

T-MATRIX PERTURBATION THEORY IN THE THREE-NUCLEON BOUND STATE

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Abstract

A T -matrix perturbation method has been used to calculate three-body binding energies for two local potentials. The results obtained indicate that the method provides one of the most attractive ways of solving by computation the three-body bound state problem for realistic interactions.

I. INTRODUCTION

One of the many successes of the Faddeev (1961) equations has been a renewal of interest in the three-nucleon bound state as a means of investigating the off-shell behaviour of the two-body T -matrix (Afnan and Serduke 1973; Hadjimichael and Jackson 1972). Although a large number of calculations for the bound three-nucleon system have been made with separable potentials (see the review by Mitra 1969), the ultimate aim of these investigations has always been to calculate the binding energy and wavefunction of the three nucleons with realistic two-body interaction potentials such as the Reid (1968) potential. There have been a number of recent advances in this direction with the work of Malfliet and Tjon (1970) and Harper *et al.* (1972) on the direct solution of the two-dimensional Faddeev equations and that of Levinger's group (Harms 1970; Bhatt *et al.* 1972) who have used the unitary pole approximation. However, the binding energies obtained from these different methods and from the variational calculations of Jackson *et al.* (1971) and Hennell and Delves (1972), who used the Reid potential, do not all agree.

In the present paper, we describe the application of a T -matrix perturbation theory to the calculation of the binding energy of the three-nucleon system (Fuda 1968; Lu 1970; Kowalski and Pieper 1972; Sloan 1972). Our starting point is the solution of the Faddeev equations for a unitary pole expansion (hereinafter designated UPE) potential (Harms 1970), which is separable. The difference between the actual two-body T -matrix and that of the UPE potential is treated as a perturbation. The first few terms of the UPE are sufficient to yield a good approximation to the three-body binding energy and wavefunction. Any attempt to improve the results by increasing the number of terms involves an enormous increase in the necessary computer time and storage. This is apparent for central potentials from the results of Harms (1970) and the situation is even more pronounced in the presence of a tensor force (Afnan and Read 1972). The present perturbation approach appears capable of yielding very reliable results and has the advantage that it is much faster than methods which involve direct inversion of the Faddeev equations.

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II. TWO-BODY T -MATRIX IN UPE

In the present section we consider the UPE for a central two-body potential, summarizing the results of Harms (1970), and demonstrate that the T -matrix of the original local potential can be reproduced if a sufficient number of terms are taken in the expansion. Our aim is to use the UPE to form a separable potential V^* (hereinafter, asterisks are used to denote quantities obtained from the UPE) that gives the same T -matrix as does the original potential V in the neighbourhood of the bound state pole. To accomplish this we start with the homogeneous Lippmann–Schwinger equation for the wavefunction

$$|\psi\rangle = -G_0(-E_D)V|\psi\rangle, \quad (1)$$

where $G_0(E) = (H_0 - E)^{-1}$ and E_D is the bound state energy. We assume that equation (1) is partial wave expanded and that the channel under consideration has a bound state energy E_D . (In the 1S_0 channel we choose $E_D = 0$, which is justified by the proximity to zero of the energy of the antibound state.) Since $G_0(-E_D)$ is positive definite, we may define $G_0^\frac{1}{2} = (H_0 + E_D)^{-\frac{1}{2}}$ in order to rewrite the wavefunction (1) in the form

$$|\phi\rangle = -G_0^\frac{1}{2}VG_0^\frac{1}{2}|\phi\rangle, \quad \text{with} \quad |\psi\rangle = G_0^\frac{1}{2}|\phi\rangle. \quad (2, 3)$$

The advantage of equation (2) is that it represents a homogeneous integral equation with a symmetric kernel $K = G_0^\frac{1}{2}VG_0^\frac{1}{2}$ and so may be transformed to the eigenvalue problem

$$|\phi_n\rangle = -\lambda_n G_0^\frac{1}{2}VG_0^\frac{1}{2}|\phi_n\rangle = -\lambda_n K|\phi_n\rangle. \quad (4)$$

Since K is Hermitian, the states $|\phi_n\rangle$ form a complete set of orthonormal functions, in terms of which the kernel may be expanded as

$$K = \sum_{n,m=1}^{\infty} |\phi_n\rangle\langle\phi_n|K|\phi_m\rangle\langle\phi_m| = -\sum_{n=1}^{\infty} |\phi_n\rangle\lambda_n^{-1}\langle\phi_n|. \quad (5)$$

