Properties of One-Dimensional Correlated Gaussian Wave Functions

T. R. KOEHLER
IBM Research Laboratory, San Jose, California
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The properties of a certain class of unsymmetrized one-dimensional correlated Gaussian wave functions—those which are ground-state eigenfunctions of some coupled harmonic-oscillator Hamiltonian—are investigated in detail. It is shown that a properly symmetrized wave function constructed from these may be used to calculate the expectation value E_0 of the Hamiltonian appropriate to a system of interacting one-dimensional atoms and that this energy is, to a high degree of accuracy, equal to the value obtained when the unsymmetrized wave function is used. A method is given by which correction terms to E_0 may be obtained. In addition, it is found that even though the number of particles be very large, the necessary multivariable integrals may be performed quite simply.

I. INTRODUCTION

In a previous paper,[1] a two-parameter, many-body, correlated Gaussian wave function was used to calculate the expectation value of a Hamiltonian for N one-dimensional particles interacting through the one-dimensional analog of an atomic potential. A detailed discussion of the following two points was not given in that paper: the proper treatment of terms involving products of different permutations, and the mathematical details of integrating the wave function over all but two coordinates. The first point was avoided by restricting the size of the system, and the second, by a trick. A fuller discussion of these issues will be given in this paper.

The specific problems are those one encounters in calculating the expectation value of a Hamiltonian

$$H=\sum_i(p_i^2/2m)+\sum_{j<i}V(|x_i-x_j|), \tag{1}$$

using a wave function

$$\Phi=\sum P\Psi(x_1,x_2,\cdots,x_n), \tag{2}$$

with

$$\Psi=\exp[-\alpha^2(\tilde{x}-\tilde{b})G(x-b)]. \tag{3}$$

In the above, V is assumed to be a one-dimensional atomic potential, $\sum P$ means the appropriately symmetrized sum over all permutations of the variables $x_1,\cdots,x_N$, $\tilde{x}=(x_1,x_2,\cdots,x_N)$ and $\tilde{b}=(b,2b,\cdots,Nb)$. Thus b is the interatomic spacing, if it is assumed that G is such that Ψ is a maximum at $x=b$.

Noting that $\langle\Phi|H|\Phi\rangle/\langle\Phi|\Phi\rangle=\langle\Psi|H|\Phi\rangle/\langle\Psi|\Phi\rangle$, we wish to establish

$$\frac{\langle\Psi|H|\Phi\rangle}{\langle\Psi|\Phi\rangle}\approx\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}, \tag{4}$$

and to devise a procedure which obtains correction terms to this equation. Equation (4) is the relationship necessary to obtain Eq. (3) of I. In addition, a more general procedure than was used in I for obtaining

$$\psi(x_i,x_j)\equiv\int\Psi^2(x_1,x_2,\cdots,x_N)\prod_{n\neq i,j}dx_n \tag{5}$$

will be derived.

[1] T. Koehler, Phys. Rev. **139**, A1097 (1965). This paper will be referred to as I.

II. MATHEMATICAL PRELIMINARIES

A. Integration Techniques

Expressions for integrals involving correlated Gaussian wave functions are well known[2,3]; in particular

$$\int\exp(-\alpha^2\tilde{x}Mx)dx_2=(\pi/\alpha^2)^{(N_2/2)}|M_{22}|^{-1/2}\times\exp[-\alpha^2\tilde{x}_1(M_{11}-M_{12}(M_{22})^{-1}M_{21})x_1]. \tag{6}$$

Notation which will be used throughout the paper has been introduced for the breaking up of matrices and vectors into components which are themselves matrices and vectors:

$$x=\begin{pmatrix}x_1\\x_2\end{pmatrix},$$

and

$$M=\begin{pmatrix}M_{11}&M_{12}\\M_{21}&M_{22}\end{pmatrix},$$

with the components having dimensions N_1 and N_2. A special notation which will be employed for denoting components of inverse matrices and inverses of component matrices is illustrated below:

$$\begin{pmatrix}M_{11}&M_{12}\\M_{21}&M_{22}\end{pmatrix}\begin{pmatrix}M^{-1}{}_{11}&M^{-1}{}_{12}\\M^{-1}{}_{21}&M^{-1}{}_{22}\end{pmatrix}=\begin{pmatrix}I&0\\0&I\end{pmatrix},$$

$M_{11}(M_{11})^{-1}=I$ and $M_{22}(M_{22})^{-1}=I$, where I is the unit matrix of appropriate dimensions. If x_1 contains the variables $x_{i_1},x_{i_2},\cdots,x_{i_n}$, then $dx_1\equiv dx_{i_1}dx_{i_2}\cdots dx_{i_n}$.

