Erratum

Erratum: Green's functions for the rapid computation of nonrelativistic wave functions [Phys. Rev. A 26, 1173 (1982)]

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S. R. Patterson has pointed out to us that Eq. (7) is not an appropriate form for $\psi(\vec{r})$ in the case that the generalized potential $\mathscr{U}$ is taken to be a function of $\rho \equiv |\vec{r} - \vec{r}\,'|$. In that case, an additional term is needed in Eq. (7), as follows:

$$\psi = \mathscr{G}(\mathscr{U} - \mathscr{V} + E - E_0)\psi + \mathscr{Q}\psi \ . \tag{7'}$$

Here the $\mathscr{Q}$ operator is defined so that

$$\mathscr{Q}\psi = \int d\,\vec{r}\,' Q(\vec{r}, \vec{r}\,')\psi(\vec{r}\,') \ , \tag{75}$$

where $Q(\vec{r}, \vec{r}\,')$ must satisfy the relation

$$(\mathscr{T} - E_0)Q(\vec{r}, \vec{r}\,') + (\mathscr{T} - E)G(\vec{r}, \vec{r}\,')\mathscr{U}(\vec{r}, \vec{r}\,') + G(\vec{r}, \vec{r}\,')\mathscr{U}(\vec{r}, \vec{r}\,')\mathscr{V}(\vec{r}\,') = 0 \ . \tag{76}$$

Equation (11) then must also contain an additional term

$$\Delta W_{\mu\sigma} \equiv \langle \mu | \mathscr{G}(\mathscr{U} - \mathscr{V}) + \mathscr{Q} | \sigma \rangle \ . \tag{11'}$$

With these two changes and the change to Eq. (23) described below, the error is corrected. The remainder of the equations in the original paper are unaffected.

However, the presence of the function $Q(\vec{r}, \vec{r}\,')$ forces the computational process to be extended to include it and its effects.

From the form of (76) one may deduce that Q must depend on x and $\vec{r}\,'$ in the following fashion:

$$Q = Q_0(x) + Q_1(x)\mathscr{V}(\vec{r}\,') \ . \tag{77}$$

The Q_i may then be evaluated in series in powers of x, just as was done for G in (32)–(34):

$$Q_i = Q_i^{(-)} + Q_i^{(+)}, \quad i = 0, 1 \tag{78}$$

$$Q_i^{(-)}(x) = \gamma U_0 \left[\sum_{s=0}^{2\nu} h_{si} X^{-2\nu+s-1} + (t_{0i}/x)\ln(x) \right] \ , \tag{79}$$

$$Q_i^{(+)}(x) = \gamma U_0 \left[\sum_{s=2\nu+1}^{\infty} h_{si} x^{-2\nu+s-1} + \ln(x) \sum_{s=1}^{\infty} t_{si} x^{s-1} \right] \ . \tag{80}$$

By substituting these series into the defining equation (76) the coefficients h_{si} and t_{si} may be determined in terms of the coefficients a_s and b_s of the original paper:

$$h_{00} = -a_0 \ , \tag{81}$$

$$h_{10} = -a_1 \ , \tag{82}$$

$$t_{00} = -b_0 \ , \tag{83}$$

$$t_{10} = -b_1 + (1/2\nu)(h_{2\nu-1,0} + \epsilon a_{2\nu-1}) \ , \tag{84}$$

$$h_{s+2,0}=-a_{s+2}+\eta_s^{(-)}[h_{s,0}+\epsilon a_s-2(s-\nu+1)(t_{s-2\nu+2,0}+b_{s-2\nu+2})],\quad s\neq 2\nu-1\ , \tag{85}$$

$$t_{s+2,0}=-b_{s+2}+\eta_s^{(+)}(t_s+\epsilon b_s)\ , \tag{86}$$

$$h_{01}=h_{11}=t_{01}=0\ , \tag{87}$$

$$t_{11}=(1/2\nu)h_{2\nu-1,1}+(1/\nu\gamma^2)a_{2\nu-1}\ , \tag{88}$$

$$h_{s+2,1}=\eta_s^{(-)}[h_{s,1}+2a_s/\gamma^2-2(s-\nu+1)t_{s-2\nu+2,1}],\quad s\neq 2\nu-1\ , \tag{89}$$