By introducing a set of states $|\chi_n\rangle$ defined by

$$|\phi_n\rangle = G_0^\frac{1}{2}|\chi_n\rangle, \quad (6)$$

that is, the $|\chi_n\rangle$ satisfy the conditions

$$|\chi_n\rangle = -\lambda_n VG_0(-E_D)|\chi_n\rangle, \quad (7)$$

we obtain from equation (5) that

$$V = -\sum_{n=1}^{\infty} |\chi_n\rangle\lambda_n^{-1}\langle\chi_n|. \quad (8)$$

The UPE potential V^* is then formed by truncating the summation (8) after a finite number N of terms

$$V^* = -\sum_{n=1}^N |\chi_n\rangle\lambda_n^{-1}\langle\chi_n| \quad (9)$$

and the UPE T -matrix may be written as

$$T^* = \sum_{n,m=1}^N |\chi_n\rangle [M^{-1}(E)]_{nm} \langle \chi_m|, \quad (10)$$

where

$$M_{nm}(E) = -\lambda_n \delta_{nm} + \langle \chi_n | G_0(E) | \chi_m \rangle. \quad (11)$$

This truncation turns out to yield a better approximation for the T -matrix than for the potential, the explanation being that the bound state pole dominates the behaviour of the T -matrix on the negative energy axis and the series (9) reproduces the two-body bound state energy and wavefunction exactly for any N .

TABLE 1
EXACT AND UPE S-STATE PHASE SHIFTS FOR POTENTIALS (12) AND (13)

Columns listing UPE phase shifts are labelled by the number of attractive (A) and repulsive (R) terms retained in the expansion (9) (for example, 4A+2R implies that the first four attractive and the first two repulsive terms have been used)

E_{cm} (MeV)	Exact	Phase shift for potential (12)							
		1A	2A	4A	6A	10A	12A	20A	30A
12	1.5053	1.3374	1.3882	1.4659	1.4913	1.5015	1.5023	1.5034	1.5053
24	1.2818	1.0263	1.1377	1.2560	1.2712	1.2721	1.2723	1.2793	1.2818
48	1.0803	0.7283	0.9422	1.0475	1.0496	1.0656	1.0688	1.0767	1.0803
72	0.9725	0.5695	0.8493	0.9163	0.9366	0.9616	0.0629	0.9688	0.9725
104	0.8810	0.4407	0.7660	0.8053	0.8513	0.8636	0.8639	0.8771	0.8810
152	0.7928	0.3262	0.6718	0.7134	0.7614	0.7688	0.7734	0.7872	0.7928
176	0.7604	0.2875	0.6325	0.6840	0.7231	0.7377	0.7429	0.7558	0.7602

E_{cm} (MeV)	Exact	Phase shift for potential (13)							
		2A + 1R	3A + 1R	4A + 1R	4A + 2R	6A + 5R	7A + 5R	10A + 6R	16A + 8R
12	1.0997	1.0841	1.0908	1.0943	1.0940	1.0961	1.0977	1.0997	1.0997
24	0.8370	0.8100	0.8248	0.8315	0.8304	0.8336	0.8357	0.8370	0.8370
48	0.5501	0.5222	0.5445	0.5513	0.5479	0.5488	0.5492	0.5499	0.5501
72	0.3730	0.3578	0.3756	0.3784	0.3717	0.3698	0.3700	0.3731	0.3731
104	0.2083	0.2094	0.2152	0.2152	0.2031	0.2011	0.2043	0.2084	0.2084
152	0.0358	0.0438	0.0449	0.0506	0.0282	0.0291	0.0345	0.0364	0.0361
176	-0.0311	-0.0258	-0.0179	-0.0078	-0.0363	-0.0358	-0.0318	-0.0301	-0.0307

