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# Self-consistent pseudopotentials in the thermodynamic limit. II. The state-dependent one-body field

E. S. Hernández*
*Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, 1428 Buenos Aires, Argentina*

A. Plastino and L. Szybisz
*Departamento de Física, Universidad Nacional de La Plata, 1900 La Plata, Argentina*
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We explore the concept of the pseudopotential, introduced in a previous paper, within the context of the exact boundary condition for a system of fermions interacting through a pair-wise, hard-core potential, in the thermodynamic limit. We discuss several *Ansätze* for the Lagrange multipliers that allow the inclusion of the boundary conditions into the variational principle. It is found that under a given *Ansatz*, a dynamical, microscopic interpretation of the pseudopotential can be put forward. A comparison between this situation and the coherent approximation induced by the use of the correlation function is also presented.

[NUCLEAR STRUCTURE Hard-core interactions, boundary condition, variational principle constrained Hartree-Fock problem; *Ansatz*, structure of the pseudopotential, state dependence.]

## I. INTRODUCTION

The self-consistent treatment of correlations induced by two-body interactions characterized by the presence of a hard core has recently been the subject of detailed analysis.[1,2] The central idea, suggested in an early paper of de Llano and Ramirez,[3] is that of working with Slater determinants of spatially localized, nonoverlapping, single-particle (s.p.) wave functions which, contrary to general belief, make Hartree-Fock (HF) calculations with hard cores possible, as shown in Ref. 1.

In a previous work,[2] hereafter referred to as I, we have tackled the problem of singular two-body forces via the well-known pseudopotential method[4-8] and tried to relate it to the variational principle, in order to attempt a connection with the HF theory. We showed that the effect of the hard core in the two-body interaction can be included as a constraint into the variational principle. We derived the corresponding Euler-Lagrange equations for a one-dimensional system and found that they were of the HF type, but with a modified one-body field, the pseudopotential. This extra term was seen to provide complementary correlations in momentum and coordinate space, allowing us to suggest a tentative explanation for the origin of density waves in nuclear matter whose existence, conjectured by Overhauser,[9] has motivated a great amount of research lately (see for example Refs. 10–12).

In I the construction of the psuedopotential was based on a particular representation of the geometrical (boundary) condition imposed on the two-fermion relative wave function.[1] This must vanish inside the hard-core radius and, in order to fulfill this requirement, a restriction was introduced into the variational principle in terms of the so-called correlation function for the interacting system.[13] Such an approach is obviously not the best one. The boundary condition can be represented in more adequate terms, with greater fidelity.

The purpose of this paper is twofold. On the one hand, we shall examine in further detail the consequences of the approach given in I. On the other hand, we shall discuss several possibilities that allow for the introduction of more detailed microscopic information into the mean field. In particular, attention will be drawn to the fact that the use of the correlation function implies significant phase cancellations which result in a state-independent pseudopotential. Better descriptions of the boundary condition generate state-dependent ones, which admit an appealing microscopic interpretation.

In Sec. II we show how the "true" boundary condition is described in our model and we present the approximations whose features and consequences are discussed in Sec. III. Conclusions and perspectives are summarized in Sec. IV.

## II. THE BOUNDARY CONDITION

For the sake of economy of notation, we shall restrict our presentation to a one-dimensional system of $N$ fermions in a container of length $L$. Both $N$ and $L$ are supposed to be very large, but the average density $\rho_0 = \lim_{N,L\to\infty} N/L$ is a well-

 

defined quantity (thermodynamic limit). The fermionic Hamiltonian is

$$H_0 = \int dk\, t(k) a_k^\dagger a_k + \tfrac{1}{4} \int\int\int\int dk_1 dk_2 dk_3 dk_4 \times \langle k_1 k_2 | V | k_3 k_4 \rangle a_{k_1}^\dagger a_{k_2}^\dagger a_{k_4} a_{k_3} , \quad (1)$$

where the continuous variable $k$ labels a momentum eigenstate created on the s.p. vacuum $|0\rangle$ by the operator $a_k^\dagger$,

$$|k\rangle = a_k^\dagger |0\rangle \quad (2)$$

and $V$ is a regular pair-wise interaction. Although we are assuming that our system interacts through a singular, i.e., hard-core, two-body potential, in the spirit of I we consider that $V$ is the analytical continuation of the regular portion of the actual interaction inside the forbidden region. We will take care of the singularity by means of the boundary condition in a constrained variational procedure.[2]

