اگر هامیلتونی تحت وارونی زمان ناوردا باشد و ویژه حالت انرژی آن ناتبهگن باشد، آیا تابع موج حتما حقیقی است؟

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Wave Function

Suppose at some given time, say at $t = 0$, a spinless single-particle system is found in a state represented by $|\alpha\rangle$.

Its wave function $\langle x'|\alpha\rangle$ appears as the expansion coefficient in the position representation

$$|\alpha\rangle = \int d^3x' \, |\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle$$

Applying the time-reversal operator

$$\Theta|\alpha\rangle = \int d^3x' \,\Theta|\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle^*$$

$$= \int d^3x' |\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle^*,$$

where we have chosen the phase convention so that $\Theta|x'\rangle$ is $|x'\rangle$ itself.

We then recover the rule

$$\psi(\mathbf{x}') \rightarrow \psi^*(\mathbf{x}')$$

inferred earlier by looking at the Schrodinger wave equation [see $\psi(x,t) = u_n(x)e^{-iE_t/\hbar}, \psi^*(x,-t) = u_n^*(x)e^{-iE_t/\hbar}$].

The angular part of the wave function is given by a spherical harmonic Y_l^m.

With the usual phase convention we have

$$Y_l^m(\theta,\phi) \rightarrow Y_l^{m*}(\theta,\phi) = (-1)^m Y_l^{-m}(\theta,\phi)$$

Now $Y_l^m(\theta,\varphi)$ is the wave function for $|l,m\rangle$ [see $\langle\hat{n}|l,m\rangle = Y_l^m(\theta,\varphi) = Y_l^m(\hat{n}\ )$]; therefore, from $\psi(x') \rightarrow \psi^*(x')$ we deduce

$$\Theta|l,m\rangle = (-1)^m|l,-m\rangle$$

If we study the probability current density $j(x,t) = \frac{\hbar}{m} Im(\psi^* \nabla \psi)$ for a wave function of type $\langle x'|n,l,m\rangle = R_{nl}(r)Y_l^m(\theta,\varphi)$ going like $R(r)Y_l^m$, we shall conclude that for m > 0 the current flows in the counterclockwise direction, as seen from the positive z-axis.

The wave function for the corresponding time-reversed state has its probability current flowing in the opposite direction because the sign of m is reversed.

All this is very reasonable.

As a nontrivial consequence of time-reversal invariance, we state an important theorem on the reality of the energy eigenfunction of a spinless particle.

Theorem.

Suppose the Hamiltonian is invariant under time reversal and the energy eigenket $|n\rangle$ is nondegenerate; then the corresponding energy eigenfunction is real (or, more generally, a real function times a phase factor independent of $\mathbf{x}$).

Proof:

To prove this, first note that

$$H\Theta|n\rangle = \Theta H|n\rangle = E_n\Theta|n\rangle$$

so $|n\rangle$ and $\Theta|n\rangle$ have the same energy.

The nondegeneracy assumption prompts us to conclude that $|n\rangle$ and $\Theta|n\rangle$ must represent the same state; otherwise there would be two different states with the same energy E_n, an obvious contradiction!

Let us recall that the wave functions for $|n\rangle$ and $\Theta|n\rangle$ are $\langle x'|n\rangle$ and $\langle x'|n\rangle^*$ respectively.

They must be the same—that is,

$$\langle \mathbf{x}'|n\rangle = \langle \mathbf{x}'|n\rangle^*$$

for all practical purposes—or, more precisely, they can differ at most by a phase factor independent of $\mathbf{x}$. ■

Thus if we have, for instance, a nondegenerate bound state, its wave function is always real.

On the other hand, in the hydrogen atom with $l \neq 0, m \neq 0$, the energy eigenfunction characterized by definite (n, l, m) quantum numbers is complex because Y_l^m is complex; this does not contradict the theorem because $|n, l, m\rangle$ and $|n, l, -m\rangle$ are degenerate.

Similarly, the wave function of a plane wave $e^{i\mathbf{p}.\mathbf{x}/\hbar}$ is complex, but it is degenerate with $e^{-i\mathbf{p}.\mathbf{x}/\hbar}$.

We see that for a spinless system, the wave function for the time-reversed state, say at t = 0, is simply obtained by complex conjugation.

In terms of ket $|\alpha\rangle$ written as in

$$|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \xrightarrow{K} |\tilde{\alpha}\rangle = \sum_{a'} \langle a'|\alpha\rangle^* K |a'\rangle$$
$$= \sum_{a'} \langle a'|\alpha\rangle^* |a'\rangle.$$

or in

$$|\alpha\rangle = \int d^3x' |\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle$$

the Θ operator is the complex conjugate operator K itself because K and Θ have the same effect when acting on the base ket |a'> (or |x'>).