Harms (1970) has shown that, for $N \approx 3$, T^* is a good approximation to the T -matrix from the potential V on the negative energy axis. To complement Harm's result and at the same time show that for large enough N we can reproduce the T -matrix for the potential V , we have made UPE calculations of the s-state phase shifts and half-off-shell function (Kowalski 1965; Noyes 1965) for different values of N and compared the results with the exact values obtained from V directly. The comparison of the phase shifts at different centre-of-mass energies E_{cm} is given in Table 1 and of the half-off-shell functions at different momenta p for fixed $E_{cm} = 72$ MeV is given in Table 2. Two potentials were used: a one-term attractive Yukawa potential

$$V(r) = -V_0 \exp(-\mu r)/r \quad (12)$$

with $V_0 = 65.246$ MeV and $\mu = 0.6329$ fm $^{-1}$, which has a single bound state at an

energy $E_D = 2.240$ MeV; and the two-term Yukawa potential of Malfliet and Tjon (1969)

$$V(r) = -V_A \exp(-\mu_A r)/r + V_R \exp(-\mu_R r)/r \quad (13)$$

with $V_A = 181.5422$ MeV, $V_R = 457.8828$ MeV, $\mu_A = 1.55 \text{ fm}^{-1}$, $\mu_R = 3.11 \text{ fm}^{-1}$, and $E_D = 0.35$ MeV, which was used to test the effect of short-range repulsion on the UPE. For potentials with both attraction and repulsion, the eigenvalues λ_n of equation (4) can be positive (designated by A) or negative (designated by R) whereas for purely attractive potentials all the eigenvalues are positive. The order in which the attractive and repulsive terms were added was that of increasing $|\lambda_n|$, so that terms with smallest $|\lambda_n|$ were included first, this choice being justified by the definition (9) of the UPE potential.

TABLE 2
EXACT AND UPE S-STATE HALF-OFF-SHELL FUNCTIONS FOR POTENTIALS (12) AND (13)
The half-off-shell function is given for a centre-of-mass energy $E_{cm} = 72$ MeV

p (fm $^{-1}$)	Half-off-shell function for potential (12)					Half-off-shell function for potential (13)			
	Exact	1A	3A	12A	30A	Exact	2A+1R	6A+5R	16A+8R
0.0064	0.777	2.173	0.668	0.803	0.777	1.550	1.697	1.539	1.549
0.1535	0.781	2.136	0.692	0.800	0.781	1.547	1.690	1.540	1.547
0.4885	0.816	1.851	0.850	0.812	0.817	1.514	1.618	1.526	1.513
1.007	0.942	1.276	1.021	0.958	0.942	1.292	1.307	1.307	1.291
2.041	0.786	0.588	0.782	0.797	0.786	0.032	0.129	0.035	0.033
2.780	0.511	0.369	0.546	0.512	0.511	-0.691	-0.576	-0.688	-0.690
3.772	0.305	0.221	0.334	0.306	0.305	-0.893	-0.899	-0.900	-0.892
5.182	0.170	0.125	0.179	0.173	0.170	-0.614	-0.665	-0.615	-0.614
7.355	0.087	0.064	0.085	0.086	0.087	-0.257	-0.278	-0.263	-0.258
11.070	0.039	0.029	0.034	0.040	0.039	-0.074	-0.131	-0.078	-0.075
14.051	0.024	0.018	0.021	0.024	0.024	-0.039	-0.095	-0.037	-0.037
18.42	0.014	0.011	0.012	0.014	0.014	-0.020	-0.061	-0.016	-0.019
25.239	0.008	0.006	0.006	0.008	0.008	-0.010	-0.035	-0.010	-0.011

Tables 1 and 2 show that the agreement is remarkably good in general provided N is taken large enough. Together with the results of Harms (1970) at negative energy, this leads to the conclusion that, with a suitable choice of N , the UPE can reproduce the T -matrix of a local potential. The method has been tested for the Reid potential in the 1S_0 and $^3S_1 - ^3D_1$ channels (Afnan and Read 1972) with comparable success in reproducing the on-shell T -matrix. Finally we note that to reproduce the T -matrix for the original potential we require $N \approx 12$. This makes it very difficult to use T^* in the Faddeev equations because of time and storage problems on present computers. However, this problem can be overcome by the use of T -matrix perturbation theory.

