1 Dirac–Frenkel variational principal

Time dependant Shroedinger equation:

$$i\hbar\frac{\partial|\Phi_{ex}\rangle}{\partial t} = \hat{H}|\Phi_{ex}\rangle \tag{1}$$

We will consider the following mean value:

$$W = \frac{\langle\Phi|\hat{H} - i\hbar\frac{\partial}{\partial t}|\Phi\rangle}{\langle\Phi|\Phi\rangle}$$

which, if calculated on exact solutions $|\Phi_{ex}\rangle$ of (1), equals to zero, and its variation: $\delta W = 0$

If $|\Phi_{ex}\rangle$ is an exact solution of (1), then the norm conservation condition is satisfied:

$$\frac{\partial\langle\Phi_{ex}|\Phi_{ex}\rangle}{\partial t} = 0$$

But we do not know beforehand about norm of arbitrary function $|\Phi\rangle$. We can consider mean value of $i\hbar\frac{\partial}{\partial t}$:

$$\langle\omega\rangle = \frac{\langle\Phi|i\hbar\frac{\partial}{\partial t}|\Phi\rangle}{\langle\Phi|\Phi\rangle}$$

Let us will calculate difference between $\langle\omega\rangle$ and its complex conjugate:

$$\langle\omega\rangle - \langle\omega\rangle^* = \frac{i\hbar(\langle\Phi|\frac{\partial\Phi}{\partial t}\rangle + \langle\frac{\partial\Phi}{\partial t}|\Phi\rangle)}{\langle\Phi|\Phi\rangle}$$

$$\frac{i}{\hbar}\left(\langle\omega\rangle^* - \langle\omega\rangle\right) = \frac{\partial}{\partial t}\ln\langle\Phi|\Phi\rangle$$

Now we will solve this equation to obtain time dependance of norm:

$$N(t) = N(0)e^P,\ \text{where } P = \frac{i}{\hbar}\int_0^t \left(\langle\omega\rangle^* - \langle\omega\rangle\right)\, dt'$$

We see, that if function has a conserved norm, then $P = 0,\ \langle\omega\rangle \in \mathbb{R}$ and hence $W \in \mathbb{R}$ But if it is an approximate solution we can not guarantee conservation of norm!

But let us assume, that we can construct function $|\Phi'\rangle$, that differes from $|\Phi\rangle$ by angular multiplier:

$$|\Phi'\rangle = |\Phi\rangle \cdot e^Q,\ \text{where } Q = \frac{i}{\hbar}\int_0^t \alpha(t')\, dt',\ \alpha(t') \in \mathbb{C}$$

We need to find parameter $\alpha(t)$, so that norm $\langle \Phi' | \Phi' \rangle$ is conserved. Once again, we will consider a mean value:

$$\langle \omega' \rangle = \frac{\langle \Phi' | i\hbar \frac{\partial}{\partial t} | \Phi' \rangle}{\langle \Phi' | \Phi' \rangle} = \frac{\langle \Phi | e^{-Q} i\hbar \cdot \frac{i}{\hbar} \alpha(t) e^{Q} + i\hbar \frac{\partial}{\partial t} | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \langle \omega \rangle - \alpha$$

If $\langle \omega' \rangle \in \mathbb{R}$, then:

$$0 = \langle \omega' \rangle - \langle \omega' \rangle^* = \langle \omega \rangle - \langle \omega \rangle^* - 2iIm(\alpha)$$

$$iIm(\alpha) = \frac{1}{2} \left(\langle \omega \rangle - \langle \omega \rangle^* \right)$$

$$\alpha = Re(\alpha) + iIm(\alpha) = Re(\alpha) + \frac{1}{2} \left(\langle \omega \rangle - \langle \omega \rangle^* \right)$$

$$\langle \omega' \rangle = \langle \omega \rangle - \alpha = \langle \omega \rangle - \frac{1}{2} \left(\langle \omega \rangle - \langle \omega \rangle^* \right) - Re(\alpha) = \frac{1}{2} \left(\langle \omega \rangle + \langle \omega \rangle^* \right) - Re(\alpha)$$

$$|\Phi' \rangle = |\Phi \rangle \cdot e^{Q} = |\Phi \rangle \cdot e^{R} \cdot e^{-0.5P}, \text{ where } R = \frac{i}{\hbar} \int_0^t Re(\alpha(t'))\, dt'$$

As $N(t) = N(0) \cdot e^{P}$, we have:

$$|\Phi' \rangle = |\Phi \rangle \cdot e^{R} \cdot \left(\frac{N(0)}{N(t)} \right)^{1/2}$$