It is apparent that the momentum-space wave function of the time-reversed state is not just the complex conjugate of the original momentum-space wave function; rather, we must identify $\phi^*(-\mathbf{p}')$ as the momentum-space wave function for the time-reversed state. This situation once again illustrates the basic point that the particular form of Θ depends on the particular representation used.

Time Reversal for a Spin $\frac{1}{2}$ System

The situation is even more interesting for a particle with spin—spin ½ , in particular.

We recall from Section 3.2 that the eigenket of $S.\hat{n}$ with eigenvalue $\frac{\hbar}{2}$ can be written as

$$|\hat{\mathbf{n}};+\rangle = e^{-iS_z\alpha/\hbar}e^{-iS_y\beta/\hbar}|+\rangle$$

where $\hat{n}$ is characterized by the polar and azimuthal angles β and α, respectively.

$$\Theta|\hat{\mathbf{n}};+\rangle = e^{-iS_z\alpha/\hbar}e^{-iS_y\beta/\hbar}\Theta|+\rangle = \eta|\hat{\mathbf{n}};-\rangle$$

Why?

$$\Theta|\hat{\boldsymbol{n}};+\rangle = \Theta e^{-iS_z\alpha/\hbar}e^{-iS_y\beta/\hbar}\Theta^{-1}\Theta|+\rangle$$

$$\Theta J\Theta^{-1} = -J$$

$$\Theta i\Theta^{-1} = -i$$

$$\Theta|\hat{\boldsymbol{n}};+\rangle = e^{-iS_z\alpha/\hbar}e^{-iS_y\beta/\hbar}\Theta|+\rangle$$

$$\Theta|+\rangle = +|-\rangle$$

Why?

$$S_z|+\rangle = \frac{\hbar}{2}|+\rangle$$

$$\Theta S_z\Theta^{-1}\Theta|+\rangle = \frac{\hbar}{2}\Theta|+\rangle$$

$$\Theta S_z \Theta^{-1} \Theta|+\rangle = \frac{\hbar}{2}\Theta|+\rangle$$

$$-S_z \Theta|+\rangle = \frac{\hbar}{2}\Theta|+\rangle$$

$$S_z(\Theta|+\rangle) = -\frac{\hbar}{2}(\Theta|+\rangle)$$

$$S_z|-\rangle = -\frac{\hbar}{2}|-\rangle$$

$\Theta|+\rangle = |-\rangle$ *up to a phase*

$\Theta|+\rangle = \eta|-\rangle$

for $\eta = 1$ we have

$$\Theta|\hat{\boldsymbol{n}};+\rangle = e^{-iS_z\alpha/\hbar}e^{-iS_y\beta/\hbar}|-\rangle$$

$\Theta|-\rangle = -|+\rangle$

$\Theta^2 = -1$

More generally for spin j system

$\Theta^2 = (-1)^{2j}$

On the other hand, we can easily verify that

$$|\hat{\mathbf{n}};-\rangle = e^{-i\alpha S_z/\hbar}e^{-i(\pi+\beta)S_y/\hbar}|+\rangle$$

Why?

$$e^{-iS_y\pi/\hbar}|+\rangle = |-\rangle$$

In general, we saw earlier that the product UK is an antiunitary operator.

Comparing the above two equations with Θ set equal to UK, and noting that K acting on the base ket |+> gives just |+>, we see that

$$\Theta = \eta e^{-i\pi S_y/\hbar} K = -i\eta\left(\frac{2S_y}{\hbar}\right)K$$

where η stands for an arbitrary phase (a complex number of modulus unity).

$\Theta = UK = -i\delta_y K$

$\Theta^{-1} = -\Theta = i\delta_y K$

Why?

$$\exp\left(\frac{-i\sigma_3\alpha}{2}\right)\exp\left(\frac{-i\sigma_2\beta}{2}\right)\exp\left(\frac{-i\sigma_3\gamma}{2}\right)$$

$$= \begin{pmatrix} e^{-i\alpha/2} & 0 \\ 0 & e^{i\alpha/2} \end{pmatrix} \begin{pmatrix} \cos(\beta/2) & -\sin(\beta/2) \\ \sin(\beta/2) & \cos(\beta/2) \end{pmatrix} \begin{pmatrix} e^{-i\gamma/2} & 0 \\ 0 & e^{i\gamma/2} \end{pmatrix}$$

