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Application of Schrödinger Equation to an Alpha Field in Nanorobotics

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As it is well known, nanorobotics is the field that deals with the controlled manipulation with atomic and molecular-sized objects [1]. At the nanoscale the control dynamics is very complex because there are very strong interactions between nanorobots, manipulated objects and nanoenvironment in a multipotential field. The problem is to design the control dynamics that will compensate or/and control the mentioned interactions. Generally, at the nanoscale the well known quantum efects can not be neglected. Therefore one has to include the Schrödinger equation that describes how the quantum state of a physical system changes in time. Thus, for a general quantum system one can employ time dependent Schrödinger equation [2]:

$$i\hbar \frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \hat{\boldsymbol{H}}\,\Psi(\mathbf{r},t). \tag{1}$$

Here $\Psi(\mathbf{r},t)$ is the wave function, which is the probability amplitude for different configurations of the system. Parameter $\hbar$ is the reduced Planck's constant and $\mathbf{r} = (x, y, z)$ is the particle position in three-dimensional space. With $\hat{\boldsymbol{H}}$ is denoted the related Hamiltonian operator. Thus, for application of Schrödinger equation to a multipotential Alpha Field one should found out the related Hamiltonian operator $\hat{\boldsymbol{H}}_\alpha$ as the function of the field parameter α and α' of that field. Generally, there are four solutions for field parameters α and α' (like in Dirac's theory) as the dimensionless functions of the total potential energy U_α of a particle in the related potential field. For the simplicity here will be presented the first solution only [3]:

$$\alpha = 1 + i\sqrt{\frac{2U_\alpha}{m_0c^2} + \left(\frac{U_\alpha}{m_0c^2}\right)^2}, \quad \alpha' = 1 - i\sqrt{\frac{2U_\alpha}{m_0c^2} + \left(\frac{U_\alpha}{m_0c^2}\right)^2}, \quad \alpha - \alpha' = 2\,i\sqrt{\frac{2U_\alpha}{m_0c^2} + \left(\frac{U_\alpha}{m_0c^2}\right)^2},$$
$$\alpha\alpha' = \left(1 + \frac{2U_\alpha}{m_0c^2} + \left(\frac{U_\alpha}{m_0c^2}\right)^2\right) = \left(1 + \frac{U_\alpha}{m_0c^2}\right)^2, \quad \rightarrow \quad U_\alpha = \left(\sqrt{\alpha\alpha'} - 1\right)m_0c^2. \tag{2}$$

In the equations (2) m_o is a rest mass of a particle, c is the speed of the light in a vacuum and $i = \sqrt{(-1)}$ is an imaginary unit. The relations in (2) are valid for a strong potential field. Meanwhile, in the case of a weak potential field ($U_\alpha << m_oc^2$) the quadratic term $(U_\alpha/m_oc^2)^2$ can be neglected in the relations (2). Now, we can define an Alpha Field as any potential field that can be described by the field parameters α and α'. To this category belong, among the others, an electromagnetic field and a gravitational field.

At the nanoscale control of a particle (sample) motion or/and manipulation with nanorobots, we usually have the multi-potential field with n-potentials, plus an artificial control field of the nanorobot that influents to the particle with a potential energy U_c. Thus, the related potential energy of the particle (sample) in that case can be calculated by using the following equation:

$$U_\alpha = U_1 + U_2 + .. + U_n + U_c = \Sigma U_j + U_c, \qquad j = 1, 2, .., n. \tag{3}$$

In the relation (3) U_j is a potential energy of the particle in the j-th potential field. Starting with (2) and (3), the relativistic Hamiltonian $\boldsymbol{H}$ has been derived in the reference [4], with the following form:

$$\left(\frac{\boldsymbol{H}}{\sqrt{\alpha\alpha'}}\right)^2\frac{1}{c^2}-\left(\frac{P}{\sqrt{\alpha\alpha'}}\right)^2=m_0c^2,\quad \boldsymbol{H}_e=\frac{\boldsymbol{H}}{\sqrt{\alpha\alpha'}},\quad P_e=\frac{P}{\sqrt{\alpha\alpha'}}\quad\rightarrow\quad\frac{\boldsymbol{H}_e^2}{c^2}-P_e^2=m_0c^2. \tag{4}$$

