Deterministic technique of path summation

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A numerical method, based on the Euclidean path integral formulation of quantum mechanics, to evaluate the ground state energy and wave function of a quantum system is discussed. The method is illustrated in one-dimensional cases, and then applied to a two-body system interacting through central and tensor potentials. A detailed discussion of the deuteron problem with a realistic nuclear potential is given.

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Monte Carlo evaluation of path integrals is often useful in situations difficult to handle by analytical techniques such as stationary phase approximation or perturbation theory. An important feature of Monte Carlo techniques is the possibility of facing problems with arbitrary dimensionality, but two fundamental limits are the missing of the tunneling effects (partially cured by simulated annealing) [1] and the need of high statistics, and then large CPU time, to reduce the statistical errors.

An alternative method [2,3] for evaluating path integrals is the following: (i) Take the Euclidean "short time" propagator

$$K(x,\varepsilon;x_0,0) = \frac{1}{\sqrt{2\pi\varepsilon}} \exp\left\{-\frac{1}{2\varepsilon}(x-x_0)^2 - f(x,\varepsilon;x_0,0)\right\}; \quad (1)$$

where the first term in the exponential corresponds to the kinetic part of the Hamiltonian, $\hbar = m = 1$, and the function $f(x,\varepsilon;x_0,0)$ is equal to the symmetric expression $\varepsilon\,[V(x)+V(y)]/2$; with this choice the short time propagator is correct to $O(\varepsilon^2)$ [1]. (ii) Build the finite time propagator through the semigroup composition law

$$K(x,t;x_0,t_0) = \int dx'\, K(x,t;x',t')K(x',t';x_0,t_0). \quad (2)$$

This convolution integral has to be evaluated for any x, x_0, and it is essentially equivalent to the product of square matrices with dimension N. (iii) Evaluate the ground state energy and wave function in a standard way [2], by stopping the iteration when convergence is attained. In the practical case this happens after 5–10 iterations only.

The iteration allows us to project out just the ground state. An equivalent and interesting technique is to diagonalize directly the short time propagator; this gives some advantages, as the possibility of obtaining immediately the excited states. The results of the two methods are exactly the same.

We must, now, consider the fact that the interval of integration in (2) goes from $-\infty$ to $+\infty$, and so taking finite matrices, and consequently finite interval, corresponds to putting the system in an infinite potential well. This affects the tail of the wave functions but, if the interval is large enough, it gives only small corrections to the energies and the wave functions. These corrections can be evaluated perturbatively [4].

The method has been tested and it works very well for simple solvable systems like harmonic and Poschen-Teller potentials; with $N = 21$ we get a precision better than 0.1%. As a more sophisticated example we analyze the double-well potential

$$V(x) = (x^2 - x_0^2)^2. \quad (3)$$

We vary the strength of the potential barrier by tuning the parameter x_0. In Table I we compare the "exact" ($N = 100$) numerical value for the first level with the numerical result obtained by discretizations with 17 and 33 points, and after n steps ($t = 2^n\varepsilon$). The result is quite good. The relatively long time needed to reach convergence is related to the separation of the second level, which is almost degenerate with the first (the splitting is exponentially small with the tunneling barrier).

A Monte Carlo approach needs a much larger computer time and more refined tricks to work. Furthermore, even if specific sampling methods are able to recover the instanton contributions, in the less simple case of a slightly asymmetric double well, where the wave function local-

TABLE I. Ground state energy of the double-well potential. n is the number of iterations. N is the number of points. $E_{\text{g.s.}}$ is the numerical value of the energy obtained with 100 points.

	$x_0 = 1$		$x_0 = 2$	
	$N = 17$	$N = 33$	$N = 17$	$N = 33$
n=5	0.85675	0.48563	2.5298	2.3202
n=10	0.86518	0.86930	2.6347	2.7400
n=15	0.86518	0.86930	2.6381	2.7535
$E_{\text{g.s.}}$	0.86958		2.7624	

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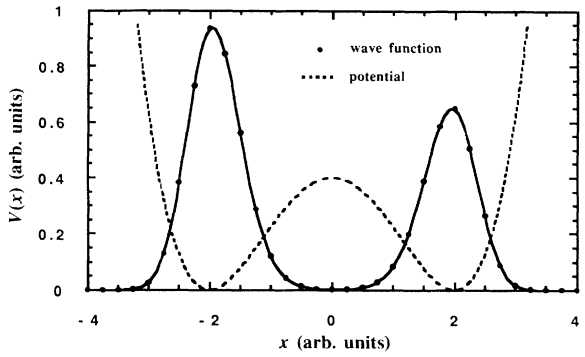

FIG. 1. Ground state wave function of the slightly asymmetric double well.

ization is a delicate problem, the Monte Carlo approach fails completely while this method works very well. As an example we give in Fig. 1 the wave function of the slightly asymmetric double-well potential:

$$V(x) = (x^2 - 4)^2[1 + 10^{-5}/(1 + e^{-10(x-2)})]. \quad (4)$$

We analyze now a three-dimensional problem with a central potential. In this case it is possible to separate the angular and the radial variables; then the kernel factorizes in a product of spherical harmonics and a radial part given by [5]

$$g_l(\mathbf{u}) = k_l(\mathbf{u}) \exp\{-f(\mathbf{u})\}, \quad (5)$$

where $\mathbf{u} \equiv (r, \varepsilon; r_0, 0)$, $f(\mathbf{u})$ has been defined above,

$$k_l(\mathbf{u}) = \frac{1}{\sqrt{2\pi\varepsilon}} \sqrt{2\pi \frac{r\, r_0}{\varepsilon}}\, e^{-r r_0/\varepsilon}\, I_{l+\frac{1}{2}} \left(\frac{r\, r_0}{\varepsilon}\right) \times e^{-(r-r_0)^2/2\varepsilon}, \quad (6)$$

and $I_{l+1/2}(z)$ are modified Bessel functions. This short time propagator can be used in the same way as for the one-dimensional case and we have tested the stability of the method by studying the Krazer potential

$$V(r) = \frac{A}{r^2} - \frac{1}{r} \quad (7)$$

and the limit for $A \to 0$ (Coulomb potential). The results (reported in Table II) are encouraging. They become more stable for angular momenta different from zero since the centrifugal barrier acts like a natural cutoff and regularizes the solution at the origin.

