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SIGN SOLVED PROPAGATOR OF A TWO ELECTRONS 2D ATOM AND APPLICATION

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Abstract

In the present paper, we calculate the sign solved propagator of a two electrons two dimensional (2D) atom by solving the sign problem. We apply the sign solved propagator expression to the evaluation of the geometric phase of the ground state of the 2D helium atom that is derived variationally. 2D quantum dots are another possible area of application of the present theory.

1. Introduction

In the present paper, we calculate the sign solved propagator (SSP) of a two dimensional (2D) helium like atom. The SSP propagator theory began as an attempt to solve [1] the sign problem, a well known problem in quantum physics and chemistry. Then we applied that solution in [2] and [3] and numerically observed the existence of the SSP and further of the sign solved influence functional. In those two references the author studied the solution of the sign problem in systems concerning the interaction of radiation with matter. There followed the severe foundation of the whole theory in [4, 5, 6]. Other systems were considered in [7, 8, 9].

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Instead to the use of the single word "propagator" in the development of the theory of the above series of papers we have preferred to introduce the naming "sign solved propagator" as in contrast with the usual case the being extracted includes a delta function which forbids its connection with a zeta function although it obeys the semigroup property. The importance and the power of the extracted being is that it gives closed expressions even in the case of interacting systems and therefore it introduces a completely new approach in solving differential equations, like the Schrödinger one, and consequently performing analytical and further numerical calculations. Moreover, although till now we have restricted our interest in quantum mechanical systems the applicability of the SSP theory is wider as we discuss in the conclusions of [5].

To handle the present system of a 2D two electrons atom and calculate its SSP we combine standard methods of the path integral theory with our methods (see next section). Further, we consider the calculation of the geometric phase of the ground state of the present system that has been derived variationally. 2D quantum dots are another area of application of the present theory as the Hamiltonian term of each single electron appears just in a phase in the final result. Moreover, that phase is canceled in most of the expressions of interest. What matters in the present theory is the interaction term.

The paper proceeds as follows. In Section 2, we study the path integral of a 2D helium like atom and handle it in such a way that we can apply the usual SSP theorem. In Section 3, we consider the numerical evaluation of the geometric phase of the ground state of the present system. In Section 4, we give our conclusions. Finally, in Appendix A we give certain necessary integrals.

2. System Hamiltonian and Path Integration

The Hamiltonian H of a 2D two electrons atom has the form

$$H = \frac{\vec{p}_1^{\,2}}{2} + \frac{\vec{p}_2^{\,2}}{2} - \frac{Z}{|\vec{\rho}_1|} - \frac{Z}{|\vec{\rho}_2|} + \frac{1}{|\vec{\rho}_1 - \vec{\rho}_2|}, \tag{1}$$

where Z is the atomic number. $\vec{\rho}_1$ and $\vec{\rho}_2$ are the positions of the first and the second electron respectively, with respect the nucleus placed at the origin. Moreover, $\vec{p}_1$ and $\vec{p}_2$ are their corresponding momentums.

The corresponding path integral in its discrete form is

$$\widetilde{K}(\vec{\rho}_{1f}, \vec{\rho}_{2f}, t_f; \vec{\rho}_{1i}, \vec{\rho}_{2i}, t_i)$$

$$= \lim_{N\to\infty} \prod_{n=1}^{N} \int_{-\infty}^{\infty} d\vec{\rho}_{1n} \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{d\vec{p}_{1n}}{(2\pi)^2} \right] \prod_{n=1}^{N} \int_{-\infty}^{\infty} d\vec{\rho}_{2n} \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{d\vec{p}_{2n}}{(2\pi)^2} \right]$$

$$\times \exp\left\{ i \sum_{n=1}^{N+1} \left[\begin{array}{l} \vec{p}_{1n} \cdot (\vec{\rho}_{1n} - \vec{\rho}_{1n-1}) + \vec{p}_{2n} \cdot (\vec{\rho}_{2n} - \vec{\rho}_{2n-1}) \\ - \varepsilon \left(\dfrac{\vec{p}_{1n}^{\,2}}{2} + \dfrac{\vec{p}_{2n}^{\,2}}{2} - \dfrac{Z}{|\vec{\rho}_{1n}|} - \dfrac{Z}{|\vec{\rho}_{2n}|} + \dfrac{1}{|\vec{\rho}_{1n} - \vec{\rho}_{2n}|} \right) \end{array} \right] \right\}, \tag{2}$$