$$= \begin{pmatrix} e^{-i(\alpha+\gamma)/2}\cos(\beta/2) & -e^{-i(\alpha-\gamma)/2}\sin(\beta/2) \\ e^{i(\alpha-\gamma)/2}\sin(\beta/2) & e^{i(\alpha+\gamma)/2}\cos(\beta/2) \end{pmatrix}, \qquad (3.3.21)$$

$$d^{(j)}_{m'm}(\beta) \equiv \langle j, m' | \exp\left(\frac{-iJ_y\beta}{\hbar}\right) | j, m\rangle$$

$$\Theta = \eta e^{-i\pi S_y/\hbar}K = -i\eta\left(\frac{2S_y}{\hbar}\right)K$$

$$d^{(1/2)} = \begin{pmatrix} \cos\left(\frac{\beta}{2}\right) & -\sin\left(\frac{\beta}{2}\right) \\ \sin\left(\frac{\beta}{2}\right) & \cos\left(\frac{\beta}{2}\right) \end{pmatrix}$$

$$\Theta = UK = -i\delta_y K$$

$$\Theta^{-1} = -\Theta = i\delta_y K$$

$$\boldsymbol{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \boldsymbol{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\Theta\begin{pmatrix}1\\0\end{pmatrix} = UK\begin{pmatrix}1\\0\end{pmatrix} = -i\delta_y K\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}=\begin{pmatrix}0\\1\end{pmatrix}=\begin{pmatrix}0\\1\end{pmatrix}$$

$$\Theta\begin{pmatrix}0\\1\end{pmatrix} = UK\begin{pmatrix}0\\1\end{pmatrix} = -i\delta_y K\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix}=\begin{pmatrix}-1\\0\end{pmatrix}=-\begin{pmatrix}1\\0\end{pmatrix}$$

Another way to be convinced of the last equation is to verify that if $\chi(\hat{\boldsymbol{n}};+)$is the two-component eigenspinor corresponding to $|\hat{\boldsymbol{n}};+\rangle$ [in the sense that $\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{n}}\chi(\hat{\boldsymbol{n}};+) = \chi(\hat{\boldsymbol{n}};+)$], then$-i\sigma_y\chi^*\,(\hat{\boldsymbol{n}};+)$ (note the complex conjugation!) is the eigenspinor corresponding to $|\hat{\boldsymbol{n}};-\rangle$, again up to an arbitrary phase, see Problem 7 of this chapter.

7. a. Let $\psi(\mathbf{x}, t)$ be the wave function of a spinless particle corresponding to a plane wave in three dimensions. Show that $\psi^*(\mathbf{x}, -t)$ is the wave function for the plane wave with the momentum direction reversed.

b. Let $\chi(\hat{\mathbf{n}})$ be the two-component eigenspinor of $\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}$ with eigenvalue $+1$. *Using the explicit form of* $\chi(\hat{\mathbf{n}})$ (in terms of the polar and azimuthal angles β and γ that characterize $\hat{\mathbf{n}}$) verify that $-i\sigma_2\chi^*(\hat{\mathbf{n}})$ is the two-component eigenspinor with the spin direction reversed.

Let us now note

$$e^{-i\pi S_y/\hbar}|+\rangle = +|-\rangle, \qquad e^{-i\pi S_y/\hbar}|-\rangle = -|+\rangle$$

Using the above relations, we are in a position to work out the effect of Θ, written as $\Theta = \eta e^{-i\pi S_y/\hbar}$, on the most general spin ½ ket:

$$\Theta\left(c_+|+\rangle + c_-|-\rangle\right) = +\eta c_+^*|-\rangle - \eta c_-^*|+\rangle$$

Let us apply Θ once again:

$$\Theta^2(c_+|+\rangle + c_-|-\rangle) = -|\eta|^2 c_+|+\rangle - |\eta|^2 c_-|-\rangle$$
$$= -(c_+|+\rangle + c_-|-\rangle)$$

Or

$$\Theta^2 = -1$$

(where -1 is to be understood as -1 times the identity operator) for any spin orientation.

This is an extraordinary result.

It is crucial to note here that our conclusion is completely independent of the choice of phase;

$\Theta^2 = -1$ holds no matter what phase convention we may use for η.

In contrast, we may note that two successive applications of Θ to a spinless state give

$$\Theta^2 = +1$$

as is evident from, say, $\Theta|l, m\rangle = (-1)^m |l, -m\rangle$.

More generally, we now prove

$$\Theta^2 |j \text{ half-integer}\rangle = -|j \text{ half-integer}\rangle$$

$$\Theta^2 |j \text{ integer}\rangle = +|j \text{ integer}\rangle.$$

Thus the eigenvalue of Θ^2 is given by $(-1)^{2j}$.

Having worked out the behavior of angular-momentum eigenstates under time reversal, we are in a position to study once again the expectation values of a Hermitian operator.