III. T -MATRIX PERTURBATION THEORY

We now consider the three-body bound state, for which we require the two-body T -matrix to be on the negative energy axis where its behaviour is largely determined by the two-body bound state pole. Since the UPE with only three terms gives a reasonable result for the three-body binding energy, the remaining terms in the expansion may be treated by perturbation theory. This overcomes the numerical problem of solving the Faddeev equations with a large number of terms. The perturbation is introduced via

the truncated potential

$$v^* = - \sum_{n=1}^{N_1} |\chi_n\rangle \lambda_n^{-1} \langle \chi_n| \quad \text{for} \quad N_1 \ll N, \quad (14)$$

where the N of the expansion (9) is taken to be large enough to reproduce the T -matrix for the potential V . The Faddeev equations are then solved for the energy and wavefunction of the three-body system by using the T -matrix corresponding to v^* ,

$$\tau^*(E) = \sum_{n,m=1}^{N_1} |\chi_n\rangle [M^{-1}(E)]_{nm} \langle \chi_m|, \quad (15)$$

and treating the difference between the actual T -matrix and τ^* by perturbation theory. Explicitly the perturbation is

$$t(E) = T(E) - \tau^*(E) \approx T^*(E) - \tau^*(E), \quad (16)$$

the separability of which, as is shown below, constitutes the crucial simplification of our method.

The formalism for such a T -matrix perturbation theory has been presented by Fuda (1968) who gives as the first-order correction for three identical particles

$$\Delta E^{(1)} = 12 \langle \Phi_3 | (123) t_3(E_0) (123) | \Phi_3 \rangle, \quad (17)$$

where (123) is the permutation operator (Harper *et al.* 1970), $t_3(E_0)$ is the perturbing T -matrix for particles 1 and 2, and E_0 is the binding energy for the three-body system with τ^* . The wavefunction $|\Phi_3\rangle$ in equation (17) is a solution of the Faddeev equation for the bound state

$$|\Phi_3\rangle = -2 G_0(E_0) \tau_3^*(E_0) (123) |\Phi_3\rangle, \quad (18)$$

with normalization chosen such that

$$\langle \Phi | \Phi \rangle = 1, \quad \text{where} \quad |\Phi\rangle = \sum_{\alpha=1}^3 |\Phi_\alpha\rangle. \quad (19, 20)$$

The advantage of using T^* instead of T in equation (16) may be seen on transforming equation (17) to a momentum space representation and considering the case of three identical bosons interacting only in relative s-states, whence

$$\Delta E^{(1)} = 12 \iiint \eta(p, q) t(p, p'; E_0 - \frac{3}{4}q^2) \eta(p', q) p^2 dp p'^2 dp' 4\pi q^2 dq, \quad (21)$$

where

$$\eta(p, q) = 2\pi \int_{-1}^1 \Phi_3(\frac{1}{2}\mathbf{p} + \frac{3}{4}\mathbf{q}, \mathbf{p} - \frac{1}{2}\mathbf{q}) d(\hat{\mathbf{p}} \cdot \hat{\mathbf{q}}). \quad (22)$$

Since $t(p, p'; E)$ is the difference between two separable terms we can write equation (21) as

$$\Delta E^{(1)} = E^{(1)}(N) - E^{(1)}(N_1), \quad (23)$$

where

$$E^{(1)}(L) = -12 \sum_{n,m=1}^L \int_0^\infty dq q^2 A_n(q) [M^{-1}(E_0 - \frac{3}{4}q^2)]_{nm} A_m(q) \quad (24)$$

and

$$A_n(q) = \int_0^\infty dp p^2 \chi_n(p) \eta(p, q). \quad (25)$$

Equation (25) can be reduced to (see Appendix)

$$A_n(q) = - \sum_{\mu=1}^{N_1} \int_0^\infty dk k^2 K_{n\mu}(q, k) F_\mu(k), \quad (26)$$

where $F_\mu(k)$ is related to the spectator function and $K_{n\mu}(q, k)$ is the kernel of the integral equation for $F_\mu(k)$. Hence the problem of calculating $E^{(1)}(L)$ is reduced to the evaluation of a one-dimensional integral and two sums. The advantages of this approach over that of performing the three-dimensional integration are: there are no errors in the sums, the integrand is very simple to calculate, and the problem of calculating the full off-shell T -matrix for a local potential as a function of energy has been avoided. The latter point leads to a considerable saving of time in the numerical solution.