where $\varepsilon = \dfrac{t_f - t_i}{N+1}$. We have also set $\vec{\rho}_{10} = \vec{\rho}_{1i}, \vec{\rho}_{20} = \vec{\rho}_{2i}, \vec{\rho}_{1N+1} = \vec{\rho}_{1f}$ and $\vec{\rho}_{2N+1} = \vec{\rho}_{2f}$. Now, we observe that the two electrons interaction term can be written as

$$\frac{1}{|\vec{\rho}_{1n} - \vec{\rho}_{2n}|} = \frac{1}{\sqrt{\rho_{1n}^2 + \rho_{2n}^2 - 2\vec{\rho}_{1n}\cdot\vec{\rho}_{2n}}} = \frac{1}{\sqrt{\rho_{1n}^2 + \rho_{2n}^2 - 2\rho_{1n}\rho_{2n}\cos\varphi_{12n}}}$$

$$= \frac{1}{\sqrt{\rho_{1n}^2 + \rho_{2n}^2}} \frac{1}{\sqrt{1 - \dfrac{2\rho_{1n}\rho_{2n}}{\rho_{1n}^2 + \rho_{2n}^2}\cos\varphi_{12n}}}$$

$$= \frac{1}{\sqrt{\rho_{1n}^2 + \rho_{2n}^2}} \frac{1}{\sqrt{1 - \dfrac{2}{\dfrac{\rho_{1n}}{\rho_{2n}} + \dfrac{\rho_{2n}}{\rho_{1n}}}\cos\varphi_{12n}}}$$

$$= \frac{1}{\sqrt{\rho_{1n}^2 + \rho_{2n}^2}} \frac{1}{\sqrt{1 - \alpha(\rho_{1n}, \rho_{2n})\cos\varphi_{12n}}}. \tag{3}$$

In the last equality we have set

$$\alpha(\rho_{1n}, \rho_{2n}) = \frac{2}{\dfrac{\rho_{1n}}{\rho_{2n}} + \dfrac{\rho_{2n}}{\rho_{1n}}} \leq 1. \tag{4}$$

Moreover, $\rho_{1n} = |\vec{\rho}_{1n}|$, $\rho_{2n} = |\vec{\rho}_{2n}|$. Then the path integral (2) becomes

$$\widetilde{K}(\vec{\rho}_{1f}, \vec{\rho}_{2f}, t_f; \vec{\rho}_{1i}, \vec{\rho}_{2i}, t_i)$$

$$= \lim_{N\to\infty} \prod_{n=1}^{N} \int_{-\infty}^{\infty} d\vec{\rho}_{1n} \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{d\vec{p}_{1n}}{(2\pi)^2}\right] \prod_{n=1}^{N} \int_{-\infty}^{\infty} d\vec{\rho}_{2n} \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{d\vec{p}_{2n}}{(2\pi)^2}\right]$$

$$\times \exp\left\{ i \sum_{n=1}^{N+1} \left[\begin{array}{l} \vec{p}_{1n} \cdot (\vec{\rho}_{1n} - \vec{\rho}_{1n-1}) + \vec{p}_{2n} \cdot (\vec{\rho}_{2n} - \vec{\rho}_{2n-1}) \\ - \varepsilon \left(\frac{\vec{p}_{1n}^{\,2}}{2} + \frac{\vec{p}_{2n}^{\,2}}{2} - \frac{Z}{\rho_{1n}} - \frac{Z}{\rho_{2n}} \right. \\ \left. + \frac{1}{\sqrt{\rho_{1n}^2 + \rho_{2n}^2}} \frac{1}{\sqrt{1 - \alpha(\rho_{1n}, \rho_{2n}) \cos\varphi_{12n}}} \right) \end{array} \right] \right\}. \tag{5}$$

