J.Sci.Soc.Thailand, 21(1995) 253-269

THE PROPAGATOR CORRESPONDING TO A MODEL QUADRATIC ACTION

J. POULTER AND W. TRIAMPO

Department of Mathematics, Faculty of Science, Mahidol University, Rama 6 Road, Bangkok 10400, Thailand.

(Received May 23, 1995)

ABSTRACT

In this paper we give a complete expression for the one-particle propagator corresponding to an action containing a series of any number of non-local harmonic oscillators, a local harmonic oscillator and a term due to an arbitrary driving force. We also outline how the diagonal matrix elements may be applied in variational calculations concerning two interacting particles in a field.

1. INTRODUCTION

There exists a variety of problems involving quantum mechanics which require a suitable non-perturbative treatment. In many instances path-integral techniques have provided satisfactory results as, for example, in Feynman's celebrated work on the polaron [1] and in disordered systems [2]. For problems of this nature, the retarded propagator can be expressed in terms of a path integral with a non-local action. Physical quantities are then generally estimated using variational techniques which simulate the actual system with a trial quadratic action which must also be non-local.

The polaron [1] is an example of a particle in a field with which it interacts. The trace over the field coordinates is taken exactly to leave a one-particle action which is entirely non-local. This development has been extended to the case of two [3,4], or more [5,6], interacting particles in a field. For such cases the best trial actions involve both local and non-local terms.

There have been published a number of articles on the subject of general quadratic actions, including [7-9]. The methods developed are, however, difficult to apply to certain more complicated specific examples. In this paper we present an explicit derivation of the propagator corresponding to the following action :

$$S=\frac{1}{2}m\int_0^t d\tau\ \dot{\vec{r}}(\tau)^2-\frac{1}{2}m\omega_0^2\int_0^t d\tau\ \vec{r}(\tau)^2$$

$$-\frac{1}{8}\sum_{i=1}^{n}\kappa_i\Omega_i\int_0^t d\tau\int_0^t d\sigma\frac{\cos\Omega_i(\frac{t}{2}-|\tau-\sigma|)}{\sin\frac{1}{2}\Omega_i t}(\vec{r}(\tau)-\vec{r}(\sigma))^2$$

$$+\int_0^t d\tau\ \vec{F}(\tau)\cdot\vec{r}(\tau) \tag{1.1}$$

This action contains the kinetic energy of a particle of mass m, a local harmonic potential, a series of n non-local terms and a term due to an arbitrary driving force $\vec{F}$. We assume that ω_o^2 and the κ_i are not zero and that the Ω_i are distinct. In the case of one non-local term ($n=1$), the propagator has been given by Castrigiano and Kokiantonis [10]. The derivation for any number of non-local terms but no local term was reported in [11].

Since the action S is a quadratic function it is known [12] that the propagator must take the form

$$K(\vec{r}(t),t;\vec{r}(0),0)=G(t)\exp[\tfrac{i}{\hbar}S_{cl}(\vec{r}(t),\vec{r}(0),t)] \tag{1.2}$$

where S_{cl} is the classical action and $G(t)$ is the prefactor given by

$$G(t)=K_{F=0}(0,t;0,0) \tag{1.3}$$

The propagator is a path integral over all paths starting at time zero from $\vec{r}(0)$ and ending at time t at $\vec{r}(t)$.

We obtain the solution to the classical equation of motion by generalising the approach of [10]. The prefactor is then derived from the classical action using a generating functional. We also include a brief discussion of how our propagator might be used to improve variational estimates of the energy of two particles in a field.

2. THE CLASSICAL SOLUTION

For notational convenience we will first work in one dimension. The classical equation of motion reads

$$m\ddot{x}(\tau)\ +\ (m\omega_0^2+\sum_{i=1}^{n}\kappa_i)x(\tau)$$

$$=\ \frac{1}{2}\sum_{i=1}^{n}\kappa_i\Omega_i\int_0^t d\sigma\frac{\cos\Omega_i(\frac{t}{2}-|\tau-\sigma|)}{\sin\frac{1}{2}\Omega_i t}x(\sigma)\ +\ F(\tau) \tag{2.1}$$

and the Fourier transform

$$X(z) = \int_0^t d\tau \ e^{-i\tau z} \ x(\tau) \tag{2.2}$$

is given by

$$m\left[\omega_0^2 - z^2\left(1 + \frac{1}{m}\sum_{i=1}^{n}\frac{\kappa_i}{\Omega_i^2 - z^2}\right)\right] X(z)$$

$$= m(\dot{x}(0) + izx(0)) - me^{-itz}(\dot{x}(t) + izx(t)) + \int_0^t d\tau \, e^{-i\tau z} F(\tau)$$

$$+\frac{1}{2}i(1 - e^{-itz})\sum_{i=1}^{n}\frac{\kappa_i\Omega_i}{\sin\frac{1}{2}\Omega_i t}\frac{1}{\Omega_i^2 - z^2}\left(z\,\mathrm{Re}(e^{\frac{1}{2}i\Omega_i t}X(\Omega_i)) + i\Omega_i\,\mathrm{Im}(e^{\frac{1}{2}i\Omega_i t}X(\Omega_i))\right) \tag{2.3}$$