If one substitutes the matrix identities[4]

$$M_{11}-M_{12}(M_{22})^{-1}M_{21}=(M^{-1}{}_{11})^{-1}, \tag{7}$$

and

$$|M|=|M_{22}|\,|M^{-1}{}_{11}|^{-1}, \tag{8}$$

into Eq. (6), one obtains an expression which is more

[2] S. F. Boys, Proc. Roy. Soc. (London) **A253**, 402 (1960).
[3] K. Singer, Proc. Roy. Soc. (London) **A253**, 412 (1960).
[4] The type of matrix manipulation necessary to obtain Eq. (7) is discussed in R. A. Frazer, W. J. Duncan, and A. R. Collar, *Elementary Matrices* (The Macmillan Company, New York, 1947), p. 112.

useful in this paper than Eq. (6):

$$\int \exp(-\alpha^2\tilde{x}M\tilde{x})d\tilde{x}_2=\left(\frac{\pi}{\alpha^2}\right)^{(N_2/2)}|M|^{-1/2}|M^{-1}{}_{11}|^{-1/2}\times\exp\{-\alpha^2[\tilde{x}_1(M^{-1}{}_{11})^{-1}x_1]\}. \quad (9)$$

This form is convenient when N_1 is small, N_2 is large, and M^{-1} can be found because it is then necessary only to invert a small matrix to perform the integration.

B. Matrix Construction

If the matrix G of Eq. (3) be defined by

$$G_{mn}=N^{-1}\sum_s \omega_s e^{is(m-n)}, \quad (10)$$

then, providing $\omega_0\neq 0$,

$$G_{mn}{}^{-1}=N^{-1}\sum \omega_s{}^{-1}e^{is(m-n)}, \quad (11)$$

where $s=2\pi l/N$, $\frac{1}{2}N<l\leqslant\frac{1}{2}N$. The definition of s is conventional; i.e.,

$$N^{-1}\sum_s e^{i(m-n)s}=\delta_{mn}, \quad N^{-1}\sum_m e^{im(s-s')}=\delta_{ss'}.$$

Problems which arise when $\omega_0=0$ will be discussed later.

The wave function Ψ of Eq. (3) with G as defined in Eq. (10) is a generalization of the ground-state eigenfunction of the one-dimensional, nearest-neighbor coupled, harmonic-oscillator Hamiltonian; stated alternately, it is the ground-state eigenfunction of some one-dimensional, coupled harmonic-oscillator Hamiltonian. With $\omega_s=|\sin(\frac{1}{2}s)|$, it is readily found that

$$[-\tfrac{1}{2}\sum \nabla_i{}^2+\tfrac{1}{2}\alpha^4\sum(q_{i+1}-q_i)^2]\Psi=\alpha^2\sum\omega_s\Psi, \quad (12)$$

where $\tilde{q}=\tilde{x}-\tilde{b}$. Then it can be found that

$$G_{mn}=\frac{1}{N}\frac{\sin(\pi/N)}{\cos[2\pi(m-n)/N]-\cos(\pi/N)}, \quad (13)$$

$$\approx(2/\pi)[1-4(m-n)^2]^{-1}, \quad (14)$$

where $(m-n)^2$ is the smaller of $(m-n)^2$ or $(m-n\pm N)^2$. The notation used here is slightly different from that used in I; here $G_{mn}=2/\pi$ rather than unity.

Since the ability to perform integrals over correlated Gaussian wave functions depends upon inverting matrices, the construction of G according to Eq. (10) is particularly useful since, by considering the ω_s as variation parameters, one can generate matrices for which an explicit expression for the elements of the inverse matrix exists. However, in the general case the summations must be performed numerically.

The proof of Eq. (4) is considerably simplified if compact expressions for the matrix elements of G exist, so the wave function satisfying Eq. (12) will be used. However, the insight into the problem gained from this work enables one to check the validity of Eq. (4) for a more general wave function.

It is apparent that $\omega_0=0$ if Ψ satisfies a translationally invariant Schrödinger equation, since $\sum_m G_{mn}=\omega_0$, and Ψ is translationally invariant if $\sum_m G_{mn}=0$. This invariance implies that $\psi(x_i,x_j)=\psi(x_i-x_j)$. Therefore, it is convenient to define $\psi(x_i)\equiv\psi(x_i,x_N)$, and to eliminate the dependence of Φ on x_N by setting $x_N=0$. This also eliminates all permutations involving the index N from Φ which is equivalent to eliminating all permutations in which each coordinate is replaced by that of the particle occupying the next lattice site. Such permutations do not change the form of Ψ because of the translational invariance of Ψ. Then

$$\Psi=\exp[-\alpha^2(\tilde{x}-\tilde{b})F(x-b)], \quad (15)$$

where F is a $(N-1)\times(N-1)$ matrix given by

$$F_{mn}=G_{mn}, \quad m,n=1,\cdots,N-1. \quad (16)$$

The vectors x and b similarly do not contain x_N and b_N. Vectors and matrices will henceforth be used in this sense exclusively unless stated otherwise.