To proceed we insert in equation (5) a delta function in order to get

$$\widetilde{K}(\vec{\rho}_{1f}, \vec{\rho}_{2f}, t_f; \vec{\rho}_{1i}, \vec{\rho}_{2i}, t_i)$$

$$= \lim_{N\to\infty} \prod_{n=1}^{N} \int_{-\infty}^{\infty} d\vec{\rho}_{1n} \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{d\vec{p}_{1n}}{(2\pi)^2}\right] \prod_{n=1}^{N} \int_{-\infty}^{\infty} d\vec{\rho}_{2n} \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{d\vec{p}_{2n}}{(2\pi)^2}\right]$$

$$\times \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} dw_n\right] \prod_{n=1}^{N+1} [\delta(w_n - \alpha(\rho_{1n}, \rho_{2n}) \cos\varphi_{12n})]$$

$$\times \exp\left\{ i \sum_{n=1}^{N+1} \left[\begin{array}{l} \vec{p}_{1n} \cdot (\vec{\rho}_{1n} - \vec{\rho}_{1n-1}) + \vec{p}_{2n} \cdot (\vec{\rho}_{2n} - \vec{\rho}_{2n-1}) \\ - \varepsilon \left(\frac{\vec{p}_{1n}^{\,2}}{2} + \frac{\vec{p}_{2n}^{\,2}}{2} - \frac{Z}{\rho_{1n}} - \frac{Z}{\rho_{2n}} + \frac{1}{\sqrt{\rho_{1n}^2 + \rho_{2n}^2}} \frac{1}{\sqrt{1 - w_n}} \right) \end{array} \right] \right\}. \tag{6}$$

Now, we observe that the delta functions in equation (6) have the representation

$$\delta(w_n - \alpha_n \cos\varphi_{12n})$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\lambda_n e^{-i\lambda_n w_n} e^{i\lambda_n \alpha_n \cos\varphi_{12n}}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\lambda_n e^{-i\lambda_n w_n} J_0(\lambda_n \alpha_n) + \frac{1}{\pi} \sum_{k_n=1}^{\infty} i^{k_n} \cos(k_n \varphi_{12n}) \int_{-\infty}^{\infty} d\lambda_n e^{-i\lambda_n w_n} J_{k_n}(\lambda_n \alpha_n)$$

$$= \frac{1}{\pi}\int_0^\infty d\lambda_n \cos(\lambda_n w_n) J_0(\lambda_n \alpha_n)$$

$$+ \frac{1}{\pi}\sum_{k_n=1}^{\infty} i^{k_n} \cos(k_n \varphi_{12n}) \int_0^\infty d\lambda_n [e^{-i\lambda_n w_n} + (-1)^{k_n} e^{i\lambda_n w_n}] J_{k_n}(\lambda_n \alpha_n), \tag{7}$$

where $\alpha_n = \alpha(\rho_{1n}, \rho_{2n})$. Moreover, the integrals appearing in equation (7) are given by the expressions [10]

$$f_{2k}^c(w, \alpha) = \int_0^\infty d\lambda \cos(\lambda w) J_{2k}(\lambda\alpha) = \begin{cases} \dfrac{\cos[2k \arcsin(w/\alpha)]}{\sqrt{\alpha^2 - w^2}}, & |w| < \alpha, \\ 0, & |w| > \alpha, \end{cases} \tag{8}$$

$$f_{2k+1}^s(w, \alpha) = \int_0^\infty d\lambda \sin(\lambda w) J_{2k+1}(\lambda\alpha) = \begin{cases} \dfrac{\sin[(2k+1) \arcsin(w/\alpha)]}{\sqrt{\alpha^2 - w^2}}, & |w| < \alpha, \\ 0, & |w| > \alpha, \end{cases} \tag{9}$$

and particularly in the case of the first integral in the last equality of equation (7) we have the expression

$$f_0^c(w, \alpha) = \int_0^\infty d\lambda \cos(\lambda w) J_0(\lambda\alpha) = \begin{cases} \dfrac{1}{\sqrt{\alpha^2 - w^2}}, & |w| < \alpha, \\ 0, & |w| > \alpha. \end{cases} \tag{10}$$