It is useful to introduce n parameters ω_i, as in [11], which are solutions of

$$\sum_{j=1}^{n}\frac{\kappa_j}{\omega_i^2 - \Omega_j^2} = m \tag{2.4}$$

Then

$$1 + \frac{1}{m}\sum_{i=1}^{n}\frac{\kappa_i}{\Omega_i^2 - z^2} = \prod_{i=1}^{n}\frac{\omega_i^2 - z^2}{\Omega_i^2 - z^2} \tag{2.5}$$

and the left-hand side of (2.3) is zero if

$$\omega_0^2\prod_{i=1}^{n}(\Omega_i^2 - z^2) = z^2\prod_{i=1}^{n}(\omega_i^2 - z^2) \tag{2.6}$$

This equation has $2(n+1)$ roots z_l which are distributed symmetrically about zero.

Provided that the z_l are distinct we can write

$$X(z) = \sum_l \frac{S_l(z) - S_l(z_l)}{z - z_l} \tag{2.7}$$

where

$$S_l(z) = a_l e^{-it(z - z_l)} + b_l\int_0^t d\tau \, e^{-i\tau z} F(\tau) \tag{2.8}$$

with coefficients a_l and b_l to be determined. This result is obtained from (2.3) while demanding that $X(z)$ is always finite. If the initial parameters are chosen so that the z_l are not distinct we can take appropriate limits afterwards.

The coefficients b_l are easily found by comparing terms in (2.3), with $X(z)$ given by (2.7) and (2.8), which involve the arbitrary driving force F. We find that

$$b_l = -\frac{1}{2mz_l}\frac{\prod_{i=1}^{n}\left(z_l^2-\Omega_i^2\right)}{\prod_{k=0}^{n}{}'\left(z_l^2-z_k^2\right)} \tag{2.9}$$

where the lower product contains n factors, the prime indicating the exclusion of the $k=l$ factor. Clearly

$$\sum_l b_l = 0 \tag{2.10}$$

It can also be shown that

$$-m\sum_l b_l z_l = 1 \tag{2.11}$$

and that, for any of the Ω_i,

$$\sum_l \frac{b_l z_l}{z_l^2-\Omega_i^2} = 0 \tag{2.12}$$

The solution for $x(\tau)$ is now given by

$$ix(\tau) = \sum_l e^{i\tau z_l}\left(a_l + b_l\int_\tau^t d\sigma\, e^{-i\sigma z_l}F(\sigma)\right) \tag{2.13}$$

Differentiating twice and using (2.10) and (2.11) yields

$$im\ddot{x}(\tau) = -m\sum_l z_l^2 e^{i\tau z_l}\left(a_l + b_l\int_\tau^t d\sigma\, e^{-i\sigma z_l}F(\sigma)\right) + iF(\tau) \tag{2.14}$$

Comparison with the equation of motion (2.1) now gives that

$$\sum_{i=1}^{n}\kappa_i\Omega_i^2\sum_l \frac{e^{i\tau z_l}}{\Omega_i^2 - z_l^2}\left(a_l + b_l\int_\tau^t d\sigma\, e^{-i\sigma z_l}F(\sigma)\right)$$

$$=\frac{1}{2}\sum_{i=1}^{n}\kappa_i\Omega_i\int_0^t d\sigma\frac{\cos\Omega_i(\frac{t}{2}-|\tau-\sigma|)}{\sin\frac{1}{2}\Omega_i t}ix(\sigma) \qquad (2.15)$$

in view of the fact that the z_l obey

$$m(\omega_0^2 - z_l^2) = z_l^2\sum_{i=1}^{n}\frac{\kappa_i}{\Omega_i^2 - z_l^2} \qquad (2.16)$$

We next substitute for $x(\sigma)$ in (2.15) and perform some integrals. Using (2.12), we can then demonstrate that

$$\sum_{i=1}^{n}\frac{\kappa_i\Omega_i}{\sin\frac{1}{2}\Omega_i t}\sum_l\left(\frac{e^{i\Omega_i(\frac{t}{2}-\tau)}}{\Omega_i + z_l} - \frac{e^{-i\Omega_i(\frac{t}{2}-\tau)}}{\Omega_i - z_l}\right)$$

$$\cdot\left((1-e^{itz_l})a_l + b_l\int_0^t d\sigma\, e^{-i\sigma z_l}F(\sigma)\right) = 0 \qquad (2.17)$$