Let $\varphi_k(x)$ be the wave function associated with the orbital $|k\rangle$

$$\varphi_k(x) = \langle x | k \rangle = \frac{1}{\sqrt{2\pi}} e^{ikx} . \quad (3)$$

We assume that the Hamiltonian (1) can be approximately linearized via a unitary transformation that yields a basis of self-consistent orbitals $|\lambda\rangle$. The corresponding creation operators are

$$b_\lambda^\dagger = \int C_\lambda(k) a_k^\dagger dk , \quad (4)$$

In coordinate representation, this transformation reads

$$\psi_\lambda(x) = \frac{1}{\sqrt{2\pi}} \int C_\lambda(k) e^{ikx} dk \quad (5)$$

and fulfills the unitarity requirements

$$\int dk\, C_\mu^*(k) C_\lambda(k) = \delta_{\lambda\mu} , \quad (6)$$

$$\int d\lambda \sqrt{\mathfrak{D}(\lambda)}\, C_\lambda^*(k) C_\lambda(k') = \delta(k - k') . \quad (7)$$

Here the function $\mathfrak{D}(\lambda)$ is the density of states of the self-consistent basis,

$$\mathfrak{D}(\lambda) = dn/d\lambda , \quad (8)$$

which at the moment is an unknown of the problem, as well as the orbitals $|\lambda\rangle$ themselves. It has been explicitly displayed in Eq. (7) in order to recall that, in principle, $\lambda$ is a continuous label. In this sense, $\mathfrak{D}(\lambda)$ is the self-consistent equivalent of the well-known density of states of the (unperturbed) momentum eigenstates

$$\mathfrak{D}_0(k) = \frac{dn}{dk} = \frac{L}{2\pi} . \quad (9)$$

For simplicity, in most of this paper we shall represent $\lambda$ as a discrete label, bearing in mind that in any actual calculation we should use the identity

$$\sum_\lambda \equiv \int d\lambda\, \mathfrak{D}(\lambda) . \quad (10)$$

Now the essence of a constrained HF calculation resides in the fact that one looks for the s.p. orbitals that minimize the expectation value of the following Hamiltonian:

$$\langle H \rangle = \langle H_0 \rangle - F\{\alpha\} - \sum_\lambda \epsilon_\lambda \int dk\, |C_\lambda(k)|^2 , \quad (11)$$

where $F$ contains the constraint and a set of Lagrange multipliers $\{\alpha\}$, and the last term in the right-hand side accounts for the proper normalization of the s.p. orbitals. The expectation values are taken with respect to a Slater determinant of s.p. wave functions $\psi_\lambda$. Variation of (11) with respect to the Fourier transforms $C_\lambda$ (or their complex conjugates) leads to a system of coupled integral equations

$$\int dk\, h(k, q) C_\eta(k) - \frac{\partial F}{\partial C_\eta^*(q)} = \epsilon_\eta C_\eta(q) , \quad (12)$$

where $h$ is the well-known HF Hamiltonian.[2] Whenever we can express the variation of the constraint in the form

$$\frac{\partial F}{\partial C_\eta^*(q)} = - \int dk\, \Gamma_2(k, q, \{\alpha\}) C_\eta(k) , \quad (13)$$

the kernel $\Gamma_2$ plays the role of a self-consistent one-body potential to be added to $h$.[2] It originates in the constraint and is, in a way, a fictitious entity. However, it contains the important correlations induced in the system by the superimposed condition $F\{\alpha\}$. In I we have given the name pseudopotential to this quantity, preserving a concept that has been used in pioneering works,[4-8] since we have generated a given $F$ out of a constraint that simulates the boundary condition.