A more sophisticated system is the deuteron, with the two nucleons interacting through a realistic potential which has also a tensor part that does not commute with the orbital angular momentum. The Euclidean propagator of the deuteron is

$$\begin{aligned}\langle \mathbf{r}, S, \sigma | \hat{P}_J \hat{P}_W\, e^{-\hat{H}(t-t_0)} \hat{P}_J \hat{P}_W | \mathbf{r}_0, S, \sigma_0 \rangle = \frac{1}{r r_0} \{ & g^{00}(r, t; r_0, t_0)\, \delta_{\sigma 0}\, \delta_{0 \sigma_0} Y_{00}(\theta, \phi)\, Y^*_{00}(\theta_0, \phi_0) \\ & + g^{02}(r, t; r_0, t_0)\, \delta_{\sigma 0}\, C^{10}_{2 -\sigma_0 1 \sigma_0} Y_{0 0}(\theta, \phi)\, Y^*_{2 -\sigma_0}(\theta_0, \phi_0) \\ & + g^{20}(r, t; r_0, t_0)\, C^{10}_{2 -\sigma 1 \sigma}\, \delta_{0 \sigma_0} Y_{2 -\sigma}(\theta, \phi)\, Y^*_{00}(\theta_0, \phi_0) \\ & + g^{22}(r, t; r_0, t_0)\, C^{10}_{2 -\sigma 1 \sigma}\, C^{10}_{2 -\sigma_0 1 \sigma_0} Y_{2 -\sigma}(\theta, \phi)\, Y^*_{2 -\sigma_0}(\theta_0, \phi_0) \}, \end{aligned} \quad (8)$$

where $\hat{P}_J$ and $\hat{P}_W$ are the projectors on the total angular momentum $J = 1$ and on the parity $W = +$, and $C^{JM}_{LmS\sigma}$ are the Clebsch-Gordan coefficients. Without loss of generality, we have taken into account the term $J_z = 0$ only. Moreover, if we define the matrix

$$G(\mathbf{u}) = \begin{pmatrix} g^{00} & g^{02} \\ g^{20} & g^{22} \end{pmatrix}, \quad (9)$$

it satisfies formally the usual composition law

$$G(r, t; r_0, t_0) = \int dr'\, G(r, t; r', t') G(r', t'; r_0, t_0), \quad (10)$$

where GG is a matrix product. The main problem in evaluating the discretized forms of the g^{ab} is due to the fact that the exponential of the tensor operator $\hat{S}_{12}$ is a function of the angular variables too. Then the separation of angular and radial coordinates is not so straightforward as in the case of a radial potential; this difficulty can be overcome by using the fact that the exponential of the tensor potential can be written

$$e^{\alpha \hat{S}_{12}} = A(\alpha) + B(\alpha) \hat{S}_{12}. \quad (11)$$

Then, for the short time radial functions g^{ab}, we obtain

$$g^{00}(\mathbf{u}) = k_0(\mathbf{u}) e^{-f_C(\mathbf{u})} A(\alpha), \quad (12a)$$

TABLE II. Ground and excited state energies of the Krazer potential. The number of points is equal to 33. E_l, E_l^{th} are, respectively, the numerical and theoretical values of the energy.

A	E_0	E_0^{th}	E_1	E_1^{th}
5.0	-0.036508	-0.036492	-0.031253	-0.031250
1.0	-0.125435	-0.125000	-0.076226	-0.076201
0.5	-0.192690	-0.190983	-0.094334	-0.094290
0.2	-0.299304	-0.293044	-0.110501	-0.110427

$$g^{02}(\mathbf{u}) = \frac{\sqrt{8}}{2}[k_0(\mathbf{u}) + k_2(\mathbf{u})]e^{-f_C(\mathbf{u})-\frac{1}{2}f_{LS}(\mathbf{u})}B(\alpha), \quad (12b)$$

$$g^{20}(\mathbf{u}) = \frac{\sqrt{8}}{2}[k_0(\mathbf{u}) + k_2(\mathbf{u})]e^{-f_C(\mathbf{u})-\frac{1}{2}f_{LS}(\mathbf{u})}(\alpha), \quad (12c)$$

$$g^{22}(\mathbf{u}) = k_2(\mathbf{u})e^{-f_C(\mathbf{u})-f_{LS}(\mathbf{u})}\{A(\alpha) - 2B(\alpha)\}, \quad (12d)$$

where $\alpha = -f_T(\mathbf{u})$.

We can, now, build up the finite time propagator through the composition law (10). The results for the binding energy of deuteron are given in Table III (we used the Argonne V14 potential). As shown by the data, the deuteron case is particularly difficult, because the very long tail of the wave function requires the use of a large range of integration, and consequently large N, to have the full contribution to the energy.

TABLE III. Deuteron binding energy. N is the number of points. E_0 is the numerical value of the binding energy. $r_{\max}$ is the range of integration.

N	$r_{\max}$ (fm)	E_0[a]
51	20.0	-4.074
101	20.0	-2.425
201	20.0	-2.243

[a] $E_{\text{Argonne}} = -2.225$ MeV.

Work on further applications and improvements of the method is in progress.

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