This result must be true for any value of τ in the interval $(0,t\ )$ This allows us to write

$$\sum_l\frac{1}{\Omega_i^2 - z_l^2}\left((1-e^{itz_l})a_l + b_l\int_0^t d\sigma\, e^{-i\sigma z_l}F(\sigma)\right)$$

$$=\sum_l\frac{z_l}{\Omega_i^2 - z_l^2}\left((1-e^{itz_l})a_l + b_l\int_0^t d\sigma\, e^{-i\sigma z_l}F(\sigma)\right)$$

$$=0 \qquad (2.18)$$

for each of the Ω_i. The two remaining equations necessary for solving for the a_l are obtained from (2.13). These are

$$ix(t) = \sum_l e^{itz_l}a_l \qquad (2.19)$$

and

$$ix(0) = \sum_l\left(a_l + b_l\int_0^t d\sigma\, e^{-i\sigma z_l}F(\sigma)\right) \qquad (2.20)$$

To solve for the a_l we need to invert a (2n +2) x (2n +2) matrix M. With the a_l contained in a vector $\vec{a}$, we can arrange this as

$$\mathrm{M}\,\vec{a} = \vec{R} \tag{2.21}$$

with

$$R_1 = i\big(x(t) + x(0)\big) - \sum_l b_l \int_0^t d\sigma\, e^{-i\sigma z_l} F(\sigma) \tag{2.22}$$

$$R_2 = i\big(x(0) - x(t)\big) - \sum_l b_l \int_0^t d\sigma\, e^{-i\sigma z_l} F(\sigma) \tag{2.23}$$

and, for $1 \le i \le n$;

$$R_{2i+1} = -\sum_l \frac{b_l}{\Omega_i^2 - z_l^2} \int_0^t d\sigma\, e^{-i\sigma z_l} F(\sigma) \tag{2.24}$$

$$R_{2i+2} = -\sum_l \frac{b_l z_l}{\Omega_i^2 - z_l^2} \int_0^t d\sigma\, e^{-i\sigma z_l} F(\sigma) \tag{2.25}$$

The inverse of the matrix M is given by

$$\left(M^{-1}\right)_{l1} = \frac{b_l}{2 s_l \sum_k b_k c_k} e^{-\frac{1}{2} i t z_l} \tag{2.26}$$

$$\left(M^{-1}\right)_{l2} = -\frac{1}{2} i m \frac{b_l z_l}{s_l} e^{-\frac{1}{2} i t z_l} \tag{2.27}$$

and, for $1 \le i \le n$;

$$\left(M^{-1}\right)_{l,2i+1} = \frac{i}{2 s_l} \frac{b_l z_l}{\Omega_i^2 - z_l^2} \frac{e^{-\frac{1}{2} i t z_l}}{\sum_k \frac{b_k z_k}{\left(\Omega_i^2 - z_l^2\right)^2}} \tag{2.28}$$

$$\left(M^{-1}\right)_{l,2i+2} = -\left(M^{-1}\right)_{l,2i+1} \frac{\sum_k \frac{b_k c_k (z_k^2 - z_l^2)}{\Omega_i^2 - z_k^2}}{z_l \sum_k b_k c_k} \tag{2.29}$$

In these expressions

$$s_l = \sin \frac{1}{2} t z_l \tag{2.30}$$

and

$$c_l = \cot\frac{1}{2}tz_l \tag{2.31}$$

The a_l are now given by

$$a_l = \frac{b_l}{2s_l}\frac{e^{-\frac{1}{2}itz_l}}{\sum_k b_k c_k} \cdot \left[i(x(0)+x(t)) + mz_l(x(0)-x(t))\sum_k b_k c_k - \int_0^t d\sigma\, F(\sigma)\sum_k b_k e^{-i\sigma z_k}\left(1 - imz_l\sum_p b_p c_p + iA_{lk}\right)\right] \tag{2.32}$$

where

$$A_{lk} = \sum_{i=1}^{n}\frac{1}{\Omega_i^2 - z_l^2}\frac{1}{\Omega_i^2 - z_k^2}\frac{1}{\sum_p \frac{b_p z_p}{\left(\Omega_i^2 - z_p^2\right)^2}} \cdot \left(z_l\sum_p b_p c_p - z_k\sum_p \frac{b_p c_p (z_p^2 - z_l^2)}{\Omega_i^2 - z_p^2}\right) \tag{2.33}$$