IV. NUMERICAL RESULTS

To test the perturbation method described in Section III, we have examined the case of three bosons interacting via an s-wave potential. The reason for choosing this simple case is that it enables us to compare our results for different values of N_1 in the expansion (14) for $1 \leq N_1 \leq N$, where N is taken large enough to enable $T^*(E)$ to be a good approximation to the T -matrix for the local potential. It is worth noting that a similar calculation for a realistic potential with $N_1 = N$ would require the storage of a matrix of dimension $3N$ times the number of quadratures needed to approximate the integral in the Faddeev equations; a matrix larger than 360×360 for $N = 12$. The results of the perturbation theory for the binding energy of three bosons interacting via potentials (12) and (13) are given in Table 3. In this table, N_1 is the number of terms in the UPE used to solve the Faddeev equations for zero-order energy while N is the number of terms used in representing the T -matrix for the local potential.

If we consider the results for the one-term attractive Yukawa potential (12), we observe that $N = 9$ is sufficient to reproduce the exact T -matrix as far as the three-body binding energy is concerned. However, the number of terms used in solving the Faddeev equations is very important in determining the accuracy of the results. Thus with $N_1 = 1$, the error is about 1 MeV even after using perturbation theory because $T^* - \tau^*$ is too large for the second-order perturbation correction to be neglected. This is apparent from Tables 1 and 2 for potential (12), where the difference between the exact and the $N_1 = 1$ unitary pole approximation (UPA) results is large, and from Table 3 for potential (12), where the difference between the results for $N = 1$ and 9 is of the order of 2.1 MeV. The latter is in contrast with the case $N_1 = 3$, where the difference between the results for $N = 3$ and 9 is about 0.2 MeV, thereby indicating that the second-order terms are small. It is clear from Table 3 that the case $N_1 > 6$ need not be treated since the correction will be less than

0.001 MeV. These results show very convincingly that a definite minimum number of terms are required for the solution of the Faddeev equations in order to obtain the binding energy to a predetermined accuracy.

We now consider the results in Table 3 for the Malfliet and Tjon (1969) potential (13). Using one repulsive term in v^* , we present results for an increasing number of attractive terms until the required accuracy is obtained. It is clear that two attractive terms are sufficient in v^* and that the rest may be accurately treated by perturbation theory. Also it can be seen that the inclusion of a second repulsive term in v^* does not change the results and that therefore one repulsive term is sufficient.

TABLE 3

UPE THREE-BODY BINDING ENERGIES FOR BOSONS INTERACTING VIA POTENTIALS (12) AND (13)

The table consists of two 2-dimensional arrays, one for potential (12) and the other for potential (13), in which the columns are labelled by N_1 , the number of terms retained in the expansion (14) for v^* , and the rows are labelled by N , the number of terms retained in the expansion (9) for V^* . The diagonal elements were obtained by direct inversion of the Faddeev equations while the off-diagonal elements were obtained by T -matrix perturbation theory

N	Binding energy (MeV) for potential (12)						N	Binding energy (MeV) for potential (13)			
	1A	2A	3A	4A	5A	6A		2A + 1R	3A + 1R	4A + 1R	4A + 2R
1A	21.947							2A + 1R	7.491		
2A	23.285	24.021						3A + 1R	7.522	7.522	
3A	23.868	24.829	24.886					4A + 1R	7.537	7.537	7.538
4A	24.023	24.974	25.037	25.040				5A + 1R	7.550	7.551	7.551
5A	24.065	25.008	25.069	25.072	25.072			6A + 1R	7.555	7.556	7.556
6A	24.077	25.017	25.076	25.080	25.080	25.080		4A + 2R			7.525
7A	24.082	25.021	25.080	25.083	25.083	25.083		5A + 2R			7.539
8A	24.083	25.022	25.080	25.083	25.084	25.084		6A + 2R	7.543	7.543	7.544
9A	24.085	25.023	25.081	25.084	25.085	25.085		6A + 3R	7.540	7.540	7.540
10A	24.085	25.023	25.082	25.084	25.085	25.085		6A + 4R	7.539	7.539	7.539
11A	24.085	25.023	25.082	25.084	25.085	25.085		6A + 5R	7.538	7.539	7.539
12A	24.085	25.023	25.082	25.084	25.085	25.085					

From the foregoing discussion we conclude that, although v^* with three terms does not accurately reproduce the T -matrix for the local potential, the approximation is sufficiently good that the difference may be treated by perturbation theory. For potentials (12) and (13), it was only necessary to solve the Faddeev equations for a three-term UPE in order to calculate the three-body binding energy to within 0.1%. Such accuracy is sufficient to study the dependence of the three-nucleon observables on the off-shell behaviour of the two-body T -matrix. On the other hand, if the UPA potential (that is, $N_1 = 1$) is used, the difference between the UPA and the actual T -matrices may be too large for first-order perturbation theory to be sufficient, as is shown by the results in Table 3 for potential (12).