In the relation (4) $\boldsymbol{H}_e$ is the extended Hamiltonian and P_e is the extended momentum. Now, including the relations (2), where the total potential energy U_α is a nonlinear function of the relativistic invariant term αα', we can derive the nonlinear form of the relativistic Hamiltonian $\boldsymbol{H}_\alpha$:

$$\boldsymbol{H}_\alpha=c\sqrt{m_0^2c^2+\left(P-\frac{P\,U_\alpha}{m_0c^2}\right)^2}+U_\alpha,\quad P_e=\left(P-\frac{P\,U_\alpha}{m_0c^2}\right),\quad P=Hm_0v,\quad H=\left(1-\frac{v_\alpha^2}{c^2}\right)^{-1/2}. \tag{5}$$

This Hamiltonian is a function of the extended momentum P_e and potential energy U_α of the particle in the related multipotential field. Here v is a particle velocity in a vacuum, while v_α is a particle velocity in an Alpha Field, v_α= v-(α-α')c/2. In a nonrelativistic case ($v_\alpha << c$), the parameter H from (5) is close to one (H ≅ 1) and momentum P = m_ov. For that case the relation (5) is transformed into the form:

$$\boldsymbol{H}_\alpha\cong m_0c^2+\frac{1}{2m_0}\left(P-\frac{v\,U_\alpha}{c^2}\right)^2+U_\alpha,\qquad \boldsymbol{H}_{\alpha_R}\cong\frac{1}{2m_0}\left(P-\frac{v\,U_\alpha}{c^2}\right)^2+U_\alpha. \tag{6}$$

Here $\boldsymbol{H}_\alpha$ is a nonrelativistic approximation of the Hamiltonian in a weak potential Alpha Field. The reduced nonrelativistic approximation of the Hamiltonian, $\boldsymbol{H}_{\alpha R}$, is without rest-mass energy, m_oc^2.

In order to apply nonrelativistic Hamiltonian (6) into the nonrelativistic quantum systems one should employ the reduced nonrelativistic approximation of the Hamiltonian, $\boldsymbol{H}_{\alpha R}$. Thus, starting with the second equation in (6), the related Hamiltonian operator can be derived in the following form:

$$\hat{\boldsymbol{H}}_\alpha=-\frac{\hbar^2}{2m_0}\nabla_e^2+U_\alpha(\mathbf{r})=-\frac{\hbar^2}{2m_0}[\left(\frac{\partial}{\partial x}-i\frac{v_xU_\alpha}{\hbar c^2}\right)^2+\left(\frac{\partial}{\partial y}-i\frac{v_yU_\alpha}{\hbar c^2}\right)^2+\left(\frac{\partial}{\partial z}-i\frac{v_zU_\alpha}{\hbar c^2}\right)^2]+U_\alpha(\mathbf{r}). \tag{7}$$

Here ∇_e^2 is the extended Laplacian operator. Applying the Hamiltonian operator from (7) to (1) we obtain the time dependent Schrödinger equation for a single particle in three dimensional space:

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t)=-\frac{\hbar^2}{2m_0}\nabla_e^2\,\Psi(\mathbf{r},t)+U_\alpha(\mathbf{r})\Psi(\mathbf{r},t). \tag{8}$$

Here Ψ(**r**,t) is the wave function, which is the amplitude for the particle to have a given position **r** at any given time t, and U_α(**r**) is the potential energy of the particle at each position **r** in an Alpha Field.

For every time independent Hamiltonian operator $\hat{\boldsymbol{H}}_\alpha$ there exists a set of quantum states $|\Psi_n\rangle$ known as energy eigenstates and corresponding real numbers E_n satisfying the eigenvalue equation:

$$\boldsymbol{H}_\alpha\,|\Psi_n\rangle=E_n\,|\Psi_n\rangle,\quad\rightarrow\quad\boldsymbol{H}_\alpha=-\frac{\hbar^2}{2m_0}\nabla_e^2+U_\alpha=\frac{1}{2m_0}\left(P-\frac{v\,U_\alpha}{c^2}\right)^2+U_\alpha. \tag{9}$$

This is the time independent Schrödinger equation. For the case of a single particle, the Hamiltonian $\boldsymbol{H}_\alpha$ is the linear operator given by the second equation in (9). This is a self-adjoint operator when U_α is not too singular and does not grow too fast. The presented Schrödinger equations describe a particle dynamics in an Alpha Field, without spin effects. For inclusion of the spin effects one should employ the related Dirac's equations. Dynamics of the quantum feedback systems and control concepts and applications are presented in the references [5] and [6], respectively.

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