We can simplify (2.32) by using the following results. First,

$$\sum_{i=1}^{n}\frac{1}{\Omega_i^2 - z_l^2}\frac{1}{\Omega_i^2 - z_k^2}\frac{1}{\sum_p \frac{b_p z_p}{\left(\Omega_i^2 - z_p^2\right)^2}} = m + \frac{\delta_{lk}}{2b_l z_l} \tag{2.34}$$

where δ_{lk} is equal to unity if $z_l^2 = z_k^2$ and zero otherwise. Second, for z_q^2 distinct from both z_l^2 and z_k^2,

$$\sum_{i=1}^{n}\frac{1}{\Omega_i^2 - z_l^2}\frac{1}{\Omega_i^2 - z_k^2}\frac{1}{\Omega_i^2 - z_q^2}\frac{1}{\sum_p \frac{b_p z_p}{\left(\Omega_i^2 - z_p^2\right)^2}} = \frac{\delta_{lk}}{2b_l z_l}\frac{1}{z_l^2 - z_q^2} \tag{2.35}$$

It now follows that

$$\sum_k b_k e^{-i\sigma z_k} A_{lk} = e^{-i\sigma z_l}\sum_k b_k c_k + \sum_k b_k e^{-i\sigma z_k}\left(mz_l\sum_p b_p c_p - c_k\right) \tag{2.36}$$

Substitution in (2.32) then gives

$$a_l = \frac{b_l}{2s_l}\frac{e^{-\frac{1}{2}itz_l}}{\sum_k b_k c_k} \cdot \left[i(x(0)+x(t)) + mz_l(x(0)-x(t))\sum_k b_k c_k - i\int_0^t d\sigma\, e^{-i\sigma z_l} F(\sigma)\sum_k b_k c_k + i\int_0^t d\sigma\, F(\sigma)\sum_k \frac{b_k}{s_k} e^{-i(\sigma-\frac{t}{2})z_k} \right) \quad (2.37)$$

Finally we substitute for the a_l in (2.13) and find that

$$x(\tau) = -\frac{1}{2}(x(t)-x(0))\dot{\Delta}(\tau) + \frac{1}{2}(x(t)+x(0))\frac{\Delta(\tau)}{\Delta(0)} - \frac{1}{2m}\int_0^t d\sigma F(\sigma)\left(\frac{\Delta(\tau)\Delta(\sigma)}{\Delta(0)} - \Delta(|\tau-\sigma|)\right) \quad (2.38)$$

where

$$\Delta(\tau) = -m\sum_l \frac{b_l}{s_l}\cos(\tau - \tfrac{t}{2})z_l \quad (2.39)$$

This result clearly reduces to that given in [10] if $n=1$.

The classical action is easily derived from (2.38). We find that

$$\begin{aligned} S_{cl} &= \frac{1}{2}m(x(t)\dot{x}(t) - x(0)\dot{x}(0)) + \frac{1}{2}\int_0^t d\tau\; F(\tau)x(\tau) \\ &= -\frac{1}{4}m\ddot{\Delta}(0)(x(t)-x(0))^2 - \frac{1}{4}m\frac{1}{\Delta(0)}(x(t)+x(0))^2 \\ &\quad -\frac{1}{2}(x(t)-x(0))\int_0^t d\tau\; F(\tau)\dot{\Delta}(\tau) + \frac{1}{2}(x(t)+x(0))\int_0^t d\tau\; F(\tau)\frac{\Delta(\tau)}{\Delta(0)} \\ &\quad -\frac{1}{4m}\int_0^t d\tau\int_0^t d\sigma\, F(\tau)F(\sigma)\left(\frac{\Delta(\tau)\Delta(\sigma)}{\Delta(0)} - \Delta(|\tau-\sigma|)\right) \end{aligned} \quad (2.40)$$

In more than one dimension we simply replace x and F by vectors and take scalar products where appropriate.

3. THE PREFACTOR

The prefactor $G(t)$ is given by a path integral over all paths from and back to the origin [12], that is

$$G(t) = \int_0^0 D[x(\tau)] \; e^{\frac{i}{\hbar} S_{F=0}} \tag{3.1}$$

This is obvious since the classical action is zero if $x(0) = x(t) = 0$ and $F = 0$. If we now differentiate with respect to ω_0^2 it is found that

$$-i\hbar\omega_0^2 \frac{\partial}{\partial\omega_0^2} \ln G(t) = \left\langle \omega_0^2 \frac{\partial S_{F=0}}{\partial\omega_0^2} \right\rangle$$

$$= -\frac{1}{2} m\omega_0^2 \int_0^t d\tau \left\langle x(\tau)^2 \right\rangle \tag{3.2}$$

where the average $\langle A \rangle$, of any quantity A, is defined by

$$\langle A \rangle = \frac{1}{G(t)} \int_0^0 D[x(\tau)] A \; \exp\left(\frac{i}{\hbar} S_{F=0} \right) \tag{3.3}$$