If one uses Eq. (7), the inverse matrix can then be unambiguously obtained by

$$F^{-1}{}_{mn}=\lim_{\omega_0\to 0}(G^{-1}{}_{mn}-G^{-1}{}_{mN}G^{-1}{}_{Nn}/G^{-1}{}_{NN}) \quad (17)$$

$$=S_0+S_{m-n}-S_m-S_n, \quad (18)$$

where

$$S_m=N^{-1}\sum_{s\neq 0}e^{ims}/\omega_s. \quad (19)$$

As an alternative procedure one can use Eq. (9) to obtain the expression that results from integrating Ψ^2 over all coordinates except x_m and x_N. This expression is of the form $\exp[-A^+(x_m+x_N)^2]\times\exp[-A^-(x_m-x_N)^2]$. If one then takes limit $\omega_0\to 0$, it is found that $A^+\to 0$ and A^- is finite. The approach which has been adopted results in some notational simplification. An illustration of the alternate method is contained in the derivation given in Appendix C.

Explicit expressions for quantities which will be used later are:

$$S_m=S_0-\frac{2}{N}\sum_{n=0}^{m-1}\cot\left[\frac{\pi}{N}(m+\tfrac{1}{2})\right], \quad (20)$$

$$F^{-1}{}_{mn}=\frac{2}{N}\sin\frac{\pi m}{N}\sum_{l=0}^{n-1}\csc\left[\frac{\pi}{N}(m-l-\tfrac{1}{2})\right]\times\csc\left[\frac{\pi}{N}(l+\tfrac{1}{2})\right], \quad m>n \quad (21)$$

with $F^{-1}{}_{mn}=F^{-1}{}_{nm}$ and

$$F^{-1}{}_{m1}\approx\frac{4}{\pi}\sin\frac{\pi m}{N}\Big/\sin\left[\frac{\pi}{N}(m+\tfrac{1}{2})\right]. \quad (22)$$

Note in particular that $F^{-1}{}_{m1}\to$ constant for large m as this fact will be used extensively in Appendix B.

III. RESOLUTION OF PERMUTATION PROBLEM

By using Eq. (12) and certain symmetry properties of Ψ, one can obtain

$$\langle\Psi|H|\Phi\rangle/\langle\Psi|\Phi\rangle = \alpha^2\sum\omega_s - (N\alpha^4/2)\langle\Psi|(x_1-b)^2|\Phi\rangle/\langle\Psi|\Phi\rangle + N\langle\Psi|\sum_{n=1}^{N/2-1}V(x_n)|\Phi\rangle/\langle\Psi|\Phi\rangle, \quad (23)$$

where $x_N=Nb\equiv 0$ has been used. Since $V(x)$ is considered to have the form of an atomic potential and is, therefore, small for large x, and since Ψ is only large when $x_b\simeq nb$, the $n=1$ piece of the third term on the right-hand side of Eq. (23) corresponds to the nearest-neighbor interaction and should make the largest contribution to that term. Because of this and for notational convenience, the mathematical effort will be applied to the evaluation of the $n=1$ piece. However, it will be clear that other terms could be treated similarly.

The standard notation[5] for the cycles into which a permutation can be resolved will be used as a superscript on symbols representing quantities pertaining to that particular permutation. Using this notation, one can write

$$\psi^{(n_1,\cdots,n_m)}(x_1)\equiv\int\Psi P^{(n_1,\cdots,n_m)}\Psi\prod_{i\neq 1}dx_i = c^{(n_1,\cdots,n_m)}\exp[-\alpha^2\gamma^{(n_1,\cdots,n_m)}(x_1-\rho^{(n_1,\cdots,n_m)}b)^2], \quad (24)$$

where

$$P\Psi=\exp[-\alpha^2(\tilde{x}\tilde{P}-\tilde{b})F(Px-b)] \quad (25)$$

with P being represented by the appropriate permutation matrix on the right-hand side of Eq. (25). The constants $c^{(m_1,\cdots,m_n)}$ will be normalized such that the constant $c^{(0)}$, which results when no variables are permuted, is equal to unity.

The expression which we now wish to evaluate is

$$\langle\Psi|V(x_1)|\Phi\rangle\Big/\langle\Psi|\Phi\rangle=\int V(x_1)\phi(x_1)\Big/\int\phi(x_1), \quad (26)$$

where

$$\phi(x_1)\equiv\psi^{(0)}(x_1)+\textstyle\sum_{ij}\psi^{(ij)}(x_1)+\sum_{ijk}\psi^{(ijk)}(x_1)+\cdots. \quad (27)$$

Equation (27) is correct for bosons; the fermion case will be discussed later. Consider a particular set of terms which contribute to $\phi(x_1)$, namely, $\psi^{(ij)}$. It is shown in Appendices A and B that $c^{(ijk\cdots l)}\approx J^{[(i-j)^2+(j-k)^2+\cdots+(l-i)^2]/2}$, where $J=e^{-2\alpha^2b^2/\pi}$; in order that the cores of neighboring particles do not appreciably overlap, it is necessary that $J\ll 1$. In the examples treated in I, J was of the order 10^{-13}. However, if a potential with a softer core had been used, the variational calculation would have yielded a lower value for J, but one can still assume that $c^{(i,i+1)}\ll 1$. In fact, if this criterion is not satisfied, the wave function of Eq. (2) is not a good choice for a wave function.

