$$\beta p = \rho + \sum_{n=2}^{\infty} B_n \rho^n \ , \tag{18}$$

with a corresponding equation for $p^c$, and the radial distribution function in a density series,

$$g(r) = e^{-\beta v(r)} \sum_{n=0}^{\infty} \rho^n y_n(r) \ , \tag{19}$$

then substituting in (17) and equating powers of $\rho$ gives

$$B_n = B_n^c + (n-1)2^{-1/2}\pi a^2 e^{-\beta v(a+)} y_{n-2}(a)\lambda + O(\lambda^2) \ . \tag{20}$$

$B_n$ is the direct part of $n$th virial coefficient and $B_n^c$ is its classical counterpart. $y_0(r) = 1$, so for $n = 2$ (20) reduces to (14). For $n > 2$, $y_{n-2}(a)$ depends on the detailed nature of the potential, so for virial coefficients higher than the second the leading quantum correction is not determined solely by the depth of the potential at the hard core.

If the potential fails to be continuous for $r > a$, there will be additional first-order quantum corrections from the neighborhood of the discontinuities. For example, for the square-well potential

$$\begin{aligned} v(r) &= \infty, \quad && r < a \\ v(r) &= -\epsilon, && a < r < b \\ v(r) &= 0, && r > b \ , \end{aligned} \tag{21}$$

the $n$th virial coefficient is[1]

$$B_n = B_n^c + (n-1)2^{-1/2}\pi[a^2 e^{\beta\epsilon} y_{n-2}(a) + b^2\theta(\beta\epsilon) y_{n-2}(b)]\lambda + O(\lambda^2) \ , \tag{22}$$

where

$$\theta(x) \equiv 1 + e^x - 2e^{x/2} I_0(\tfrac{1}{2}x) \ . \tag{23}$$

Comparing (22) with (20) shows that the contribution from the neighborhood of the hard core is the same in each case, but we now have an additional contribution from the discontinuity at $r = b$.

In the above we have considered only the first-order quantum correction to the virial coefficients. Higher-order corrections to the second virial coefficient can be obtained using its expression as the inverse Laplace transform of the logarithmic derivative of the Jost function,[4] and this is the method employed by D'Arruda in his calculation for the hard-core-plus-attractive-well potential.[3] Another possible method is the modified Wigner–Kirkwood expansion given recently by Derderian and Steele,[5] in which hard-sphere basis functions rather than free-particle functions are used.

For the higher coefficients, the only method available seems to be that of I. The theory given there is quite general, and includes all higher corrections. However, even for the second-order term computational difficulties are severe. Not only does one require $G(\vec{\mathbf{r}}, \vec{\mathbf{r}}; \beta)$ to the next order, but one also needs the leading term in the function $U_3^m(1, 2, 3)$, and this involves solving a three-body problem.[6]

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# Variation-Iteration Solution of the Variable-Phase Equation

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It is pointed out that the variation-iteration method offers a fast and accurate means for solving the variable-phase equation. The method is especially useful for problems involving many partial waves.

In a recent paper by Landman,[1] a perturbation-variation treatment of the variable-phase function has been proposed. The method consists of two parts. First, the standard technique of perturbation theory is applied to the variable-phase equation.[2] A variational principle[3] is then employed to optimize the choice for the main part of the potential.

We wish to point out the limitations of Landman's method and offer a remedy. We shall adopt Land-

man's notation and refer to equations in his paper as (L. 1), (L. 2), etc.

The procedure for optimizing $V_0(r;\tilde{c})$ relies on the maximum-minimum property of the functional

$$T_l[\tilde{t}_l(x);r] \equiv -k^{-1}\int_0^r dx\, U(x)[\hat{j}_l^2 - \tilde{t}_l^2(x)\hat{n}_l^2(kx)] \times \exp\{2k^{-1}\int_x^r dy\; U(y)\hat{n}_l(ky) \times [\hat{j}_l(ky) - \tilde{t}_l(y)\hat{n}_l(ky)]\}. \quad (1)$$

[Note that the corresponding expression, Eq. (L. 31), contains a misprint.] This property, however, is known to hold only for a special class of potentials $U(r)$, namely, real potentials which do not change sign.[3,4]