We should now remark that in the presence of a hard-core interaction, the "true" boundary condition demands exact cancellation of every relative wave function $\psi_{\lambda\mu}$ inside the region of strong repulsion. This requirement can be formalized as

$$|\psi_{\lambda\mu}(x)|^2 = 0 \text{ when } |x| \leq c \text{ for all } \lambda, \mu , \quad (14)$$

where we explicitly choose to represent the condition in terms of the probability rather than the amplitude. Moreover, we can summarize the information displayed in (14) into a compact constraint,

$$F\{\alpha\}=\sum_{\lambda<\mu}\int_{-c}^{c}dx\,\alpha_{\lambda\mu}(x)|\psi_{\lambda\mu}(x)|^2=0\,, \tag{15}$$

where we have introduced the Lagrange multiplier matrix $\alpha_{\lambda\mu}(x)$. Equation (15) is the exact representation of the "true" boundary condition. It becomes evident that it entails a set of unknown functions whose determination in any practical calculation would be overwhelmingly hard, if not impossible. It is then essential, if we decide to pursue the subject, to introduce some simplifying *Ansatz* on $\alpha_{\lambda\mu}(x)$.

We quote here a few elementary choices that will enable us to gain some insight with relation to the correlations induced in our system by condition (15). They will be examined more closely in the next section, where we will discuss the following four examples. In example (1), $\alpha_{\lambda\mu}(x)=\alpha_{\lambda\mu}$, independent of $x$ for all $\lambda,\mu$. In this case the constraint reads

$$F_1(\{\alpha\})=\tfrac{1}{2}\sum_{\lambda\neq\mu}\alpha_{\lambda\mu}\int_{-c}^{c}dx\,|\psi_{\lambda\mu}(x)|^2=0\,. \tag{16}$$

In particular, $\alpha_{\lambda\mu}$ can be chosen to be a constant, i.e., independent of $\lambda,\mu$; for example (2),

$$\alpha_{\lambda\mu}(x)=\alpha_{\lambda\mu}[\delta(x+c)+\delta(x-c)]\,. \tag{17}$$

Evidently,

$$F_2(\{\alpha\})=\tfrac{1}{2}\sum_{\lambda\neq\mu}\alpha_{\lambda\mu}[|\psi_{\lambda\mu}(c)|^2+|\psi_{\lambda\mu}(-c)|^2]=0\,. \tag{18}$$

Before going into a detailed analysis of the consequences of (17) and (18), we should quote, for comparison, the approach presented in I. In that work, the constraint was expressed in terms of the correlation function $g(x_1,x_2)$ that represents the average probability of finding a two-particle configuration with coordinates $x_1$ and $x_2$, in any available pair state below the self-consistent Fermi level. One has

$$g(x_1,x_2)=\frac{2}{N^2}\sum_{\lambda,\mu\leq F}|\Psi_{\lambda\mu}(x_1,x_2)|^2\,, \tag{19}$$

where $\Psi_{\lambda\mu}$ is the antisymmetrized two-particle wave function

$$\Psi_{\lambda\mu}(x_1,x_2)=\frac{1}{\sqrt{2}}[\psi_\lambda(x_1)\psi_\mu(x_2)-\psi_\lambda(x_2)\psi_\mu(x_1)]\,, \tag{20}$$

and $N^2/2$ is the number of pairs. We should also notice that the thermodynamic limit (10) requires the self-consistent density of states $\mathcal{D}(\lambda)$ to be of order $N$ (or $L$) thus ensuring the finiteness of expression (19). If we write $\Psi_{\lambda\mu}$ in the center-of-mass system of the pair and integrate away the center-of-mass coordinate $X$, we can select an approximation to the "true" boundary condition in the form of example (3),

$$F_3(\alpha)=\int_{-c}^{c}dx\,\alpha(x)G(x)=0\,, \tag{21}$$

where

$$G(x)=\int dX\,g(x,X)\,. \tag{22}$$

One obvious advantage of this choice is the fact that the matrix $\alpha_{\lambda\mu}(x)$ is replaced by a single function. In addition, we could also try the *Ansatz* of example (4),

$$\alpha(x)=\alpha[\delta(x+c)+\delta(x-c)] \tag{23}$$

which leads to

$$F_4(\alpha)=\alpha[G(c)+G(-c)]=0\,. \tag{24}$$

This last case is the situation presented and discussed in I. An important point is to be remarked: While the "true" boundary condition (15) implies that the sum is to be taken after integrating away the center-of-mass coordinate and taking the square modulus, these procedures have been reversed in order to build the correlation function. Schematically,

$$F\propto\left|\int dX\Psi_{\lambda\mu}(x,X)\right|^2\neq\int dX|\Psi_{\lambda\mu}(x,X)|^2\propto G\,. \tag{25}$$

In this sketch we can appreciate that $F$ (and its approximations $F_{1,2}$) contains all the interference effects and phase correlations induced by the sum of the amplitudes over the center-of-mass position. These are lost in $G$; actually, the phase correlations are canceled when we add probabilities, the outcome being a coherent function. We could say, with abuse of language, that $G$ is the "random phase approximation" to $F$. This concept will be kept in mind during the forthcoming discussion.