Since $c^{(i,i+1)}\gg c^{(i,i+2)}\gg c^{(i,i+3)}\cdots$, one can immediately make the approximation that $\sum\psi^{(ij)}\approx\sum\psi^{(i,i+1)}$. There are approximately N terms in $\sum\psi^{(i,i+1)}$ so that this sum of functions will be small compared to $\psi^{(0)}$ if $NJ\ll 1$ and may be neglected in Eq. (27) as was done in I. This criterion is obviously not valid in the limit $N\to\infty$ and so further work is necessary before Eq. (26) can be meaningfully applied to very large systems. In the remainder of this section, it will be shown that the quantity on the right-hand side of Eq. (26), is to a very good approximation, independent of N, because, for an overwhelming majority of terms, $\psi^{(P)}\approx c^{(P)}\psi^{(0)}$ so that $\phi\approx$ constant$\times\psi^{(0)}$, where the constant depends on N.

It is shown in Appendix B that there exists a number $N_c\ll N$ such that if P involves the variables whose indices are $n_1,n_2,\cdots,n_m$, if $m\ll N_c$ and if $N_c<n_1<n_2\cdots<n_m<N-N_c$, then $\rho^{(P)}\approx\rho^{(0)}$ and $\gamma^{(P)}\approx\gamma^{(0)}$. One can therefore write

$$\sum\psi^{(i,j)}(x_1)\approx(\sum_{i=N_c}^{N-Nc-1}c^{(i,i+1)})\psi^{(0)}(x_1) + (\sum_{i=2}^{Nc}+\sum_{i=N-N_c}^{N-2})\psi^{(i,i+1)}(x_1) \approx C^{(I,I+1)}\psi^{(0)}(x_1), \quad (28)$$

where $C^{(I,I+1)}$ is of order NJ. Other terms for which the number of permuted variables is small compared to N_c, but may be very large compared to unity, can be treated similarly.

The contribution to $\phi(x_1)$ from permutations which can be resolved into one cycle becomes negligible rather quickly. For example, such permutations involving the variables $(i,i+1,i+2)$ and $(i,i+1,i+2,i+3)$ give a contribution of order $2NJ^3$ and $2N(J^5+J^6+J^9)$, respectively. The contribution from terms in which m different nearest-neighbor pairs of variables are permuted will be of order $(NJ)^m/m!$. Other permutations involving more than one cycle give smaller contributions. Thus it is clear that, while some of the $C^{(P)}$ may be considerably larger than unity, the series on the right-hand side of Eq. (27) can be truncated to exclude all permutations involving more than a certain number of variables. Furthermore, the approximations given in Appendices A and B are valid for all the terms which need be retained.

One may then, after deriving an expression similar to Eq. (28) for each of the retained terms, obtain

$$\phi(x_1)\approx(1+C^{(I,I+1)}+C^{(I,I+1),I+2)} + C^{(I,I+1)(J,J+1)}+\cdots)\psi^{(0)}(x_1) \quad (29)$$

$$\approx(1+NJ+2NJ^2+\tfrac{1}{2}(NJ)^2+\cdots)\psi^{(0)}(x_1)$$

$$\approx\exp(+NJ)\psi^{(0)} \quad \text{(bosons)}, \quad (30)$$

[5] See, e.g., E. P. Wigner, *Group Theory* (Academic Press Inc., New York, 1959), p. 124.

where $J \ll 1$ has been used. Equation (4) follows directly from Eqs. (23), (26), (27), and (29).

For a system of Fermi particles, a sign $(-1)^P$ must be affixed to each $C^{(P)}$, whereupon Eq. (30) becomes

$$\phi(x_1) \approx \exp(-NJ)\psi^{(0)} \quad \text{(fermions)}. \tag{31}$$

It should be noted that the method used in deriving Eqs. (30) and (31) is also applicable to the case where $\Psi(x_1,x_2,\cdots,x_N)=\prod_i \phi(x_i-x_{0,i})$, where $x_{0,i}$ are the equilibrium positions of particles on a one-dimensional lattice. In this case, the derivation is simpler because $\gamma^{(P)}=\gamma_0$ and $\rho^{(P)}=\rho^{(0)}$ for all permutations which do not involve the variables 1 or N. While Eqs. (30) and (31) are convenient approximations to Eq. (29), it is the latter equation which is used to verify Eq. (4).

The leading correction term to Eqs. (30) and (31) is that resulting from the permutation $(1N)$; an expression for $\psi^{(1N)}$ is obtained in Appendix C where it will be found that $\psi^{(1N)}(x_N,x_1)$ is a maximum at $x_N=x_1$ rather than at $x_N=x_1-b$. The term

$$\int V(x_N-x_1)\psi^{(1,N)}(x_N,x_1)dx_n\ dx_1$$

corresponds to the nearest-neighbor exchange terms which are encountered in working with determinantal wave functions.