Substitution of the force

$$F(\sigma) = \hbar k \delta(\tau - \sigma) \tag{3.4}$$

into the classical action (2.40) with $x(0) = x(t) = 0$ shows that

$$\left\langle e^{ikx(\tau)} \right\rangle = \exp\left[\frac{-i\hbar k^2}{4m} \left(\frac{\Delta(\tau)^2}{\Delta(0)} - \Delta(0) \right) \right] \tag{3.5}$$

Then, expanding in powers of k and comparing coefficients of k^2 , we have

$$\left\langle x(\tau)^2 \right\rangle = \frac{i\hbar}{2m}\left(\frac{\Delta(\tau)^2}{\Delta(0)} - \Delta(0)\right) \tag{3.6}$$

and, substituting into (3.2),

$$\frac{\partial}{\partial\omega_0^2}\ln G(t) = \frac{1}{4}\int_0^t d\tau\left(\frac{\Delta(\tau)^2}{\Delta(0)} - \Delta(0)\right) \tag{3.7}$$

Consider next the polynomial

$$P(z^2) = z^2\prod_{i=1}^{n}(z^2 - \omega_i^2) - \omega_0^2\prod_{i=1}^{n}(z^2 - \Omega_i^2) \tag{3.8}$$

According to (2.6) $P(z_l^2) = 0$. Differentiation with respect to ω_0^2, with constant Ω_i and ω_i , yields

$$\frac{\partial z_l^2}{\partial\omega_0^2}P'(z_l^2) = \prod_{i=1}^{n}(z_l^2 - \Omega_i^2) \tag{3.9}$$

where $P'(z^2)$ is the derivative of $P(z^2)$ with respect to z^2 . Now,

$$P'(z_l^2) = \prod_{k=0}^{n}{}'(z_l^2 - z_k^2) \tag{3.10}$$

and, comparing (2.9), we have that

$$\frac{\partial z_l^2}{\partial\omega_0^2} = -2mb_l z_l \tag{3.11}$$

This result is necessary to manipulate the left-hand side of (3.7).

Returning to (2.9) we see that, if z_l^2 and z_k^2 are not equal,

$$\frac{\partial b_k}{\partial z_l^2} = \frac{b_k}{z_k^2 - z_l^2} \tag{3.12}$$

Also, using (2.11), it is found that

$$z_l\frac{\partial b_l}{\partial z_l^2} = -\frac{b_l}{2z_l} - \sum_{k=0}^{n}{}'\frac{b_k z_k}{z_k^2 - z_l^2} \tag{3.13}$$

where the summation is over half of the z_k. If z_k is included then $-z_k$ is not. The $k=l$ term is of course excluded as indicated by the prime on the summation. Using this summation scheme,

$$\Delta(\tau) = -2m\sum_{l=0}^{n}\frac{b_l}{s_l}\cos(\tau-\tfrac{t}{2})z_l \tag{3.14}$$

and, with (3.12) and (3.13),

$$\frac{\partial}{\partial z_l^2}\Delta(0) = \frac{mb_l}{2z_l}\left(\frac{2c_l}{z_l}+\frac{t}{s_l^2}\right) - \frac{2m}{z_l}\sum_{k=0}^{n}{}' \frac{b_k}{z_k^2-z_l^2}\left(c_k z_l - c_l z_k\right) \tag{3.15}$$

It is now easy to show that

$$\int_0^t d\tau\ \Delta(\tau)^2 = 4m\sum_{l=0}^{n} b_l z_l \frac{\partial}{\partial z_l^2}\Delta(0) \tag{3.16}$$

Finally, since

$$\Delta(0) = \frac{-8m}{t}\sum_{l=0}^{n} b_l z_l \frac{\partial}{\partial z_l^2}\ln s_l \tag{3.17}$$

we see that, using (3.11) and (3.16) in (3.7),

$$\frac{\partial}{\partial z_l^2}\ln G(t) = -\frac{\partial}{\partial z_l^2}\left(\tfrac{1}{2}\ln\Delta(0) + \ln s_l\right) \tag{3.18}$$

Integrating and comparing with the result in [11] for $\omega_0 = 0$ the final result for the prefactor is

$$G(t) = \left(\frac{m}{4\pi i\hbar\Delta(0)}\right)^{\frac{1}{2}} \frac{\prod_{i=1}^{n}\sin\frac{1}{2}\Omega_i t}{\prod_{l=0}^{n}\sin\frac{1}{2}z_l t} \tag{3.19}$$

In d dimensions we simply raise this whole expression to the power d. For $n=1$ the prefactor given in [10] is recovered.