We finish this section quoting the actual expressions for the relative wave function and the relative correlation function. These can be easily deduced from (5) and (20) and read

$$|\Psi_{\lambda\mu}(x)|^2=2\int\int dk\,dk'C_\lambda(k)C_\mu(-k)C_\lambda^*(k')C_\mu^*(-k')\times\sin(kx)\sin(k'x) \tag{26}$$

and

$$G(x)=\frac{2}{N^2\pi}\sum_{\lambda,\mu\leq F}\int\int\int\int dK\,dk\,dK'\,dk'\,\delta(K-K')C_\lambda(\tfrac{1}{2}K+k)\,C_\lambda^*(\tfrac{1}{2}K'+k')\,C_\mu(\tfrac{1}{2}K-k)$$
$$\times\, C_\mu^*(\tfrac{1}{2}K'-k')\sin kx\,\sin k'x. \tag{27}$$

The variables involved in these integrals are the center-of-mass and relative momenta $K$ and $k$, respectively, for particles 1 and 2. Primes correspond to variables associated with the complex conjugate wave function.

## III. VARIATIONAL PROCEDURE

In this section we shall examine the pseudopotentials generated by the constraints $F_1$ to $F_4$.

### A. Constraint $F_1$

We introduce Eq. (26) into Eq. (16), evaluate the indicated integrals, and follow prescription (13). The identification of the pseudopotentials is straightforward and can be further simplified if we take advantage of time-reversal symmetry. Since we are dealing with time-reversal invariant interactions $V$ the s.p. wave functions $\psi_\lambda$ can be chosen to be real and with definite parity. These properties lead to the consequences

$$C_\lambda(k)=(-)^{\pi_\lambda}C_\lambda(k)\,, \tag{28a}$$
$$C_\lambda^*(k)=C_\lambda(-k)=(-)^{\pi_\lambda}C_\lambda(k)\,, \tag{28b}$$

where $\pi_\lambda=0,1$ is the parity of the orbital $|\lambda\rangle$.

With the help of Eqs. (28) we find

$$\Gamma_2(k,q,\{\alpha\})=\Gamma_{2\eta}(k,q,\{\alpha\})=\left[\frac{\sin(k+q)c}{k+q}-\frac{\sin(k-q)c}{k-q}\right]\sum_{\mu\neq\eta}C_\mu(k)C_\mu^*(q)[\alpha_{\eta\mu}-(-)^{\pi_\mu+\pi_\eta}\alpha_{\mu\eta}]\,. \tag{29}$$

We observe that the pseudopotential is *state dependent*. As a matter of fact, regardless of the matrix $\alpha_{\eta\mu}$, its state dependence stems from the parity phase factors. Furthermore, the structure of $F_1$ indicates that we must impose $\alpha_{\lambda\mu}=\alpha_{\mu\lambda}$ [cf. Eq. (16)]. If we take this property into account, we immediately see from Eq. (29) that the parity of the orbitals contributing to the pseudopotential is opposite to that of the one of interest, $|\eta\rangle$. Thus, odd orbitals $|\mu\rangle$ build up the one-body field experienced by even states $|\eta\rangle$ and vice versa; the restriction $\mu\neq\eta$ under the summation symbol is now superfluous.

It is illustrative to study the coordinate space form of $\Gamma_{2\eta}$. This can be achieved by means of the double-Fourier transformation

$$\Gamma_{2\eta}(x,x')=\int\int dk\,dq\langle x|k\rangle\langle k|\Gamma_{2\eta}|q\rangle\langle q|x'\rangle\,. \tag{30}$$

The integrals can be evaluated through a simple contour integration. We obtain

$$\Gamma_{2\eta}(x,x')=-\frac{\pi}{2}\sum_\mu\alpha_{\eta\mu}[1-(-)^{\pi_\eta+\pi_\mu}]$$
$$\times\int dk|C_\mu(k)|^2\{e^{ik(x-x')}[\theta(x+x'+2c)-\theta(x+x'-2c)-\theta(-x-x'-2c)+\theta(-x-x'+2c)]$$
$$-e^{ik(x+x')}[\theta(x-x'+2c)-\theta(x-x'-2c)-\theta(-x+x'-2c)+\theta(-x+x'+2c)]\}\,, \tag{31}$$

where $\theta(x)$ is the usual step function.