It is clear that a similar derivation to the above can be used to determine, for example, $\phi(x_2)$, the term appropriate for evaluation of the second-nearest-neighbor contribution.

IV. DISCUSSION

The major purpose of this paper and of I has been the development of a formalism by which one can use certain types of correlated Gaussian wave functions—those defined according to Eqs. (3) and (10)—as variational functions in many-body problems. Although, for convenience, the bulk of the detailed work was performed using a specific wave function—the ground state eigenfunction of the nearest-neighbor coupled harmonic-oscillator Hamiltonian—the techniques introduced here are applicable to a wider variety of wave functions.

The ability to write down an explicit expression for $\psi(x_i,x_j)$ which can be evaluated simply results from Eq. (7) and the fact that the $G^{-1}{}_{ij}$ are known. Thus an integral over a large number of variables can be performed without inverting a large matrix or integrating one at a time over a large number of variables.[6] It is still necessary to perform the sum in Eq. (11), but this is a much simpler numerical problem.

The development of the appropriate expressions which indicated that $\psi^{(P)} \approx \text{constant} \times \psi^{(0)}$ for certain permutations primarily depended upon the fact that $F^{-1}{}_{1,j}$ tends towards a finite constant for large j. This result probably obtains in any system in which $\omega_s \to 0$ as $s \to 0$; however, it can be checked numerically in individual examples. In the example $\omega_0 \neq 0$, one must use $G^{-1}{}_{ij}$. Here $G^{-1}{}_{ij}$ would probably approach zero for large j. These two cases can be visualized by replacing the sum in Eqs. (19) and (11), respectively, by integrals.

We intend to extend the formalism developed in this paper to three-dimensional systems. In such a system, it will be necessary to perform the summations necessary to obtain the inverse matrices numerically. It should be pointed out that the resulting three-dimensional correlated Gaussian may prove to be the most complicated trial wave function which can be treated exactly. We also intend to explore the applicability of the viewpoint which led to Eqs. (30) and (31) to the simpler example of a Heitler-London–type wave function.

[6] It is in principle possible to do the integral in Eq. (24) over one variable at a time. Here one would hope that, after integrating over a few variables adjacent to 1 and N, one would find approximate expressions for $c^{(P)}$, $\rho^{(P)}$, and $\gamma^{(P)}$. In practice, the convergence is unsatisfyingly slow.

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APPENDIX A

The integral in Eq. (24) will be evaluated in this Appendix, and matrix expressions for the constants $c^{(P)}$, $\gamma^{(P)}$, and $\rho^{(P)}$ will be derived. Approximations for the matrix expressions will be obtained. The approximations are valid when only a small fraction of all the variables is permuted and when this small fraction includes only variables which are sufficiently far removed from x_1. Actual numerical estimates of the constants will be given in Appendix B.

The expression to be evaluated is

$$\psi^{(P)}(x_1)=\left(\frac{2\alpha^2}{\pi}\right)^{(N-2)/2} |F|^{1/2}|F^{-1}{}_{11}|^{1/2} \times \int \exp\{-\alpha^2[(\tilde{x}\tilde{P}-\tilde{b})F(Px-b) + (\tilde{x}-\tilde{b})F(x-b)]\} \prod_{i=1}^{N-1} dx_i,$$

which, after the substitution $\tilde{q}=\tilde{x}-\tilde{b}$, becomes

$$\psi^{(P)}(q_1)=\left(\frac{2\alpha^2}{\pi}\right)^{(N-2)/2} |F|^{1/2}|F^{-1}{}_{11}|^{1/2} \times \int \exp\{-\alpha^2[\tilde{q}(F+\tilde{P}FP)q+\tilde{q}\tilde{P}F(P-I)b + \tilde{b}(\tilde{P}-I)FPq+\tilde{b}(\tilde{P}-I)F(P-I)q]\}dq_x, \tag{32}$$

where $\tilde{q}=(q_1,\tilde{q}_x)$, and the constant before the integral

sign is such that

$$\psi^{(0)}(q_1)=\exp[-2\alpha^2 q_1(F^{-1}{}_{11})^{-1}q_1]$$
$$=\exp[-\pi(\alpha q_1/2)^2]. \quad (33)$$

This expression can be obtained if one sets $P=I$ in Eq. (32) and uses Eqs. (9) and (22). Thus $\gamma^{(0)}=\pi/4$, $\rho^{(0)}=0$, and $c^{(0)}=1$.