For a general complex potential, Eq. (1) provides a variational principle with the following properties[3]:

$$t_l(r) = T_l[t_l(x);r]\,, \quad (2)$$

$$t_l(r) = T_l[\tilde{t}_l(x);r] + O((t_l - \tilde{t}_l)^2)\,. \quad (3)$$

Here $t_l(r)$ is the true tangent function for the potential $U(r)$. Using this fact, Eq. (1) can be applied to calculate the tangent function iteratively:

$$\tilde{t}_l^{(i+1)}(r) = T_l[\tilde{t}_l^{(i)}(x);r]\,. \quad (4)$$

As an initial guess, one can choose, for example, the exact solution $t_l^{(0)}$ for an approximate potential $V_0(r)$, i.e.,

$$\tilde{t}_l^{(0)}(r) = t_l^{(0)}(r)\,. \quad (5)$$

This is, in fact, Landman's choice.[1] As explained, one can not in general optimize the initial choice. If $\tilde{t}_l^{(0)}$ is chosen "close enough" to the true $t_l$, the process (4) converges rapidly (in a quadratic manner). (It also diverges rapidly for a wrong initial guess!) In fact, iterating (5) once gives $t_l(r)$ correctly up to order $\lambda$. A second iteration gives $t_l(r)$ correctly to order $\lambda^3$, etc. This should be contrasted with the perturbation equations (L. 19) and (L. 20), where the same numerical effort—in fact, the same machinery—is exercised. By definition, perturbation calculations give $t_l(r)$ to order $\lambda, \lambda^2, \lambda^3$, etc. The fast convergence achieved by Landman is, of course, due to his optimization procedure for the zeroth-order potential.

The iterative process (4) has been applied[5] directly to the partial scattering amplitudes

$$c_l \equiv \frac{\exp(2i\delta_l) - 1}{2i}\,,$$

where the appropriate variational principle reads

$$C_l[\tilde{c}_l(x);r] \equiv -k^{-1}\int_0^r dx\, U(x)[\hat{j}_l^2(kx) - \tilde{c}_l^2(x)\hat{h}_l^2(kx)] \times \exp\{-2k^{-1}\int_x^r dy\, U(y)\hat{h}_l(ky)[\hat{j}_l(ky) + \tilde{c}_l(y)\hat{h}_l(ky)]\}, \quad (6)$$

with $\hat{h}_l(kr) \equiv -\hat{n}_l(kr) + i\hat{j}_l(kr)$. Table I gives successive iterations of the first four partial amplitudes for the scattering of a 100-MeV neutron by $Ca^{40}$. The optical potential employed is

$$V = \frac{-V_0}{1+e^{(r-R)/a}} - \frac{4iW_D e^{(r-R)/a}}{(1+e^{(r-R)/a})^2}$$

with $R = r_0 A^{1/3}$, $r_0 = 1.25F$, $a = 0.65F$, $V_0 = 50$ MeV, and $W_D = 10$ MeV. The initial guess was taken as $\tilde{c}_l^{(0)}(r) \equiv 0$. $R^{(i)}$ and $I^{(i)}$ stand for $\mathrm{Re}\tilde{c}_l^{(i)}(\infty)$ and $\mathrm{Im}\tilde{c}_l^{(i)}(\infty)$. In this numerical example, the third iteration coincides with the exact results. The second iteration is already adequate for most practical calculations.

TABLE I. Successive iterations for the first four partial scattering amplitudes $c_l$. The third iteration coincides with the exact results.

| $L$ | $R^{(1)}$ | $I^{(1)}$ | $R^{(2)}$ | $I^{(2)}$ | $R^{(3)}=R$ | $I^{(3)}=I$ |
|---|---|---|---|---|---|---|
| 0 | −0.221 78 | 0.471 98 | −0.271 38 | 0.629 33 | −0.271 28 | 0.629 51 |
| 1 | −0.206 41 | 0.455 95 | −0.263 87 | 0.640 33 | −0.263 61 | 0.640 60 |
| 2 | −0.202 56 | 0.431 10 | −0.248 18 | 0.660 57 | −0.247 65 | 0.660 68 |
| 3 | −0.220 07 | 0.408 36 | −0.219 62 | 0.688 18 | −0.218 87 | 0.688 60 |

Using Eq. (6), a variety of scattering problems with complex potentials have been successfully solved. The iterative procedure is especially useful for problems involving many partial waves. The fact that in these problems the partial amplitudes $c_l(r)$ vary slowly and smoothly as a function of $l$ allows one to use the result $c_l(r)$ as an input for calculating $c_{l+1}(r)$. Thus, "unrelated" problems for different partial waves become related. In fact, the same procedure, namely, using the output of one problem as an input for another (similar) problem, can be applied whenever a survey is needed. This may be helpful for, e.g., scanning bombarding energies or solving the scattering problem for a family of potentials.

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