NOTES ON THE INITIAL STATE AND THE RELATIVE PHASES OF AMPLITUDES IN QUANTUM MECHANICS

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It is shown that in constructing the initial state from given relative probability densities, one should not introduce arbitrary relative phases between the different amplitudes associated with the wave function (determined uniquely).

1. *Introduction*

When one is interested in the study of the time-evolution of a quantum mechanical system, it is imperative to specify the initial state. In the physical literature, this is often stated in various ways. Such statements can be divided into two basic categories as follows. The initial state $\Psi(t_0)$ at $t = t_0$, in general, is such that

$$(i) \qquad \Psi(t_0) = \sum_j a_j(t_0)\varphi_j(t_0), \quad \sum_j |a_j(t_0)|^2 = 1, \tag{1}$$

or

$$(ii) \qquad |(\tilde{\varphi}_j\Psi)(t_0)|^2 = |a_j(t_0)|^2, \quad \sum_j |a_j(t_0)|^2 = 1. \tag{2}$$

$\{\varphi_j\}$ is a complete set of wave functions. In most physical problems, the wave functions correspond to stationary states pertaining to a time independent Hamiltonian, but, in general, they may not necessarily be so. When φ_j are uniquely determined (including arbitrary unimodular constant phase factors in each of them), in the first case Eq. (1), the amplitudes a_j including the phase factors are known uniquely. It may not be irrelevant to mention that all the amplitudes a_j may be indeterminate because of a common (independent of j) phase factor as that of the wave function $\Psi(t_0)$. Since the Schrödinger equation is linear and homogeneous this will always appear as a constant factor. We will not dwell on this redundant unimodular common phase factor. On the other hand, in the formulation of the initial state according to the second case, Eq. (2), the amplitudes a_j are inde-

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terminate because of a unimodular phase factor; however, this formulation seems to be more adequate from the standpoint of the usual physical interpretation of wave mechanics.

This short article is devoted to the unique formulations of the initial state. As a matter of fact, in the second formulation, Eq. (2), apart from arbitrary unimodular factors in φ_j, the initial a_j may be taken as $+\sqrt{|a_j|^2} \exp i\eta_j$, ($\eta_j$ are real). Hence, the expression for the state at any other instant of time will depend explicitly on η_j. One may be tempted to say that the expectation value of an observable is obtained only after averaging over these phases. It is shown in the following section that such averages lead, in general, to results which are by no means physically acceptable. It seems that the first one may be made completely unambiguous and it should be preferred. It is of interest to note here that the ambiguity does not manifest itself only in some simple cases, *e. g.*, (*i*) when the initial state is such that $|a_j| = 1$, $a_k = 0, j \neq k$, this corresponds to a pure initial state if φ_j are stationary states, and (*ii*) when in the perturbation expansion one is confined only to first order terms. Since up to the present stage all applications of quantum mechanics are confined to these simple cases, the ambiguity discussed here is not evident.

2. The evolution in time of the amplitudes

Let the Schrödinger equation of the system be given by

$$i\hbar \frac{\partial \Psi}{\partial t} = \{H_1 + H_2(t)\}\Psi \tag{3}$$

where H_2 depends on time. Furthermore, let

$$i\hbar \frac{\partial \varphi_n}{\partial t} = H_1 \varphi_n. \tag{4}$$

If H_1 is independent of time, then φ_n are stationary states. However, we need not restrict ourselves to this case. On the other hand, we assume $\{\varphi_n(t)\}$ forms a complete set, for a fixed time t, in the configuration space. (The dependence of φ_j on time may be quite involved.) Let us seek the solution of Eq. (3) with the initial condition,

$$\Psi(t_0) = \sum_j A_j \varphi_j(t_0). \tag{5}$$

Since Eq. (3) is linear and homogeneous and $\{\varphi_j(t)\}$ forms a complete set, the solution $\Psi(t)$ is a bilinear combination of A_k and $\varphi_j(t)$. Thus

$$\Psi(t) = \sum_{j,k} \varphi_j(t) U_{jk}(t) A_k \tag{6}$$

where

$$U_{jk}(t_0) = \delta_{jk}. \tag{6'}$$

Let

$$B_j(t) = (\tilde{\varphi}_j(t) \cdot \Psi(t)) = \sum_k U_{jk}(t) A_k. \tag{7}$$