4. A TRIAL ACTION FOR TWO PARTICLES IN A FIELD

We will now give an expression for an upper bound on the ground-state energy of two interacting particles in a field which may contain any number of variational parameters.

To establish notation, our Hamiltonian is

$$H=\frac{P_1^2}{2m}+\frac{P_2^2}{2m}+V(|\vec{r}_1-\vec{r}_2|)+\sum_{\vec{k}}\hbar\omega_k b_{\vec{k}}^{+}b_{\vec{k}}$$

$$+\sum_{\vec{k}}\sqrt{\frac{\hbar}{L^d}}g_k^2(e^{i\vec{k}.\vec{r}_1}+e^{i\vec{k}.\vec{r}_2})(b_{\vec{k}}+b_{-\vec{k}}^{+}) \qquad (4.1)$$

This includes the kinetic energy of two particles of mass m , an interparticle interaction V, the kinetic energy of collective modes of frequency ω_k and an interaction term characterised by the coupling constant g_k. The $b_{\vec{k}}$ are the usual boson operators and L^d is the d-dimensional volume. Generalisation to include more than one type of collective mode, as in [3], is obvious.

Elimination of the field coordinates by the prescription of Feynman [13] reformulates the problem in terms of the two-particle propagator

$$K(\vec{r}_1(t),\vec{r}_2(t),t;\vec{r}_1(0),\vec{r}_2(0),0)=\int_{\vec{r}_1(0)}^{\vec{r}_1(t)}D[\vec{r}_1(\tau)]\int_{\vec{r}_2(0)}^{\vec{r}_2(t)}D[\vec{r}_2(\tau)]\ e^{\frac{i}{\hbar}S} \qquad (4.2)$$

The path integrations are over all paths from time zero, when the particles are at $\vec{r}_1(0)$ and $\vec{r}_2(0)$, to time t when they are at $\vec{r}_1(t)$ and $\vec{r}_2(t)$. The action S is given by

$$S=\int_0^t d\tau\left(\frac{1}{2}m(\dot{\vec{r}}_1(\tau)^2+\dot{\vec{r}}_2(\tau)^2)-V\left(\left|\vec{r}_1(\tau)-\vec{r}_2(\tau)\right|\right)\right)$$

$$+\frac{1}{2L^d}\sum_{\vec{k}}g_k^2\int_0^t d\tau\int_0^t d\sigma\frac{\cos\omega_k(\frac{t}{2}-|\tau-\sigma|)}{\sin\frac{1}{2}\omega_k t}$$

$$\cdot(e^{i\vec{k}\cdot\vec{r}_1(\tau)}+e^{i\vec{k}\cdot\vec{r}_2(\tau)})(e^{-i\vec{k}\cdot\vec{r}_1(\sigma)}+e^{-i\vec{k}\cdot\vec{r}_2(\sigma)}) \qquad (4.3)$$

The ground-state energy is given by

$$E_0 = -\lim_{\beta\to\infty}\frac{1}{\beta}\ln K(-i\hbar\beta) \tag{4.4}$$

where $K(t)$ is shorthand for $K(0,0,t;0,0,0)$ and β is the inverse temperature. An upper bound on E_0 is obtained from the approximate propagator [13]

$$K(t) \approx K_o(t)\, e^{\frac{i}{\hbar}\langle S - S_o\rangle} \tag{4.5}$$

where S_o is a trial action, K_o is the propagator for S_o and the average $\langle A\rangle$, of any quantity A, is

$$\langle A\rangle = \frac{1}{K_o(t)}\int_0^0 D(\vec{r}_1(\tau))\int_0^0 D(\vec{r}_2(\tau))\, e^{\frac{i}{\hbar}S_o} \tag{4.6}$$

For convenience we will follow Khandekar [14] and introduce a transformation of coordinates

$$\vec{x} = \frac{1}{\sqrt{2}}(\vec{r}_1 - \vec{r}_2) \tag{4.7}$$

$$\vec{y} = \frac{1}{\sqrt{2}}(\vec{r}_1 + \vec{r}_2) \tag{4.8}$$

With these definitions $\vec{x}$ is the coordinate for the relative motion and $\vec{y}$ is the coordinate for the translationally invariant centre-of-mass motion.