The variables included in q_x will be further decomposed as $\tilde{q}_x=(\tilde{q}_p\tilde{q}_r)$ where $\tilde{q}_p$ includes all variables affected by P. The components of P will not be written and P will be assumed to have the appropriate dimensions in a matrix product. Therefore, if the submatrices denoted by $x,y,\cdots$ do not contain any parts affected by P, it should be noted that $P_{xx}=I$, $P_{yy}=I,\cdots$, $P_{xy}=0$, $P_{xp}=0,\cdots$, and $P_{pp}=P$. Thus the only nonzero component of $(I-P)$ is the pp component. Then by defining $\tilde{b}'\equiv(\tilde{b})(I-\tilde{P})=(0\tilde{b}_p'0)$, one can write the expressions in the square brackets of Eq. (32) as

$$(q_1 \quad \tilde{q}_x \quad \tilde{b}_p')\begin{bmatrix} 2F_{11} & F_{1x}(I+P) & F_{1p} \\ (I+\tilde{P})F_{x1} & (F_{xx}+\tilde{P}F_{xx}P) & \tilde{P}F_{xp} \\ F_{p1} & F_{px}P & F_{pp} \end{bmatrix}\begin{bmatrix} q_1 \\ q_x \\ b_p' \end{bmatrix}.$$

The integration indicated in Eq. (33) may be performed and

$$\psi^{(P)}(q_1)=\frac{|F_{pp}|^{1/2}}{|(F+\tilde{P}FP)_{pp}/2|^{1/2}}$$
$$\times\exp\left\{-\alpha^2(q_1 \quad \tilde{b}_p')\begin{pmatrix} R_{11} & R_{1p} \\ R_{p1} & R_{pp} \end{pmatrix}\begin{pmatrix} q_1 \\ b_p' \end{pmatrix}\right\} \quad (34)$$

results, with

$$R_{11}=2F_{11}-F_{1x}(I+\tilde{P})(F_{xx}+\tilde{P}F_{xx}P)^{-1}(I+P)F_{x1}, \quad (35)$$

$$R_{p1}=\tilde{R}_{1p}=F_{p1}-F_{px}P(F_{xx}+\tilde{P}F_{xx}P)^{-1}(I+\tilde{P})F_{x1}, \quad (36)$$

$$R_{pp}=F_{pp}-F_{px}P(F_{xx}+\tilde{P}F_{xx}P)^{-1}\tilde{P}F_{xp}. \quad (37)$$

Several matrix identities which will be used in reducing Eqs. (35)–(37) are

$$P(M+\tilde{P}MP)^{-1}\tilde{P}$$
$$=M^{-1}-M^{-1}(M^{-1}+PM^{-1}\tilde{P})^{-1}M^{-1}, \quad (38)$$

$$(I+P)(M+\tilde{P}MP)(\tilde{P}+I)$$
$$=2M^{-1}-M^{-1}(P-I)(M^{-1}+\tilde{P}M^{-1}P)^{-1}$$
$$\times(\tilde{P}-I)M^{-1}, \quad (39)$$

$$P(M+\tilde{P}MP)^{-1}(I+\tilde{P})$$
$$=M^{-1}-M^{-1}P(M^{-1}+\tilde{P}M^{-1}P)^{-1}(\tilde{P}-I)M^{-1}, \quad (40)$$

$$M_{xy}(M_{yy})^{-1}=-(M^{-1}{}_{xx})^{-1}M^{-1}{}_{xy}, \quad (41)$$

$$M_{px}(M_{xx})^{-1}=\delta_{pp}, \quad (42)$$

$$(M_{xx})^{-1}M_{pr}=-M^{-1}{}_{xr}(M^{-1}{}_{rr})^{-1}. \quad (43)$$

Equation (38) is obtained from rearranging the identity $P(M+\tilde{P}MP)^{-1}(M+\tilde{P}MP)\tilde{P}M^{-1}=M^{-1}$ and Eqs. (39) and (40) can be derived similarly. Equations (41)–(43) are similar to Eq. (7); it is understood that the coordinates labeled x are further subdivided into r and p.

In addition to the above, if

$$M_{xx}+\tilde{P}M_{xx}P=\begin{pmatrix} 2M_{rr} & M_{rp}(I+P) \\ (I+P)M_{pr} & M_{pp}+\tilde{P}M_{pp}P \end{pmatrix},$$

one can write, using Eq. (7),

$$(M+\tilde{P}MP)^{-1}{}_{pp}$$
$$=[(M+\tilde{P}MP)_{pp}-(M+\tilde{P}MP)_{pr}[(M+\tilde{P}MP)_{rr}]^{-1}$$
$$\times(M+\tilde{P}MP)_{rp}]^{-1}$$
$$=[M_{pp}+\tilde{P}M_{pp}P-(I+\tilde{P})M_{pr}[2M_{rr}]^{-1}M_{rp}$$
$$\times(I+P)]^{-1}$$
$$=2[(I-\tilde{P})M_{pp}(I-P)+(I+\tilde{P})(M^{-1}{}_{pp})^{-1}(I+P)]^{-1}. \quad (44)$$

