\tau}_y$, with off-diagonal matrix elements in this basis

(ii) If we now take the entangled state $|\Xi(1,2)\rangle = \frac{1}{\sqrt{2}}[|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle e^{i\phi}]$, from (184), then the density matrix $\bar{\rho}(1)$ is

$$\bar{\rho}_{ij}(1) = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{199}$$

and all coherence has been lost - we have a simple mixture.

Finally, let's just note that reduced density matrices are actually a key part of both many-body physics & quantum field theory. We take the coordinates we are interested in to be "system 1", and the rest of the universe is "system 2". We then write the reduced density matrix, using (186), as

SYSTEM 1

$$\bar{\rho}(Q,Q') = Tr_X\left[\rho(Q,Q'; X,X)\right] \tag{200}$$

were

$$\left.\begin{array}{l} Q = (q_1, q_2 \cdots q_n) \\[6pt] X = (x_1, x_2, \ldots, x_N) \end{array}\right\} \tag{201}$$

are the coordinates of the "system" and "environment" respectively; the environmental Hilbert space can have a dimension N which is very large but finite, but the system Hilbert space is typically very small (one is normally interested in 1- or 2-particle correlation functions).

A.2.2 (c) THERMAL DENSITY MATRICES : A special case of a
reduced density matrix is that produced when the environment in eqtn (200) is considered to be in thermal eqlbm. Now in general one can vary the strength of both the coupling and the entanglement between the system and the environment. The 2 extremes here are

(i) were the coupling is very weak, and the system and environment start off

completely uncorrelated (i.e., disentangled), one can see that entanglement will slowly develop between the system and environment. Over a somewhat longer timescale, energy will be exchanged and eventually the system will come to equilibrium with the thermal bath. There are many examples of such behaviour at low temperatures - e.g., nuclear spins, or impurities, in a solid or a liquid.

The second extreme case is where the coupling is strong enough that the two reach equilibrium very quickly, and so one assumes that the system is strongly entangled with the environment.

Thus our 2 extreme cases can be described as follows:

$$\hat{\rho}(Q,Q'; X,X'; t=0) = \bar{\rho}(Q,Q') \rho(X,X'; \beta) \qquad \text{(disentangled)} \qquad (202)$$

where $\beta = 1/kT$; the initial density matrix is uncorrelated; and

$$\rho_E(Q,Q'; XX') = \sum_{j\alpha} \langle Q,X | j\alpha \rangle \, p_{j\alpha} \, \langle j\alpha | Q'x' \rangle \qquad \text{(EQUILIBRIUM)} \qquad (203)$$

where the probability $p_{j\alpha}$ is just the Boltzmann factor:

$$\left. \begin{array}{l} p_{j\alpha} = \dfrac{1}{Z} e^{-\beta E_{j\alpha}} \\[2mm] Z = \sum_{j\alpha} e^{-\beta E_{j\alpha}} \end{array} \right\} \qquad (204)$$

i.e., $Z(\beta)$ is just the partition function.

Often, in dealing with problems of this kind, and when dealing with the equilibrium thermal density matrix, one deals with the simple function

$$\hat{\rho}(\beta) = e^{-\beta \hat{\mathcal{H}}} \qquad (205)$$

This is because it satisfies the simple differential eqn $\boxed{\dfrac{\partial \hat{\rho}}{\partial \beta} = -\hat{\mathcal{H}} \hat{\rho}} \qquad (206)$

along with the simple "initial condition"
$$\hat{\rho}(\beta=0) = 1 \qquad (207)$$

In the position representation, this is $\partial_\beta \rho(xx'; \beta) = \hat{\mathcal{H}}_x \rho(xx'\beta) \qquad (208)$

with $\rho(xx'; \beta=0) = \delta(x-x')$.

It is fairly straightforward to solve this for simple Hamiltonians. Thus, for a free particle in a thermal bath, we have
$$\mathcal{H}_0 = P^2/2m \qquad (209)$$

so that
$$\frac{\partial}{\partial \beta} \rho_0(x,x';\beta) = \frac{\hbar^2}{2m} \partial_x^2 \rho_0(xx'\beta) \qquad (210)$$

which has solution
$$\rho_0(xx'\beta) = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{1}{2}} \exp\left\{-\left(\frac{m}{2\pi\hbar^2\beta}\right)(x-x')^2\right\} \qquad (211)$$

and a partition function
$$Z = \text{Tr}\,\rho = \int dx\, \rho(xx;\beta) = \left(\frac{m}{2\pi\hbar^2}\right)^{\frac{1}{2}} \qquad (212)$$

for a 1-d system.

Note that the eqn of motion (206) for $\rho(xx'\beta)$ is not the same as the usual operator eqn for the time evolution of $\hat{\rho}(xx';t)$, with the simple substitution $\beta = it$ (cf eqn (141)), although this is sometimes stated in the literature. One should view $\hat{\rho}(\beta)$ as an auxiliary quantity (albeit a very useful one).