The diagonal matrix element is specially interesting. The normalization condition (6) allows us to write

$$\Gamma_{2\eta}(x)=-\frac{\pi}{2}\sum_\mu\alpha_{\eta\mu}[1-(-)^{\pi_\eta+\pi_\mu}]\left\{\theta(x+c)-\theta(x-c)-\theta(-x-c)+\theta(-x+c)-\int dk|C_\mu(k)|^2e^{2ikx}\right\}. \tag{32}$$

We have used the fact that $\theta(2c)=\theta(c)=1$. It is easy to see that the sum of the step functions represents a centered square well of range $2c$ and intensity proportional to the sum of the $\alpha$'s. The integral is the Fourier transform of the probability $|C_\mu(k)|^2$ and its effect is to distort the square well by superimposing a wiggle and to make it vanish at $x=0$. This geometrical picture, although useful for future reference, should not be misleading; $\Gamma_{2\eta}$ is a nonlocal field, as given by Eq. (31), its actual spatial shape being much more complicated. However, Eq. (31) suggests that its structure is, essentially, a superposition of square wells with momentum-dependent weights and phases that depend on the amount of nonlocality.

### B. Constraint $F_2$

Following the lines invoked in subsection A, we find in this case

$$\Gamma_{2\eta}(k,q\{\alpha\}) = -4\sin qc\,\sin kc\sum_{\mu}\alpha_{\eta\mu}[1-(-)^{\pi_\eta+\pi_\mu}]C_\mu^*(q)C_\mu(k)\,, \tag{33}$$

We see that the parity selection rule of the preceding paragraph is preserved. In addition, Eq. (33) provides us with some interesting "edge information," since this pseudopotential is entirely generated on the hard-core walls. In order to display this more clearly, let us examine the coordinate representation of Eq. (33). We transform according to (30) and easily find, with the help of Eq. (5),

$$\Gamma_{2\eta}(x,x') = -\pi\sum_{\mu}\alpha_{\eta\mu}[1-(-)^{\pi_\eta+\pi_\mu}][\psi_\mu(x+c)\psi_\mu^*(x'+c)+\psi_\mu(x-c)\psi_\mu^*(x'-c)-\psi_\mu(x-c)\psi_\mu^*(x'+c)-\psi_\mu(x+c)\psi_\mu^*(x'-c)]\,. \tag{34}$$

It becomes apparent that $\Gamma_{2\eta}(x,x')$ presents the structure of an s.p. propagator,[14] where the "weight" of the line labeled $\mu$ is given by the sum of Lagrange multipliers and phase factors. The first and second terms in the sum can be interpreted as describing a virtual process in which an s.p. path starts at position $x'\pm c$ and ends at $x\pm c$. The third term describes the "propagation" of a particle from one hard-core radius to the right of point $x'$, to one hard-core radius to the left of $x$. The fourth term corresponds to exchanging $x$ and $x'$ in the preceding one. This dynamical picture sheds some light on the meaning of the pseudopotential, since we can see now that its fictitious nature, emphasized in I, is reflected in a spatial structure that consists of a superposition of virtual displacements that keep intact the hard-core exclusion distance.