Recalling $\langle \alpha | A | \alpha \rangle = \pm \langle \tilde{\alpha} | A | \tilde{\alpha} \rangle$, we obtain under time reversal (canceling the i^{2m} factors)

$$\langle \alpha, j, m | A | \alpha, j, m \rangle = \pm \langle \alpha, j, -m | A | \alpha, j, -m \rangle$$

Now suppose A is a component of a spherical tensor $T_q^{(k)}$.

$$T_q^{(k)} = Y_{l=k}^{m=q}(\mathbf{V})$$

Because of the Wigner-Eckart theorem, it is sufficient to examine just the matrix element of the $q = 0$ component.

In general, $T^{(k)}$ (assumed to be Hermitian) is said to be even or odd under time reversal depending on how its $q = 0$ component satisfies the upper or lower sign in

$$\Theta T_{q=0}^{(k)} \Theta^{-1} = \pm T_{q=0}^{(k)}$$

Equation $\langle\alpha, j, m|A|\alpha, j, m\rangle = \pm\langle\alpha, j, -m|A|\alpha, j, -m\rangle$ for $A = T_0^{(k)}$ becomes

$$\langle\alpha, j, m|T_0^{(k)}|\alpha, j, m\rangle = \pm\langle\alpha, j, -m|T_0^{(k)}|\alpha, j, -m\rangle$$

Due to the following realtions, we expect $|\alpha, j, -m\rangle = \mathscr{D}(0, \pi, 0)|\alpha, j, m\rangle$ up to a phase.

$$|\hat{\mathbf{n}}\rangle = \mathscr{D}(R)|\hat{\mathbf{z}}\rangle$$

$$\mathscr{D}(R) = \mathscr{D}(\alpha = \phi, \beta = \theta, \gamma = 0)$$

$$|\hat{\mathbf{n}}\rangle = \sum_l \sum_m \mathscr{D}(R)|l, m\rangle\langle l, m|\hat{\mathbf{z}}\rangle$$

$$\langle l, m'|\hat{\mathbf{n}}\rangle = \sum_m \mathscr{D}^{(l)}_{m'm}(\alpha = \phi, \beta = \theta, \gamma = 0)\langle l, m|\hat{\mathbf{z}}\rangle$$

We next use the following expression for $T_0^{(k)}$

$$\mathscr{D}^\dagger(R)T_q^{(k)}\mathscr{D}(R) = \sum_{q'=-k}^{k} \mathscr{D}_{qq'}^{(k)*}(R)T_{q'}^{(k)}$$

Or equivalently

$$\mathscr{D}(R)T_q^{(k)}\mathscr{D}^\dagger(R) = \sum_{q'=-k}^{k} \mathscr{D}_{q'q}^{(k)}(R)T_{q'}^{(k)}$$

which leads to

$$\mathscr{D}^\dagger(0,\pi,0)T_0^{(k)}\mathscr{D}(0,\pi,0) = (-1)^k T_0^{(k)} + (q \neq 0 \text{ components})$$

where we have used $\mathscr{D}_{00}^{(k)}(0,\pi,0) = P_k(\cos\pi) = (-1)^k$, and the $q \neq 0$ components give vanishing contributions when sandwiched between $\langle\alpha, j, m|$ and $|\alpha, j, m\rangle$.

The net result is

$$\langle\alpha, j, m|T_0^{(k)}|\alpha, j, m\rangle = \pm(-1)^k\langle\alpha, j, m|T_0^{(k)}|\alpha, j, m\rangle$$

As an example, taking $k=1$, the expectation value $\langle\mathbf{x}\rangle$ taken with respect to eigenstates of j, m vanishes. We may argue that we already know $\langle\mathbf{x}\rangle = 0$ from parity inversion if the expectation value is taken with respect to parity eigenstates [see (4.2.41)]. But note that here $|\alpha, j, m\rangle$ need not be parity eigenkets! For example, the $|j, m\rangle$ for spin $\frac{1}{2}$ particles could be $c_s|s_{1/2}\rangle + c_p|p_{1/2}\rangle$.

$$T_q^{(k)} = Y_{l=k}^{m=q}(\mathbf{V})$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\frac{z}{r} \to T_0^{(1)} = \sqrt{\frac{3}{4\pi}}V_z,$$

$$Y_1^{\pm1} = \mp\sqrt{\frac{3}{4\pi}}\frac{x \pm iy}{\sqrt{2}\,r} \to T_{\pm1}^{(1)} = \sqrt{\frac{3}{4\pi}}\left(\mp\frac{V_x \pm iV_y}{\sqrt{2}}\right)$$