Therefore, we can perform the integrations in equation (7) according to the expressions (8)-(10) and place the results in equation (6) after keeping leading terms with respect the k_n's. In fact the angular part of higher order terms in the expansion (7) gives infinities as $N \to \infty$. This is the case in [2, 3, 7, 8] as well, anyhow large the volume may be there. The presence of the volume just guides us to the correct route of the solution. Now, expression (6) becomes

$$\widetilde{K}(\vec{\rho}_{1f}, \vec{\rho}_{2f}, t_f; \vec{\rho}_{1i}, \vec{\rho}_{2i}, t_i)$$

$$= \lim_{N\to\infty} \prod_{n=1}^{N} \int_{-\infty}^{\infty} d\vec{\rho}_{1n} \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{d\vec{p}_{1n}}{(2\pi)^2}\right] \prod_{n=1}^{N} \int_{-\infty}^{\infty} d\vec{\rho}_{2n} \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{d\vec{p}_{2n}}{(2\pi)^2}\right]$$

$$\times \prod_{n=1}^{N+1} \left[\int_{-\alpha_n}^{\alpha_n} \frac{dw_n}{\pi}\right] \prod_{n=1}^{N} [f_0^c(w_n, \alpha_n)]$$

$$\times\left(\begin{array}{l} f_0^c(w_{N+1},\alpha_{N+1}) \\ +2\sum\limits_{k_{N+1}=1}^{\infty}(-1)^{k_{N+1}}\cos[2k_{N+1}\varphi_{12N+1}]f_{2k_{N+1}}^c(w_{N+1},\alpha_{N+1}) \\ +2\sum\limits_{k_{N+1}=1}^{\infty}(-1)^{k_{N+1}}\cos[(2k_{N+1}+1)\varphi_{12N+1}]f_{2k_{N+1}+1}^s(w_{N+1},\alpha_{N+1}) \end{array}\right)$$

$$\times\exp\left\{i\sum_{n=1}^{N+1}\left[\begin{array}{l}\vec{p}_{1n}\cdot(\vec{\rho}_{1n}-\vec{\rho}_{1n-1})+\vec{p}_{2n}\cdot(\vec{\rho}_{2n}-\vec{\rho}_{2n-1}) \\ -\varepsilon\left(\frac{\vec{p}_{1n}^{\,2}}{2}+\frac{\vec{p}_{2n}^{\,2}}{2}-\frac{Z}{\rho_{1n}}-\frac{Z}{\rho_{2n}}+\frac{1}{\sqrt{\rho_{1n}^2+\rho_{2n}^2}}\frac{1}{\sqrt{1-w_n}}\right)\end{array}\right]\right\}. \quad (11)$$

We have set the range of w_n in the interval from $-\alpha_n$ to α_n as otherwise the functions f_{2k}^c and f_{2k+1}^s are zero (see equations (8)-(10)). Moreover, for the case of the $N+1$ factor appearing in equation (11) we have kept the full series (7) as it involves the final coordinates.

Now, in the two dimensional path integral (11) we perform standard manipulations including angular decomposition according to [11] to obtain the result

$$\widetilde{K}(\vec{\rho}_{1f},\vec{\rho}_{2f},t_f;\vec{\rho}_{1i},\vec{\rho}_{2i},t_i)$$

$$=\frac{1}{\sqrt{\rho_{1f}\rho_{1i}\rho_{2f}\rho_{2i}}}\sum_{q_1=-\infty}^{\infty}\sum_{q_2=-\infty}^{\infty}\frac{1}{2\pi}e^{iq_1(\varphi_{1f}-\varphi_{1i})}\frac{1}{2\pi}e^{iq_2(\varphi_{2f}-\varphi_{2i})}$$

$$\times\left[\begin{array}{l}\widetilde{K}_{0q_1q_2}^c(\rho_{1f},\rho_{2f},t_f;\rho_{1i},\rho_{2i},t_i) \\ +\sum\limits_{k=1}^{\infty}(-1)^k(e^{2ik(\varphi_{1f}-\varphi_{2f})} \\ +e^{-2ik(\varphi_{1f}-\varphi_{2f})})\widetilde{K}_{2kq_1q_2}^c(\rho_{1f},\rho_{2f},t_f;\rho_{1i},\rho_{2i},t_i) \\ +\sum\limits_{k=0}^{\infty}(-1)^k(e^{i(2k+1)(\varphi_{1f}-\varphi_{2f})} \\ +e^{-i(2k+1)(\varphi_{1f}-\varphi_{2f})})\widetilde{K}_{2k+1q_1q_2}^s(\rho_{1f},\rho_{2f},t_f;\rho_{1i},\rho_{2i},t_i)\end{array}\right] \quad (12)$$

q_1 and q_2 have appeared after the angular decomposition and are the azimuthal quantum numbers corresponding to electrons 1 and 2, respectively. The

