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A NEW EXACT PATH INTEGRAL TREATMENT OF THE HYDROGEN ATOM *

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ABSTRACT

Using a recently developed general new-time transformation method, free of operator ordering ambiguities by construction we reconsider the hydrogen atom problem. We solve the problem directly without any dimension raising trick.

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Recently an important computational tool was introduced into the path integral formalism by Duru and Kleinert to solve the hydrogen atom, the long standing classical challenge [1]. This was the first example of one step forward beyond the gaussians which was the computational limit of the path integral (because of the nonexistence of exact integration techniques beyond that). The immediate generalization to any spherically symmetric potential is given right after [2]. An exact path integral solution of an arbitrary spherically symmetric potential is certainly very important, given the time it took to get to that point, but formulating a general procedure for path integral treatment of any arbitrary potential would be more desirable. Recently we have been able to formulate this general method [3]. The first example we have applied our method, were the Morse potential [4], and the Pösche-Teller potential [5].

Our aim in reconsidering the hydrogen atom problem in this work is twofold. Firstly we wanted to expose simplicity of our general method; furthermore reproducing the well known results would constituite a direct check of the correctness of our general method. Secondly we thought it would be more desirable to solve a simple problem like this directly without resorting to sophisticated tricks like going into one higher dimension via a Kustaanheimo-Stiefel transformation [6] as is done in Ref.1).

The propagator for an arbitrary spherically symmetric potential has the following forms:

$$K^{(2)}(\vec{r}_f,\vec{r}_i;T) = \sum_{l=-\infty}^{\infty} \frac{1}{2\pi} e^{il(\varphi_f-\varphi_i)} K_l^{(2)}(r_f,r_i;T) \tag{1}$$

$$K^{(3)}(\vec{r}_f,\vec{r}_i;T) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{lm}^{*}(\theta_f,\varphi_f) Y_{lm}(\theta_i,\varphi_i) K_l^{(3)}(r_f,r_i;T) \tag{2}$$

in two and three dimension respectively [7]. We first observe that K_l's can

be written in terms of the kernel of a generic one dimensional problem defined as

$$K_\gamma(r_f,r_i;T) = N \int \mathcal{D}r(t) \exp\left[\frac{i}{\hbar}\int_0^T dt\, \mathcal{L}(r,\dot{r})\right]$$
$$\mathcal{L}(r,\dot{r}) = \frac{1}{2}m\dot{r}^2 - \left[-\frac{(\gamma^2-\frac{1}{4})\hbar^2}{2mr^2} + V(r)\right] \tag{3}$$

These simply read:

$$K_l^{(2)} = \frac{1}{(r_f r_i)^{1/2}} K_l(r_f,r_i;T) \tag{4}$$

$$K_l^{(3)} = \frac{1}{r_f r_i} K_{l+\frac{1}{2}}(r_f,r_i;T) \tag{5}$$

Then the simultaneous solution of the hydrogen atom, $V(r) = -e^2/r$, in two and three dimensions is reduced to the solution of the one-dimensional generic problem (3), with $\gamma = l$, and $\gamma = l+1/2$ respectively. This is what we are going to do next, solve the problem defined in Eq.(3) using the general method we have developed in ref 3).

Let us first briefly outline the results of Ref 3), in the configuration space. We apply a point canonical transformation (PCT) on the coordinate followed by the corresponding new-time transformation,

$$r = f(Q) \qquad \frac{dt}{ds} = [f'(Q)]^2 \tag{6}$$

to convert the path integral into

$$K(f(Q_f),f(Q_i),T) = \int_{-\infty}^{\infty}\frac{dE}{2\pi\hbar} e^{-\frac{i}{\hbar}ET}[f'(Q_f)f'(Q_i)]^{1/2}\int_0^{\infty} dS \int \mathcal{D}Q(s)\, e^{\frac{i}{\hbar}\int_0^S ds\left[\frac{1}{2}m\dot{Q}^2 - V_{new}(Q)\right]} \tag{7}$$

where V_{new} is the new potential

$$V_{new}(Q) = [f'(Q)]^2[V(f(Q)) - E] + \Delta V(f(Q))$$
$$\Delta V(f(Q)) = \frac{\hbar^2}{m}\left[\frac{3}{8}\left(\frac{f''}{f'}\right)^2 - \frac{1}{4}\left(\frac{f'''}{f'}\right)\right] \tag{8}$$

Here the primes denote derivatives with respect to Q.