The probability of finding the system in the state $\varphi_j(t)$ at t is

$$|B_j(t)|^2 = \sum_{k,l} U^*_{jk}(t)U_{jl}(t)A^*_k A_l. \tag{8}$$

Now, if we take from Eq. (2)

$$A_k = |a_k|e^{i\eta_k}, \tag{9}$$

then $|B_j(t)|$ contains terms with $\cos(\eta_j - \eta_k)$ and $\sin(\eta_j - \eta_k)$, *i.e.* they depend upon relative phases. It should be emphasized that $U_{jk}(t)$ are independent of $|A_k|$ and $\arg A_k$. There are no physical observables associated with these phases; as a matter of fact, working rules in quantum mechanics are formulated so that these phases do not appear explicitly. At this stage one may argue that we should consider only the averages of these indeterminate phases. This is tantamount to

$$\overline{A^*_k A_l} = \delta_{kl}|A_k|^2. \tag{10}$$

But this leads to some drastic consequences as shown below.

From Eqs (3), (4), (6) and (7), it follows that

$$\frac{d}{dt}(B^*_j(t)B_k(t)) = \frac{i}{\hbar}\sum_l \{H_{2,lj}B^*_l(t)B_k(t) - H_{2,kl}B_l(t)B^*_j(t)\}. \tag{11}$$

Thus, if

$$\overline{B^*_l(t)B_k(t)} = \delta_{kl}|B_k| \tag{12}$$

at any instant t, then

$$\frac{d}{dt}\{B^*_l(t)B_k(t)\} = 0. \tag{13}$$

Hence,

$$|B_l(t)| = |B_l(t_0)| = A_l. \tag{14}$$

It should be noted that in Eq. (11) the hermiticity of the Hamiltonian has been used. Equation (14) states that relative population densities with respect to the states φ_l do not change at all with time. This is not physically agreeable, as noted in the introduction. Thus, such averages as in Eq. (10) are too severe in nature and lead to trivial results; hence, they are not acceptable. Therefore, the relative phases of a_j in Eq. (1) and A_j in Eq. (5) should be taken as zero.

What is more, Eq. (8) shows that if the initial state is such that $A_j = a_j\delta_{jk}\exp i\eta_k$ for a given k, the expressions for $|B_j|^2$ do not contain any phase as noted in the introduction. It may be emphasized that the results referred above are exact and no recourse to perturbation theory has been taken. On the other hand, if $H_2(\varepsilon, t)$ contains a small perturbation parameter ε and the perturbation expansion of the solution is taken, retaining only first order terms, then the cross terms such as $A^*_k A_l$ remain, in general. But in most physical problems $H_2(\varepsilon, t)$ is periodic (without any constant term) and these cross terms drop out when the corresponding physical quantity is averaged over time. However, even with second order terms (not to mention higher order terms), the contributions due to cross terms remain after suitable time averages are effected.

3. Discussion

It seems that in constructing the initial state, once the basis wave functions φ_j are determined without any arbitrary unimodular phase factor, all the coefficients a_j are uniquely given (but for a common phase factor) by the positive square root of the respective initial probability density. They are the only physical quantities which are needed to construct the initial state. Thus, the initial state should be given by Eq. (1) with a_j and φ_j as stated above. It should also be noted that from the point of view of the differential equation, a unique solution may be obtained only when $\Psi(t_0)$ is uniquely given as in Eq.(1). However, in writing Eq. (1) it is obvious that one may introduce $a_j \exp -i\zeta_j$ for a_j and $\varphi_j \exp i\zeta_j$ for φ_j (ζ_j are real). Such substitutions should not introduce any change in the observable quantities, as a_j and a_k^* are always associated with matrix elements formed by φ_j and $\tilde{\varphi}_k$ respectively, as well as with both φ_j and $\tilde{\varphi}_j$ simultaneously. Since they never appear separately, they are completely redundant.