$\widetilde{K}_{\left\{\begin{smallmatrix}c\\s\end{smallmatrix}\right\}\left\{\begin{smallmatrix}2k\\2k+1\end{smallmatrix}\right\}q_1q_2}(\rho_{1f},\, \rho_{2f},\, t_f;\, \rho_{1i},\, \rho_{2i},\, t_i)$ terms above correspond to the path integrals

$$\widetilde{K}_{\left\{\begin{smallmatrix}c\\s\end{smallmatrix}\right\}\left\{\begin{smallmatrix}2k\\2k+1\end{smallmatrix}\right\}q_1q_2}(\rho_{1f},\, \rho_{2f},\, t_f;\, \rho_{1i},\, \rho_{2i},\, t_i)$$

$$= \lim_{N\to\infty}\prod_{n=1}^{N}\int_0^{\infty} d\rho_{1n}\prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty}\frac{dp_{1n}}{2\pi}\right]\prod_{n=1}^{N}\int_0^{\infty} d\rho_{2n}\prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty}\frac{dp_{2n}}{2\pi}\right]$$

$$\times \exp\left\{i\sum_{n=1}^{N+1}\left[\begin{array}{l} p_{1n}(\rho_{1n}-\rho_{1n-1})+p_{2n}(\rho_{2n}-\rho_{2n-1}) \\ -\varepsilon\left(\dfrac{p_{1n}^2}{2}+\dfrac{q_1^2-1/4}{2\rho_{1n}^2}-\dfrac{Z}{\rho_{1n}}+\dfrac{p_{2n}^2}{2}+\dfrac{q_2^2-1/4}{2\rho_{2n}^2}-\dfrac{Z}{\rho_{2n}}\right)\end{array}\right]\right\}$$

$$\times F_{\left\{\begin{smallmatrix}c\\s\end{smallmatrix}\right\}\left\{\begin{smallmatrix}2k\\2k+1\end{smallmatrix}\right\}}(\rho_{11},\, \rho_{12},\, \ldots,\, \rho_{1N+1},\, \rho_{21},\, \rho_{22},\, \rho_{2N+1}). \tag{13}$$

We have set $\rho_{10} = \rho_{1i},\, \rho_{20} = \rho_{2i},\, \rho_{1N+1} = \rho_{1f}$ and $\rho_{2N+1} = \rho_{2f}$ while the factors $F_{\left\{\begin{smallmatrix}c\\s\end{smallmatrix}\right\}\left\{\begin{smallmatrix}2k\\2k+1\end{smallmatrix}\right\}}(\rho_{11},\, \rho_{12},\, \ldots,\, \rho_{1N+1},\, \rho_{21},\, \rho_{22},\, \ldots,\, \rho_{2N+1})$ appearing in the two cases of equation (13) above have the form

$$F_{\left\{\begin{smallmatrix}c\\s\end{smallmatrix}\right\}\left\{\begin{smallmatrix}2k\\2k+1\end{smallmatrix}\right\}}(\rho_{11},\, \rho_{12},\, \ldots,\, \rho_{1N+1},\, \rho_{21},\, \rho_{22},\, \ldots,\, \rho_{2N+1})$$

$$= \prod_{n=1}^{N+1}\left[\int_{-\alpha_n}^{\alpha_n}\frac{dw_n}{\pi}\right]\prod_{n=1}^{N}\left[f_0^c(w_n,\, \alpha_n)\right]$$

$$f_{\left\{\begin{smallmatrix}c\\s\end{smallmatrix}\right\}\left\{\begin{smallmatrix}2k\\2k+1\end{smallmatrix}\right\}}(w_{N+1},\, \alpha_{N+1})\exp\left\{-i\varepsilon\sum_{n=1}^{N+1}\left[\frac{1}{\sqrt{\rho_{1n}^2+\rho_{2n}^2}}\,\frac{1}{\sqrt{1-w_n}}\right]\right\}. \tag{14}$$

We can easily observe that the above multiple integral can be decomposed in $N+1$ one-dimensional integrals. We can use the results of Appendix A for their evaluation.