### C. Constraints based on the correlation function

In I we have shown that the correlation function can be written as the expectation value of the pseudopotential, which in turn is the average of the correlation field $\chi^2$. It means that we can write

$$F_{3,4}(\alpha) = -\,\mathrm{Tr}(\Gamma_2\rho) = -\,\mathrm{Tr}\{[\mathrm{Tr}(\chi\rho)]\rho\}\,, \tag{35}$$

where the one-body density $\rho$ has the matrix elements[2]

$$\rho(k,q) = \sum_{\lambda\le F} C_\lambda^*(q)C_\lambda(k)\,. \tag{36}$$

If we introduce (36) into the expression for $G$ given by (27), the quantities $\Gamma_2$ and $\chi$ can be written down by simple inspection. Since the case of the constraint $F_4$ has been discussed in I, we refer the reader to that paper. Here we will quote the corresponding results for the constraint $F_3$. We just get

$$\Gamma_2(k,q) = -\frac{4}{\pi\rho_0^2}\int\int dk'dq'\delta(k-q+k'-q')\rho(q',k')\int_{-c}^{c}dx\,\alpha(x)\sin(q-q')\frac{x}{2}\sin(k-k')\frac{x}{2}, \tag{37}$$

$$\chi(k,q,k',q') = -\frac{4}{\pi\rho_0^2}\delta(k-q+k'-q')\int_{-c}^{c}dx\,\alpha(x)\sin(q-q')\frac{x}{2}\sin(k-k')\frac{x}{2}\,, \tag{38}$$

The density factor $\rho_0^2$ arises from the thermodynamic limit, in which we must assume the density of states $\mathfrak{D}(\lambda)$ [Eq. (8)] to be of order $N$ or $L$.

Although the function $\alpha(x)$ is an unknown, it will be illustrative to study at least one particular *Ansatz* (other than the one in I). The simplest is, evidently, $\alpha$ = constant. In this case we immediately find

$$\chi(k,q,k',q') = -\frac{4\alpha}{\pi\rho_0^2}\delta(k-q+k'-q')\left[\frac{\sin(k-k'-q+q')c/2}{(k-k'-q+q')/2}-\frac{\sin(k-k'+q-q')c/2}{(k-k'+q-q')/2}\right], \tag{39}$$

which is precisely the antisymmetrized two-body matrix element, taken with respect to momentum eigenstates, of a square-well potential of width $c$ and depth

$$V_0 = -8\alpha/\rho_0^2\,. \tag{40}$$

It is clear that $\alpha=-\infty$ is an exact solution that corresponds to an infinite barrier, i.e., to the original hard core. A finite value of $\alpha$, if a solution of the constrained HF problem, would provide an upper limit to the total energy of the system. The question of the existence of such solutions remains

unanswered at the moment. However, we persist in this example, since it should be confronted with the results of subsection A. A comparison of the pseudopotentials associated with the correlation field (39) with the one in Eq. (32) allows us to draw some conclusions on the consequences of the random-phase-approximation to the "true" boundary condition [Eq. (15)]. We realize that the destruction of the intrinsic phase correlations present in Eq. (15) leads us to a simple geometrical picture for the correlation field and the pseudopotential. The s.p. contributions to both of them add coherently to a unique square well, or barrier, that reproduces the input, i.e., the hard core, in an exact fashion. By contrast, we can see in (32) that the infinite strength of the hard core acting on a particular orbital $\eta$ becomes smoothed away in a series of individual wells, each of them admitting a finite intensity. In fact, the full repulsive strength can be regarded with the sum over the orbitals $\mu$, even though the individual contributions are finite. Of course, an actual calculation of (32) entails the unknown matrix $\alpha_{\lambda\mu}$, which is a continuous function of the s.p. labels in the thermodynamic limit. This is the price we must pay if we intend to save the microscopic phase correlations that are present in the pair probability $|\Psi_{\lambda\mu}(x_1, x_2)|^2$. The numerical problem, namely the discussion of the existence and convergence of the solutions under these different constraints is currently being explored and lies beyond the scope of the present paper.

## IV. SUMMARY

We have examined the constrained variational principle that takes into account the geometrical restrictions induced by the presence of a hard-core interaction. We have expressed the "true" boundary condition and shown that its effect on the HF equations can be represented by means of a state-dependent pseudopotential. This one-body field can be analyzed under simplifying *Ansätze* for the Lagrange multiplier function $\alpha_{\lambda\mu}(x)$, and its microscopic structure in terms of elementary scattering or displacement events becomes apparent. It is shown that, by contrast, the coherence carried by the correlation function, when chosen as a representation for the boundary condition, gives rise to a macroscopic one-body field that reproduces the exact initial problem if the corresponding Lagrange multiplier becomes infinite.

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*Present address: Nuclear Theory Group, Lawrence Berkeley Laboratory, Berkeley, California 94720.

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