The trial action we consider is

$$S_o = \frac{1}{2}m\int_0^t d\tau\,(\dot{\vec{x}}(\tau)^2 + \dot{\vec{y}}(\tau)^2 - \omega_o^2\,\vec{x}(\tau)^2)$$

$$-\frac{1}{8}\sum_{i=1}^{n}\kappa_i\Omega_i\int_0^t d\tau\int_0^t d\sigma\,\frac{\cos\Omega_i(\frac{t}{2}-|\tau-\sigma|)}{\sin\frac{1}{2}\Omega_i t}(\vec{x}(\tau)-\vec{x}(\sigma))^2$$

$$-\frac{1}{8}\sum_{i=1}^{n'}\kappa_i'\Omega_i'\int_0^t d\tau\int_0^t d\sigma\,\frac{\cos\Omega_i'(\frac{t}{2}-|\tau-\sigma|)}{\sin\frac{1}{2}\Omega_i' t}(\vec{y}(\tau)-\vec{y}(\sigma))^2 \tag{4.9}$$

This choice contains $2(n+n')+1$ variational parameters. These are the κ_i and Ω_i for $1 \le i \le n$, the κ_i' and Ω_i' for $1 \le i \le n'$ and ω_o. Previous work [3,4] has used this trial action with $n=n'=1$ and $\Omega_1 = \Omega_1'$, that is four variational parameters. A constant force driving the relative motion was also included in [4] to aid in identifying the state where the particles are bound together. We find this to be unnecessary.

Finding an upper bound for E_o using the approximate propagator (4.5) is a straightforward but rather tedious operation. Essentially, we can use (2.40) to deal with terms involving the relative motion and the classical action in [11] for those involving the centre-of-mass motion. Our result is

$$E_o \le \frac{1}{2} d\hbar \sum_{l=0}^{n} z_l(1+mb_l z_l) - \frac{1}{2} d\hbar \sum_{i=1}^{n} \Omega_i + \frac{1}{2} d\hbar \sum_{i=1}^{n'} \left(\omega_i' - \Omega_i' - \frac{1}{2} m \frac{h_i}{\omega_i'} \right)$$

$$+ \frac{1}{L^d} \sum_{\vec{k}} V_k e^{\hbar k^2 \sum_{l=0}^{n} b_l} - \frac{2}{L^d} \sum_{\vec{k}} g_k^2 \int_0^\infty dx\, e^{-\omega_k x} \left(e^{-\frac{1}{4}\hbar k^2 C_+(x)} + e^{-\frac{1}{4}\hbar k^2 C_-(x)} \right) \tag{4.10}$$

where V_k is the Fourier transform of the interparticle interaction and

$$C_{\pm}(x) = -2\sum_{l=0}^{n} b_l \left(1 \pm e^{-z_l x}\right) + \sum_{i=1}^{n'} \frac{h_i}{\omega_i'^3} \left(1 - e^{-\omega_i' x}\right) + \frac{1}{m} \left(1 - m \sum_{i=1}^{n'} \frac{h_i}{\omega_i'^2}\right) x \tag{4.11}$$

The z_l are given by (2.16) and the b_l by (2.9). The ω_i' and h_i are given according to the results of [11] ;

$$\sum_{j=1}^{n'} \frac{\kappa_j'}{\omega_i'^2 - \Omega_j'^2} = m \tag{4.12}$$

and

$$h_i = \frac{1}{m}\left(\omega_i'^2 - \Omega_i'^2\right) \prod_{j=1}^{n'}{}' \frac{\Omega_j'^2 - \omega_i'^2}{\omega_j'^2 - \omega_i'^2} \tag{4.13}$$

where the $i=j$ factor is excluded.

In actual minimisations of (4.10) it is convenient to let the variational parameters be the z_l for $0 \le l \le n$, the Ω_i for $1 \le i \le n$ and the Ω_i' and ω_i' for $1 \le i \le n'$. Each of these parameters must be kept real and non-negative. Also the z_l and the ω_i' must be distinct. If the smallest of the z_l, say z_o, is set to be zero we have the state where the particles have infinite separation. Otherwise the average separation is always finite and given by

$$\left\langle \vec{x}^2 \right\rangle = -d\hbar \sum_{l=0}^{n} b_l \tag{4.14}$$

Whether or not the particles are bound depends on which state has the lowest energy.