If one now substitutes Eq. (38) and then Eq. (44) into Eq. (42),

$$R_{pp}=[(F_{xx})^{-1}+P(F_{xx})^{-1}\tilde{P}]^{-1}{}_{pp}$$
$$=2[(I-P)(F_{xx})^{-1}{}_{pp}(I-\tilde{P})$$
$$+(I+P)F_{pp}(I+\tilde{P})]^{-1} \quad (45)$$

is obtained. A convenient approximation to this expression may be obtained if one notes that

$$(I-P)(F_{xx})^{-1}{}_{pp}(I-\tilde{P})$$
$$=(I-P)[F^{-1}{}_{xx}-F_{x1}(F^{-1}{}_{11})^{-1}F_{1x}]_{pp}(I-\tilde{P})$$
$$\approx(I-P)F^{-1}{}_{pp}(I-\tilde{P}).$$

The approximation obtains because $F^{-1}{}_{1m}\to$ constant for large m so that $F^{-1}{}_{1p}(I-P)\to 0$ when p involves variables sufficiently far removed from x_1. This approximation will be used in subsequent proofs. Finally, there results

$$R_{pp}\approx 2[(I-P)F^{-1}{}_{pp}(I-\tilde{P})+(I+P)F_{pp}(I+\tilde{P})]^{-1}. \quad (46)$$

In this form, R_{pp} is expressed in terms of matrices of the same rank as P and can be evaluated numerically if the dimensions of P are small enough. A rough approximation to Eq. (46) will be given in Appendix B.

Equations (40), (41), and (43) are used to reduce Eq. (36) as follows:

$$R_{p1}=F_{p1}-F_{px}(F_{xx})^{-1}F_{x1}+F_{px}(F_{xx})^{-1}$$
$$\times P[(F_{xx})^{-1}+\tilde{P}(F_{xx})^{-1}P]^{-1}(\tilde{P}-I)(F_{xx})^{-1}F_{p1}$$
$$=-P[(F_{xx})^{-1}+\tilde{P}(F_{xx})^{-1}P]^{-1}{}_{pp}(\tilde{P}-I)F^{-1}{}_{p1}$$
$$\times(F^{-1}{}_{11})^{-1}$$
$$=R_{pp}(P-I)F^{-1}{}_{p1}(F^{-1}{}_{11})^{-1} \quad (47)$$
$$\approx 0. \quad (48)$$

Similarly, Eqs. (35), (39), (7), and (41) are used to determine R_{11}:

$$R_{11}=2F_{11}-2F_{1x}(F_{xx})^{-1}F_{x1}-F_{1x}(F_{xx})^{-1}(P-I)$$
$$\times[(F_{xx})^{-1}+\tilde{P}(F_{xx})^{-1}P]^{-1}(\tilde{P}-I)(F_{xx})^{-1}F_{p1}$$
$$=2(F^{-1}{}_{11})^{-1}-(F^{-1}{}_{11})^{-1}F^{-1}{}_{1p}(\tilde{P}-I)$$
$$\times R_{pp}(P-I)F^{-1}{}_{p1}(F^{-1}{}_{11})^{-1} \quad (49)$$
$$\approx 2(F^{-1}{}_{11})^{-1}. \quad (50)$$

Combining these results, one obtains

$$\psi^{(P)}(q_1)\approx\frac{|F_{pp}|^{1/2}}{|(F_{pp}+\tilde{P}F_{pp}P)/2|^{1/2}}\times\exp(-\alpha^2\tilde{b}_p'R_{pp}b_p')\psi^{(0)}(q_1). \quad (51)$$

Note that the $(P-I)F^{-1}{}_{p1}\approx 0$ was the only approximation used in obtaining Eqs. (46), (48), and (50) and that before this approximation was employed, each expression was reduced so as to contain only matrices whose dimensions were those of P.

APPENDIX B

This Appendix will be primarily concerned with the evaluation of Eq. (46) so that an approximate expression for $c^{(p)}$ can be obtained. We shall be exclusively concerned with the case where P affects the m indices $n_1,n_2,\cdots,n_m$ with $N_c<n_1<n_2\cdots<n_m<N-N_c$, where $1\ll N_c\ll N$.

The following identities and approximations can be derived from Eqs. (18) and (21):

$$F^{-1}{}_{mm}-F^{-1}{}_{mn}=F^{-1}{}_{m,m-n},$$

$$F^{-1}{}_{mm}\approx F^{-1}{}_{m+n,m+n}, \qquad n\ll m;\ 1\ll m\ll N, \quad (52)$$

$$F^{-1}{}_{mn}\approx F^{-1}{}_{mm}-\tfrac{1}{2}F^{-1}{}_{m-n},\ F^{-1}{}_{m-n}, \qquad n\ll m;\ 1\ll m\ll N, \quad (53)$$

and

$$F^{-1}{}_{mn}\approx-\frac{8}{\pi}\sum_{n=1}^{m}(2n-1)^{-1}, \quad m/N\ll 1. \quad (54)$$

Using Eqs. (52) and (53) one can obtain

$$[(I-P)F^{-1}{}_{pp}(I-\tilde{P})]_{n_1n_2}=-\tfrac{1}{2}F^{-1}{}_{n_2-n_1,n_2-n_1}(1-\delta_{n_2n_1}). \quad (55)$$