Now, we solve the sign problem relevant with the path integral (13). It is easy to observe that

$$\left| F_{\begin{Bmatrix} 2k \\ 2k+1 \end{Bmatrix}}^{\begin{Bmatrix} c \\ s \end{Bmatrix}} (\rho_{11}, \rho_{12}, \ldots, \rho_{1N+1}, \rho_{21}, \rho_{22}, \ldots, \rho_{2N+1}) \right| \leq b, \tag{15}$$

where b is a positive constant. The above inequalities can be derived easily if we take into account both the facts that the phase in equation (14) is bounded by unity as well as the form of the functions in equations (8), (9), (10) and further if we perform the transformation $w_n = \alpha_n \sin(\theta_n)$. Therefore, the sign solved propagator theorem of [5, 6] is applicable and the corresponding sign solved propagators are

$$\widetilde{K}_{\begin{Bmatrix} 2k \\ 2k+1 \end{Bmatrix} q_1 q_2}^{\begin{Bmatrix} c \\ s \end{Bmatrix}} (\rho_{1f}, \rho_{2f}, t_f; \rho_{1i}, \rho_{2i}, t_i)$$

$$= \delta(\rho_{1f} - \rho_{1i})\delta(\rho_{2f} - \rho_{2i})$$

$$\times \exp\{-i\langle H_0^{q_1 q_2}\rangle (t_f - t_i)\} \lim_{N\to\infty} F_{\begin{Bmatrix} 2k \\ 2k+1 \end{Bmatrix}}^{\begin{Bmatrix} c \\ s \end{Bmatrix}} \Bigg(\underbrace{\rho_{1f}, \rho_{1f}, \ldots, \rho_{1f}}_{N+1}, \underbrace{\rho_{2f}, \rho_{2f}, \ldots, \rho_{2f}}_{N+1} \Bigg). \tag{16}$$

In equation (16) we have set

$$H_0^{q_1 q_2} = \frac{p_1^2}{2} + \frac{q_1^2 - 1/4}{2\rho_1^2} - \frac{Z}{\rho_1} + \frac{p_2^2}{2} + \frac{q_2^2 - 1/4}{2\rho_2^2} - \frac{Z}{\rho_2}. \tag{17}$$

An appropriate sampling function is used in the evaluation of the expectation value of $H_0^{q_1 q_2}$ on the phase in equation (16). However, in most of the final results of interest, that phase does not appear.

3. Application to the Geometric Phase

Our intension now is to apply the above theory to the numerical evaluation of the geometric phase [12]. Let the wavefunction of the ground state of the 2D helium atom [13] at time zero be $|\psi(0)\rangle$. Then the geometric phase $\Phi_g(t)$ of the system has the form

$$\Phi_g(t) = \arg\langle\psi(0)|\psi(t)\rangle + i\int_0^t \langle\psi(\tau)|\dot{\psi}(\tau)\rangle d\tau, \tag{18}$$

where according to standard results of quantum mechanics the wavefunction $|\psi(t)\rangle$ of the system at time t has the form

$$\langle\vec{\rho}_{1f}, \vec{\rho}_{2f} | \psi(t)\rangle = \int d\vec{\rho}_{1i} d\vec{\rho}_{2i} \widetilde{K}(\vec{\rho}_{1f}, \vec{\rho}_{2f}, t; \vec{\rho}_{1i}, \vec{\rho}_{2i}, 0) \langle\vec{\rho}_{1i}, \vec{\rho}_{2i} | \psi(0)\rangle. \quad (19)$$

The SSP is given by equation (12). We notice that if we take into account equations (12) and (16), then the phase appearing in equation (16) is canceled in equation (18).

In our calculations we consider as an initial state the approximate variationally extracted wavefunction of the singlet ground state of the 2D atom. It has the form

$$\langle\vec{\rho}_{1i}, \vec{\rho}_{2i} | \psi_1(0)\rangle = \frac{8Z'^2}{\pi} \exp[-2Z'(\rho_{1i} + \rho_{2i})], \quad (20)$$

where $Z' = Z - \frac{3\pi}{32}$.

The first term on the right hand side of equation (18) is the total phase while the second one is the opposite of the dynamical one. More specifically in the case of the ground state of the 2D helium $(Z = 2)$ we give the geometric phase as a function of time in Figure 1. The range of time is arbitrary and has been extended to large enough values in order jumps in the value of the geometric phase to be observed. Larger values of time are not considered due to limited numerical accuracy. However, we can expect a structure with jumps. In fact in our calculations we use $N = 200$ and in the series of the Appendix A we have kept terms until $n = 100$.