Now let us make the following PCT for the problem defined by Equ(3):

$$r = u^2 \quad ; \quad p = \frac{1}{2u} p_u \tag{9}$$

which can be obtained from the generating function $F_2(r,p_u) = r^{1/2} p_u$. The corresponding new-time transformation is

$$\frac{dt}{ds} = 4u^2 \tag{10}$$

Next we compute the new potential :

$$V_{new}(u) = \frac{\left[(2\gamma)^2 - \frac{1}{4}\right]\hbar^2}{2mu^2} - 4Eu^2 - 4e^2 \tag{11}$$

We will express the solution of this problem in terms of the amputated kernel, P_E^γ , defined by

$$g^\gamma(f(u_f), f(u_i); E) = \left[f'(u_f) f'(u_i)\right]^{1/2} \int_0^\infty dS\, P_E^\gamma(u_f, u_i; S)$$

$$P_E^\gamma(u_f, u_i; S) = e^{i\frac{4e^2 S}{\hbar}} N \left\{ \mathcal{D}u(s) \exp\left\{ \frac{i}{\hbar} \int_0^S ds \left[\frac{1}{2} m\dot{u}^2 - \frac{\left[(2\gamma)^2 - \frac{1}{4}\right]\hbar^2}{2mu^2} + 4Eu^2 \right] \right\} \right\} \tag{12}$$

where g^γ is the Fourier transformed kernel

$$k(T) = \int_{-\infty}^{\infty} \frac{dE}{2\pi\hbar} e^{-\frac{i}{\hbar} ET} g(E) \tag{13}$$

The solution of this problem is given in the literature [7,8]. Defining $1/2\, m\omega^2 = -4E$, P_E^γ reads

$$P_E^\gamma(u_f, u_i; S) = e^{4ie^2 S/\hbar} \frac{m\omega (u_f u_i)^{1/2}}{i\hbar \sin \omega S} I_{2\gamma}\left(\frac{m\omega u_f u_i}{i\hbar \sin \omega S} \right) e^{i\frac{m\omega}{2\hbar}(u_f^2 + u_i^2)\cot g\, \omega S} \tag{14}$$

Here $I_{2\gamma}$ is the modified Bessel function. Plugging this in Equ.(12), we obtain

(15)

The next step is to perform this integral. To do this, we first make the variable change $\omega s = -iq$, and make the following definitions:

$$b = \frac{2e^2}{\hbar\omega} \quad , \quad \alpha = \frac{m\omega}{\hbar} u_f u_i \quad ; \quad \beta = \frac{m\omega}{2\hbar}(u_f^2 + u_i^2) \tag{16}$$

We can now perform the integral, using the integral formula

$$\int_0^\infty dq\, e^{-2pq} \operatorname{Cosech}(q)\, J_{2\gamma}(\alpha \operatorname{Cosech}(q))\, e^{-\beta \operatorname{Coth}(q)}$$

$$= \frac{1}{\alpha} \frac{\Gamma\left(\frac{1}{2} - p + \gamma\right)}{\Gamma(2\gamma+1)} M_{-p,\gamma}\left(\sqrt{\alpha^2+\beta^2} - \beta\right) W_{p,\gamma}\left(\sqrt{\alpha^2+\beta^2} + \beta\right) \tag{17}$$

where M and W are the Whittaker functions. Then g^γ reads

$$g^\gamma(r_f, r_i; E) = \frac{2}{\omega}(-1)^{\gamma+1} \frac{\Gamma\left(\frac{1}{2} - p + \gamma\right)}{\Gamma(2\gamma+1)} M_{-p,\gamma}\left(-\frac{m\omega}{\hbar} r_i\right) W_{p,\gamma}\left(\frac{m\omega}{\hbar} r_f\right) \tag{18}$$