The above is a good approximation. A crude but useful approximation is obtained by replacing all the nonzero elements given by Eq. (55) by a constant $-\frac{1}{2}\bar{F}$ where $\bar{F}\approx F^{-1}{}_{11}=8/\pi$. Then Eq. (55) may be rewritten

$$(I-P)F^{-1}{}_{pp}(I-P)\approx\tfrac{1}{2}\bar{F}(2I-P-\tilde{P}). \quad (56)$$

Since the off-diagonal matrix elements of F are small, one may make a second crude approximation

$$(F_{pp})^{-1}\approx(\tfrac{1}{2}\pi)I. \quad (57)$$

By substituting Eqs. (56) and (57) into Eq. (46), one now obtains

$$R_{pp}\approx 2\left[\tfrac{1}{2}\bar{F}(2I-P-\tilde{P})+\frac{\pi}{2}(2I+P+\tilde{P})\right]^{-1} \quad (58)$$

$$\approx\frac{1}{\pi}I$$

where $\bar{F}\approx\pi$ has been used. The product $\tilde{b}_p'R_{pp}b_p'$ now becomes $(1/\pi)\tilde{b}'b'$ so that

$$c^{(P)}\approx(2|F_{pp}|/|F_{pp}+\tilde{P}F_{pp}P|)^{1/2}\exp[-\alpha^2\tilde{b}'b'/\pi]. \quad (59)$$

Although the approximations made in deriving Eq. (59) were quite rough the approximate value of $\tilde{b}_p'R_{pp}b_p'$ comes out fairly close to the value—which we shall call the true value—obtained when the only approximation made is that given by Eq. (54) and the matrix work is performed numerically. The reason for this is that the $(I-P)$ factor in b' cancels certain errors in estimating R_{pp}.

When P is a 2×2 matrix, the true value of $c^{(P)}$ is easily found to be $\exp[-2b^2\alpha^2(n_1-n_2)^2/F^{-1}{}_{n_1-n_2;\,n_1-n_2}]$ whereas Eq. (59) would give $c^{(P)}\approx\exp[-2\alpha^2b^2(n_1-n_2)^2/\pi]$. Note that for the permutation $P^{(n_1,n_2,n_3,\cdots,n_m)}$,

$$\tilde{b}'b'=b^2[(n_2-n_1)^2+(n_3-n_2)^2+\cdots+(n_1-n_m)^2],$$

and also that it would be expected that the constant in front of the exponent in Eq. (59) would be of order unity so that

$$c^{(n_1,n_2,\cdots,n_m)}\approx J^{[(n_2-n_1)^2\cdots+(n_1-n_m)^2]},$$

where $J=\exp[-2\alpha^2b^2/\pi]$.

APPENDIX C

In the case where $P=P^{(1N)}$ it is more convenient to work with the G matrix. Evaluation of this permutation violates our earlier statement that all permutations involving x_N were to be omitted; however, because $\sum_n G_{mn}=0$, it is readily shown that

$$P^{(1N)}\Psi=P^{(2,3,\cdots,N-1,1)}\Psi;$$

since the first notation is more transparent, we will use it. By integrating over the variables $x_2\cdots x_{N-1}$ and denoting these by the subscript x, one can obtain an expression analogous to Eq. (34):

$$\psi^{(N,1)}(q_p)=\exp\left\{-\alpha^2(q_p\quad b_p')\begin{pmatrix}R_{qq}&R_{qb}\\R_{bq}&R_{bb}\end{pmatrix}\begin{pmatrix}q_p\\b_p'\end{pmatrix}\right\}, \quad (60)$$

with

$$R_{qq}=G_{pp}+\tilde{P}G_{pp}P-(I+P)G_{px}(2G_{xx})^{-1}G_{xp}(I+P), \quad (61)$$

$$R_{qb}=\tilde{R}_{bq}=\tilde{P}G_{pp}(P-I)-(I+P)G_{px}(2G_{xx})^{-1}G_{xp}(P-I), \quad (62)$$

$$R_{bb}=G_{pp}-G_{px}(2G_{xx})^{-1}G_{xp}. \quad (63)$$

In the above $\tilde{b}_p'=(q_N-q_1)(1-1)$, and the term analogous to $|F_{pp}|^{1/2}|\frac{1}{2}(F_{pp}+\tilde{P}F_{pp}P)|^{-1/2}$ of Eq. (34) is unity in Eq. (60).

Using Eqs. (7) and (16) and $\sum_n G_{mn}=0$, we obtain

$$G_{11}-G_{1x}(G_{xx})^{-1}G_{x1}=(F^{-1}{}_{11})^{-1}, \quad (64)$$

and

$$G_{1N}-G_{1x}(G_{xx})^{-1}G_{xN}=-(F^{-1}{}_{11})^{-1}. \quad (65)$$

Equations (60)–(65) can be combined to yield

$$\psi^{(N,1)}=\exp[-2\alpha^2b^2(F^{-1}{}_{11})^{-1}]\times\exp[-\alpha^2(G_{11}-G_{1N})(x_N-x_1)^2]. \quad (66)$$