4. Conclusions

In the present paper, we consider the path integral of a 2D two electrons atom. We have derived its SSP and specializing on helium we have presented results on the numerical calculation of the geometric phase of its ground state. The wavefunction has been derived variationally. A complete discussion of the usefulness of the 2D Helium is given in [13].

The 2D quantum dots are another domain of application of the present methodology.

Further, we notice that if we consider the interaction of the two electrons with radiation and treat the radiation term perturbatively in the relevant path integral, then the present theory is applicable in both of the above physical cases.

Concluding the present method is tractable and can be used in various problems concerning the quantum mechanics of a two electrons 2D atom. In future, we intend to consider the present calculations further when external magnetic fields are present.

Appendix A

In equations above (see for instance equation (14)) there appear integrals of the following forms (see equations (8), (9), (10) for the definition of $f_{2k}^{c}(w, \alpha)$ and $f_{2k+1}^{s}(w, \alpha)$)

$$
\begin{aligned}
I_{2k}^{c} &= \int_{-\alpha}^{\alpha} \frac{dw}{\pi} \frac{\cos[2k \arcsin(w/\alpha)]}{\sqrt{\alpha^2 - w^2}} \exp\left[-i \frac{g}{\sqrt{1-w}}\right]^{w=\alpha\sin(\theta)} \\
&= \int_{-\pi/2}^{\pi/2} \frac{d\theta}{\pi} \cos[2k\theta] \exp\left[-i \frac{g}{\sqrt{1-\alpha\sin(\theta)}}\right] \\
&= \sum_{n=0}^{\infty} \frac{(-ig)^n}{n!} \int_{-\pi/2}^{\pi/2} \frac{d\theta}{\pi} \frac{\cos[2k\theta]}{(1-\alpha\sin(\theta))^{n/2}},
\end{aligned} \tag{A1}
$$

$$
\begin{aligned}
I_{2k+1}^{s} &= \int_{-\alpha}^{\alpha} \frac{dw}{\pi} \frac{\sin[(2k+1)\arcsin(w/\alpha)]}{\sqrt{\alpha^2 - w^2}} \exp\left[-i \frac{g}{\sqrt{1-w}}\right]^{w=\alpha\sin(\theta)} \\
&= \int_{-\pi/2}^{\pi/2} \frac{d\theta}{\pi} \sin[(2k+1)\theta] \exp\left[-i \frac{g}{\sqrt{1-\alpha\sin(\theta)}}\right] \\
&= \sum_{n=0}^{\infty} \frac{(-ig)^n}{n!} \int_{-\pi/2}^{\pi/2} \frac{d\theta}{\pi} \frac{\sin[(2k+1)\theta]}{(1-\alpha\sin(\theta))^{n/2}}.
\end{aligned} \tag{A2}
$$

Therefore, for instance

$$
I_0^c = \sum_{n=0}^{\infty} \frac{(-ig)^n}{n!} F\left(\frac{n}{4} + \frac{1}{2}, \frac{n}{4}; 1; \alpha^2\right), \tag{A3}
$$

$F\left(\frac{n}{4} + \frac{1}{2}, \frac{n}{4}; 1; \alpha^2\right)$ is a Gaussian hypergeometric function [14]. Similarly

$$
I_1^s = \frac{\alpha}{4} \sum_{n=1}^{\infty} \frac{(-ig)^n}{(n-1)!} F\left(\frac{n}{4} + \frac{1}{2}, \frac{n}{4} + 1; 2; \alpha^2\right). \tag{A4}
$$

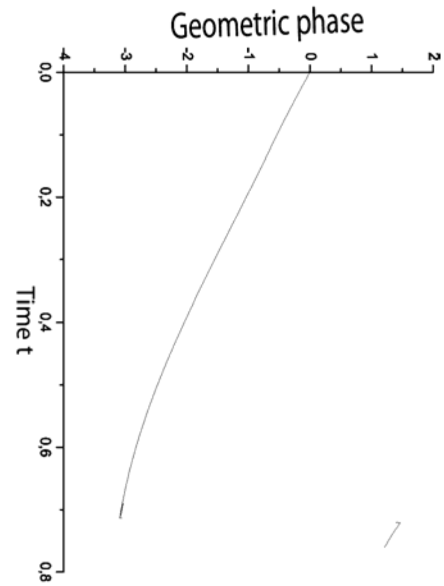

Figure 1. Geometric phase of the ground state of the 2D helium as a function of time. We have used $N = 200$.

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