Now that we have solved the generic one-dimensional problem, we can transpose this solution into Equs.(4) and (5), to get the kernels of the two and three- dimensional Hydrogen atom.

By setting $\gamma = \ell$, we get the result for the two dimensions:

$$G^{(2)}(\vec{r}_f, \vec{r}_i; E) = \sum_{\ell=-\infty}^{\infty} e^{i\ell(\varphi_f - \varphi_i)} \frac{(-1)^{\gamma+1}}{\pi\omega(r_f r_i)^{1/2}} \frac{\Gamma\left(\frac{1}{2} - p + \ell\right)}{\Gamma(2\ell+1)} M_{-p,\ell}\left(-\frac{m\omega}{\hbar} r_i\right) W_{p,\ell}\left(\frac{m\omega}{\hbar} r_f\right) \tag{19}$$

We find the energy eigenvalues from the poles of the $\Gamma(1/2 - p + \ell)$, which occur at

$$\frac{1}{2} - p + \ell = -n' \quad , \quad n' = 0, 1, 2, 3, \ldots \tag{20}$$

The corresponding energy levels are

$$E_p = -\frac{me^4}{2\hbar^2 p^2} \quad , \quad p = n + \frac{1}{2} \quad , \quad n = n' + \ell = 0, 1, 2, 3, \ldots \tag{21}$$

Next by setting $\gamma = \ell + 1/2$ in (18), we get the result for three dimensions:

$$G^{(3)}(\vec{r}_f, \vec{r}_i; E) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\theta_f, \varphi_f)\, Y_{\ell m}(\theta_i, \varphi_i)$$

$$\times \frac{2(-1)^{\ell+\frac{3}{2}}}{\omega r_f r_i} \frac{\Gamma(\ell - p + 1)}{\Gamma(2\ell+2)} M_{-p,\ell+\frac{1}{2}}\left(-\frac{m\omega}{\hbar} r_i\right) W_{p,\ell+\frac{1}{2}}\left(\frac{m\omega}{\hbar} r_f\right) \tag{22}$$

Again the energy eigenvalues are found from the poles of the $\Gamma(\ell - p+1)$ which occur at

$$\ell - p + 1 = -n_r \quad , \quad n_r = 0, 1, 2, 3, \ldots \tag{23}$$

The corresponding energy eigenvalues are

$$E_p = -\frac{m e^4}{2\hbar^2 p^2} \quad , \quad p = n_r + \ell + 1 = 1, 2, 3, \ldots \tag{24}$$

The resistance of the Hydrogen atom, which in some sense symbolizes the success of the canonical quantum mechanics, to an exact treatment in path integral formalism was one of the great puzzles in this field for a long time. Once the solution is given by Durn and Kleinert, the subtleties in their solution on the implementation of the (point) canonical transformation in the path integral have generated some discussion right after. Indeed there are subtleties in the symmetrization procedure of the short-time kernel in applying a PCT, which requires extreme care. Therefore instead of going through this procedure for the special transformations required by the individual problem, a general method of implementing a PCT, free of ordering ambiguities, independent of the particulars of the special problems, is needed. This method now exists and we have used it in this work. Another feature of our work is solving the problem direct in three (and two) dimensions without resorting to going into four dimensions via KS transformation. For, this method requires an ext constraint to specify the physical subspace, undoubtedly complicating

path integral. This problem did not become any simpler when the KS transformation were applied to the intervals rather than the coordinates by Inomata.[1)]

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