$$t_{s+2,1}=\eta_s^{(+)}(t_{s,1}+2b_s/\gamma^2)\ . \tag{90}$$

Here

$$\eta_s^{(\pm)}\equiv[(s+1)(s\pm 2\nu+1)]^{-1} \tag{91}$$

and

$$\epsilon\equiv E/E_0\ . \tag{92}$$

In writing Eqs. (85) and (89), the coefficients b_s and t_{si} have been defined as equal to zero when $s<0$.

The coefficients $h_{2\nu+1,i}$ are not defined by (81)–(92), but must be chosen so that the boundary conditions on the Q_i be satisfied ($Q_i\rightarrow 0$ as $x\rightarrow\infty$), just as was done with the $a_{2\nu}$ in satisfying the boundary conditions on G.

Therefore (81)–(92) should be regarded as supplementing (35)–(41) of our original paper.

Fourier-Laplace transforms of the $Q_i^{(\pm)}$ must next be introduced, analogous to the $g^{(\pm)}$ defined in (42) and (43).

$$Q_i^{(-)}(x)=\int_0^\infty q_i^{(-)}(\lambda)\exp(-\lambda x^2)d\lambda\ , \tag{93}$$

$$Q_i^{(+)}(x)=\int_{-\infty}^\infty q_i^{(+)}(\lambda)\exp[(\beta-i\lambda)x^2]d\lambda\ . \tag{94}$$

Because (79) and (80) have the same form as (53) and (54), respectively, the series expansions for the $q_i^{(\pm)}$ are the same as those of $u^{(\pm)}$ [Eqs. (58) and (59)] with a_s replaced by h_{si} and b_s by t_{si}.

The quantity $\langle\mu|\mathcal{Q}|\sigma\rangle$ needed in (11′) is then the following:

$$\langle\mu|\mathcal{Q}|\sigma\rangle=\int_0^\infty d\lambda[q_0^{(-)}(\lambda)\langle\mu|\exp(-\lambda x^2)|\sigma\rangle+q_1^{(-)}(\lambda)\langle\mu|\exp(-\lambda x^2)\mathscr{V}(\vec{r}')|\sigma\rangle]$$
$$+\int_{-\infty}^\infty d\lambda\{q_0^{(+)}(\lambda)\langle\mu|\exp[(i\lambda-\beta)x^2]|\sigma\rangle+q_1^{(+)}(\lambda)\langle\mu|\exp[(i\lambda-\beta)x^2]\mathscr{V}(\vec{r}')|\sigma\rangle\}\ . \tag{95}$$

The four elements $\langle\mu|\cdots|\sigma\rangle$ appearing in (95) are discussed in the original paper. Three are explicitly evaluated, in Eqs. (66), (67), and (72). The fourth is obtained from (72) by replacing $\Lambda^{(-)}$ by $\Lambda^{(+)}$ throughout.

Finally, note that the estimate for U_0, Eq. (23), must be corrected for the presence of the operator $\mathcal{Q}$ by altering (21):

$$Z_{\mu\sigma}=\langle\mu|\mathscr{G}\mathscr{L}+\mathscr{P}|\sigma\rangle\ . \tag{21′}$$

Here,

$$\mathscr{P}=\mathcal{Q}/U_0\ , \tag{96}$$

the division by U_0 being necessary since (79) and (80) show that to first order Q is proportional to U_0. The implicit dependence of $\mathcal{Q}$ on U_0 is to be neglected since the central notion used in making the estimate (23) was that the explicit dependence of ΔW on U_0 should be taken into account while the implicit dependences were to be neglected.

The result is that (23) is not altered in form provided the new definition (21′) is employed.