As we've discussed previously, for exact solution of (1) $|\Phi_{ex}\rangle$ mean value W equals to zero. Let us consider mean values W', calculated on function $|\Phi'\rangle$:

$$W' = \langle H \rangle - \langle \omega' \rangle = \langle H \rangle - \frac{1}{2} \left(\langle \omega \rangle + \langle \omega \rangle^* \right) + Re(\alpha)$$

Now we need to understand, what α should be to make W' equal to zero:

$$Re(\alpha) = -\langle H \rangle + \frac{1}{2} \left(\langle \omega \rangle + \langle \omega \rangle^* \right)$$

$$\alpha = -\langle H \rangle + \frac{1}{2} \left(\langle \omega \rangle + \langle \omega \rangle^* \right) + \frac{1}{2} \left(\langle \omega \rangle - \langle \omega \rangle^* \right) = \langle \omega \rangle - \langle H \rangle = -W$$

But if $\alpha = -W$, we will obtain:

$$|\Phi' \rangle = |\Phi \rangle \cdot e^{-\frac{i}{\hbar} \int_0^t W\, dt}$$

$$\langle \Phi' | \Phi' \rangle_t = \langle \Phi | \Phi \rangle_t \cdot e^{-\frac{i}{\hbar} \int_0^t (W - W^*)\, dt} = \langle \Phi | \Phi \rangle_0 \cdot e^{P} \cdot e^{-P} = \langle \Phi | \Phi \rangle_0$$

So we have built functions $|\Phi'\rangle$, that have conserved norm and lead to zero W'.

Let us consider for simplicity function $|\Psi\rangle$ to be from the family of functions $|\Phi'\rangle$. This function has conserved norm, and mean value W, calculated on this function, is zero. As the norm of $|\Psi\rangle$ doesn't change with time, we can write the following equation:

$$\delta\langle\Psi|\Psi\rangle = \langle\delta\Psi|\Psi\rangle + \langle\Psi|\delta\Psi\rangle = 0 \tag{2}$$

If our variation is arbitrary, then we will obtain two equations:

$$\langle\delta\Psi|\Psi\rangle = 0,\ \langle\Psi|\delta\Psi\rangle = 0$$

Thus we should consider only those variations $|\delta\Psi\rangle$, that are orthogonal to $|\Psi\rangle$.

Now we can write down variation δW. For simplicity, we shall denote $\langle\Psi|\hat{H} - i\hbar\frac{\partial}{\partial t}|\Psi\rangle$ as A and $\langle\Psi|\Psi\rangle$ as B:

$$W = \frac{A}{B},\ \delta W = \frac{B \cdot \delta A - A \cdot \delta B}{B^2} = \frac{\delta A - W\delta B}{B}$$

$$\delta A - W\delta B = \langle\delta\Psi|\hat{H} - i\hbar\frac{\partial}{\partial t}|\Psi\rangle + \langle\Psi|\hat{H} - i\hbar\frac{\partial}{\partial t}|\delta\Psi\rangle - W\langle\delta\Psi|\Psi\rangle - W\langle\Psi|\delta\Psi\rangle =$$

$$= \langle\delta\Psi|\hat{H} - i\hbar\frac{\partial}{\partial t}|\Psi\rangle + \langle\Psi|\hat{H} - i\hbar\frac{\partial}{\partial t}|\delta\Psi\rangle - W\delta\langle\Psi|\Psi\rangle$$

As $\delta\langle\Psi|\Psi\rangle = 0,\ \delta W = 0$, we obtain:

$$\langle\delta\Psi|\hat{H} - i\hbar\frac{\partial}{\partial t}|\Psi\rangle = 0 \text{ — Dirac–Frenkel variational principal} \tag{3}$$

$$\langle\Psi|\hat{H} - i\hbar\frac{\partial}{\partial t}|\delta\Psi\rangle = 0$$

We shall consider the second equation:

$$\langle\Psi|\hat{H} - i\hbar\frac{\partial}{\partial t}|\delta\Psi\rangle = \left\langle \left(\hat{H} - i\hbar\frac{\partial}{\partial t}\right)\Psi \middle| \delta\Psi \right\rangle - i\hbar\left\langle \frac{\partial\Psi}{\partial t} \middle| \delta\Psi \right\rangle - i\hbar\left\langle \Psi \middle| \frac{\partial}{\partial t}\delta\Psi \right\rangle =$$

$$= \langle\delta\Psi|\hat{H} - i\hbar\frac{\partial}{\partial t}|\Psi\rangle^* - i\hbar\frac{\partial}{\partial t}\langle\Psi|\delta\Psi\rangle = 0$$

Thus, the second equation is a mere consiquence of Dirac–Frenkel variational principal (3) and condition (2).