The best known example of this general formalism is the large bipolaron. The field consists of longitudinal optical phonons and the particles are electrons with a Coulomb interaction. The electron-lattice interaction takes the form suggested by Fröhlich [15]. Phonon dispersion is ignored and ω_k is set to be a constant. In Feynman units ($\hbar = m = \omega_k = 1$) the electron-lattice coupling constant is then given by (d =3)

$$g_k^2 = \frac{2\sqrt{2}\pi\alpha}{k^2} \tag{4.15}$$

where α is the dimensionless polaron coupling constant. With

$$V_k = \frac{4\pi U}{k^2} \tag{4.16}$$

all the sums over $\vec{k}$ in (4.10) can be performed exactly and (d =3)

$$E_o \le \frac{3}{2}\sum_{l=0}^{n} z_l(1 + b_l z_l) - \frac{3}{2}\sum_{i=1}^{n}\Omega_i + \frac{3}{2}\sum_{i=1}^{n'}\left(\omega_i' - \Omega_i' - \frac{1}{2}\frac{h_i}{\omega_i'}\right)$$
$$+ \frac{U}{\left(-\pi\sum_{l=0}^{n} b_l\right)^{\frac{1}{2}}} \frac{2\sqrt{2}\alpha}{\sqrt{\pi}} \int_0^\infty dx\, e^{-x}\left(C_+(x)^{-\frac{1}{2}} + C_-(x)^{-\frac{1}{2}}\right) \tag{4.17}$$

If $\omega_o = 0$ this reduces to twice the upper bound for the ground-state energy of a large polaron given in [16]. For d =2 there is a simple scaling relation [4] which can be used to convert (4.17).

We have investigated (4.17) numerically. Increasing the number of variational parameters always decreases the upper bound. In particular better results are found in the domain of bipolaron stability if the Ω_i and the Ω_i' are not equal. In the table we present some data for illustration. Although the improvements are not in this case remarkable, they do illustrate the general principle that the upper bound (4.10) is better optimised by increasing the number of variational parameters. It is also worth noting that the complexity of the sums over $\vec{k}$ in (4.10) is independent of the number of variational parameters. Data corresponding to ours for $n = n' = 1$ and $\Omega_1 = \Omega_1'$ has been indicated graphically in [6,17].

We believe that our estimates should be a little lower. The small improvements obtained for the large bipolaron are consistent with those for the large polaron [16].

TABLE Upper bounds on the ground-state energy of a large bipolaron with $U = \sqrt{2}\alpha$ and $n = n'$

n	α	
	10	**20**
1	-28.6490	-101.6911
2	-28.6533	-101.6920
4	-28.6534	-101.6921

5. CONCLUDING REMARKS

We have presented a complete derivation of all the matrix elements of the retarded propagator corresponding to an action containing a local harmonic oscillator, an arbitrary time-dependent driving force and a series of any number of non-local harmonic oscillators. The propagator is given by equations (1.2), (2.40) and (3.19) and is the principal result of this paper.

One application of this result is the simulation of the relative motion of two particles in a field. With n non-local oscillators in the trial action, $2n+1$ parameters are provided for use in a variational calculation. For any system described by the Hamiltonian (4.1), an upper bound on the energy is given by (4.10), which involves as many variational parameters as desired.

ACKNOWLEDGMENT

We thank the National Electronics and Computer Technology Center (NECTEC), National Science and Technology Development Agency (NSTDA), Thailand, for the use of high performance computing facilities.

REFERENCES

1. Feynman R P 1955 *Phys. Rev.* **97**: 660
2. Edwards S F and Gulyaev V V 1964 *Proc. Phys. Soc.* **83**: 495
3. Hiramoto H and Toyozawa Y 1985 *J. Phys. Soc. Jpn.* **54**: 245
4. Verbist G, Peeters F M and Devreese J T 1991 *Phys. Rev.* **B43**: 2712
5. Kochetov E A and Smondyrev M A 1991 *Theor. Math. Phys. (USSR)* **85**: 1062 (English translation)
6. Smondyrev M A, Verbist G, Peeters F M and Devreese J T 1993 *Phys. Rev.* **B47**: 2596
7. Adamowski J, Gerlach B and Leschke H 1982 *J. Math. Phys.* **23**: 243
8. Papadopoulos G J 1985 J. Phys. A : *Math. Gen.* **18**: 1945
9. Khandekar D C and Lawande S V 1986 *Phys. Rep.* **137**: 115
10. Castrigiano D P L and Kokiantonis N 1983 *Phys. Lett.* **96A**: 55
11. Poulter J and Sa-yakanit V 1992 *J. Phys. A : Math. Gen.* **25**: 1539
12. Feynman R P and Hibbs A R 1965 Quantum Mechanics and Path Integrals (New York : Mc Graw-Hill)
13. Feynman R P 1972 Statistical Mechanics (Benjamin : New York)
14. Khandekar D C 1990 *Mod. Phys. Lett.* **B4**: 1201
15. Fröhlich H 1954 *Adv. Phys.* **3**: 325
16. Poulter J and Sa-yakanit V 1993 In Lectures on Path Integration : Trieste 1991, eds Cerdeira H A *et al.* (Singapore : World Scientific) p.506
17. Verbist G, Smondyrev M A, Peeters F M and Devreese J T 1992 *Phys. Rev.* **B45**: 5262