With the success of our method for the two Yukawa potentials, we are optimistic about the inclusion of spin dependence and a tensor force. We have already shown (Afnan and Read 1972) that a UPE in the presence of a tensor force has a reasonably good convergence.

V. ACKNOWLEDGMENTS

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APPENDIX

Evaluation of $\Lambda_n(q)$

We discuss here the procedure for calculating $\Lambda_n(q)$, which is defined as

$$\Lambda_n(q) = \int_0^\infty dp p^2 \chi_n(p) \eta(p, q) = \int d\mathbf{p} \chi_n(p) \Phi_3(\frac{1}{2}\mathbf{p} + \frac{3}{4}\mathbf{q}, \mathbf{p} - \frac{1}{2}\mathbf{q}). \quad (\text{A1})$$

If we introduce a new integration variable \mathbf{k} , where

$$\mathbf{k} = \mathbf{p} - \frac{1}{2}\mathbf{q},$$

then equation (A1) becomes

$$\Lambda_n(q) = \int d\mathbf{k} \chi_n(|\mathbf{k} + \frac{1}{2}\mathbf{q}|) \Phi_3(\frac{1}{2}\mathbf{k} + \mathbf{q}, \mathbf{k}). \quad (\text{A2})$$

For an N_1 -term separable potential we can write

$$\Phi_3(\frac{1}{2}\mathbf{k} + \mathbf{q}, \mathbf{k}) = - \sum_{\mu=1}^{N_1} \frac{\chi_\mu(|\mathbf{q} + \frac{1}{2}\mathbf{k}|) F_\mu(k)}{2\pi(q^2 + k^2 + \mathbf{k} \cdot \mathbf{q} - E_0)}, \quad (\text{A3})$$

where $F_\mu(k)$ is a solution of the integral equation

$$\sum_{v=1}^{N_1} M_{\mu v}(E_0 - \frac{3}{4}k^2) F_v(k) = \sum_{v=1}^{N_1} \int_0^\infty dk' k'^2 K_{\mu v}(k, k') F_v(k') \quad (\text{A4})$$

with $M_{\mu\nu}$ given by equation (11) and $K_{\mu\nu}$ defined by

$$K_{\mu\nu}(k, k') = \int_{-1}^1 d(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}') \frac{\chi_\mu(|\mathbf{k}' + \frac{1}{2}\mathbf{k}|) \chi_\nu(|\mathbf{k} + \frac{1}{2}\mathbf{k}'|)}{(k^2 + k'^2 + \mathbf{k} \cdot \mathbf{k}' - E_0)}. \quad (\text{A5})$$

On substituting equations (A3) and (A5) in equation (A2) we obtain

$$\begin{aligned} A_n(q) &= - \int_0^\infty dk k^2 \int_{-1}^1 d(\hat{\mathbf{k}} \cdot \hat{\mathbf{q}}) \sum_{\mu=1}^{N_1} \frac{\chi_n(|\mathbf{k} + \frac{1}{2}\mathbf{q}|) \chi_\mu(|\mathbf{q} + \frac{1}{2}\mathbf{k}|)}{(q^2 + k^2 + \mathbf{k} \cdot \mathbf{q} - E_0)} F_\mu(k) \\ &= - \sum_{\mu=1}^{N_1} \int_0^\infty dk k^2 K_{n\mu}(q, k) F_\mu(k). \end{aligned} \quad (\text{A6})$$

The important point to note is that when we solve the three-body bound state problem with τ^* we obtain $F_\mu(\mu = 1, \dots, N_1)$ and that part of the kernel $K_{n\mu}(q, k)$ has been evaluated. Thus, the evaluation of $A_n(q)$ takes very little extra time and the correction to the energy is then a one-dimensional integral.

