Errata

Erratum: New approach to the calculation of density functionals [Phys. Rev. A 28, 544 (1983)]

Gil Zumbach and Klaus Maschke

We are indebted to H. Englisch, R. Englisch, E. V. Ludena, and J. K. Percus for pointing out to us that the conditions formulated in theorem 3 for obtaining all Ψ's such that $\Psi \rightarrow \rho$ are not correct. During the preparation of the present Erratum many other attentive readers have detected the same problem and the above list is only chronological and by no means complete. At this occasion we would like to give thanks for the many helpful comments which we have received.

The correct formulation of theorem 3 reads

Theorem 3. For all $\rho(\vec{r}) \in A_N$,

$$\varphi^{\vec{k}s}(\vec{r}) = [\rho(\vec{r})/N]^{1/2} e^{i\vec{k}\cdot\vec{R}} s \quad ,$$

the one-particle basis of theorem 1,

$$\psi_{\{\vec{k},s\}_i} = \frac{1}{\sqrt{N!}} \det{}_{\{\vec{k},s\}_i}(\varphi^{\vec{k}s}) \quad ,$$

the corresponding N-particle basis,

$$\mathrm{Card}\{\vec{k},s\}_i = N \quad ,$$

$$\{\vec{k},s\}_i = \{(\vec{k},s)_{p_1}, \ldots, (\vec{k},s)_{p_N}\}_i \quad ,$$

an ordered set with $p_1 < \cdots < p_N$, and

$$\Psi = \sum_i \lambda_{\{\vec{k},s\}_i} \psi_{\{\vec{k},s\}_i} \quad ,$$

an N-particle wave function, with

$$\sum_i |\lambda_{\{\vec{k},s\}_i}|^2 = 1 \quad .$$

If for all i,j with $i \neq j$ the unordered sets $\{\vec{k},s\}_i$ differ from the unordered sets $\{\vec{k},s\}_j$ (a) by at least two elements $(\vec{k},s)$, or (b) by only one element $(\vec{k},s)$, which differs either (i) by the spin s, the $\vec{k}$ vector can be different or not, or (ii) by the vector $\vec{k}$, the spins remaining unchanged, i.e., $(\vec{k},s)_{p_n} = (\vec{q},s) \in \{\vec{k},s\}_i$ is replaced by $(\vec{k},s)_{p_m} = (\vec{q}\,',s) \in \{\vec{k},s\}_j$, and

$$\sum_{i,j}{}' (-1)^{P_{i,j}} \lambda_{\{\vec{k},s\}_i} \lambda^*_{\{\vec{k},s\}_j} e^{i(\vec{q}-\vec{q}\,')\cdot\vec{R}} = 0 \quad , \quad \text{for all } \vec{R} \quad ,$$

where $P_{i,j} = P_{i,j}(\vec{q} \rightarrow \vec{q}\,')$ is the number of permutations which is necessary to obtain an ordered set $\{\vec{k},s\}_j$ after the replacement of $\vec{q}$ by $\vec{q}\,'$ in the set $\{\vec{k},s\}_i$, then

$$\Psi \rightarrow \rho \quad .$$

The important point is that the above condition for the $\lambda_{\{\vec{k},s\}_i}$ does not depend on the charge density $\rho(\vec{r})$. Note that if the condition (b) (ii) occurs, the pair of set indices i,j fixes the pair of vectors $\vec{q}$ and $\vec{q}\,'$.

To avoid any misleading interpretation we have replaced λ_i by $\lambda_{\{\vec{k},s\}_i}$. Condition (b) (ii) was omitted in the original version of our paper. The restriction to ordered sets $\{\vec{k},s\}_i$ is necessary in order to fix the sign in the definition of the basis vector $\psi_{\{\vec{k},s\}_i}$.

Proof of theorem 3: We have

$$\rho'(\vec{r}) = N \sum_\sigma \int d^3r_2 \cdots d^3r_N |\Psi(\vec{r}, \vec{r}_1, \ldots, \vec{r}_N)|^2 = N \sum_\sigma \int d^3r_2 \cdots d^3r_N \sum_{i,j} \lambda_{\{\vec{k},s\}_i} \lambda^*_{\{\vec{k},s\}_j} \psi_{\{\vec{k},s\}_i} \psi^*_{\{\vec{k},s\}_j}$$

$$= N \sum_\sigma \int d^3r_2 \cdots d^3r_N \left\{ \sum_i |\lambda_{\{\vec{k},s\}_i}|^2 |\psi_{\{\vec{k},s\}_i}|^2 + \sum_{\substack{i,j \\ i\neq j}} \lambda_{\{\vec{k},s\}_i} \lambda^*_{\{\vec{k},s\}_j} \psi_{\{\vec{k},s\}_i} \psi^*_{\{\vec{k},s\}_j} \right\} \quad .$$

All the N-particle basis functions are orthogonal, but in the relation for the charge density we have to sum over N spin coordinates, whereas we integrate over only N-1 spatial coordinates. Therefore cases (a) and (b) (i) are trivial, and we have only to worry about the sets which differ by one $\vec{k}$ vector ($\vec{q} \to \vec{q}'$). We obtain

$$\rho'(\vec{r}) = \sum_i |\lambda_{\{\vec{k},s\}_i}|^2 \sum_{(\vec{k},s)\in\{\vec{k},s\}_i} |\varphi^{\vec{k}s}|^2 + \sum_{i,j}{}' (-1)^{P_{i,j}} \lambda_{\{\vec{k},s\}_i} \lambda^*_{\{\vec{k},s\}_j} \varphi^{\vec{q}s} (\varphi^{\vec{q}'s})^*$$

$$= \rho(\vec{r}) + \rho(\vec{r}) \sum_{i,j}{}' (-1)^{P_{i,j}} \lambda_{\{\vec{k},s\}_i} \lambda^*_{\{\vec{k},s\}_j} e^{i(\vec{q}-\vec{q}')\cdot\vec{R}(\vec{r})} \ .$$

The sum $\sum'$ runs over all i,j ($i \neq j$) for which the unordered sets $\{\vec{k},s\}_i$ and $\{\vec{k},s\}_j$ differ by exactly one element, i.e., the element $(\vec{q},s)$ in $\{\vec{k},s\}_i$ is replaced by $(\vec{q}',s)$ in $\{\vec{k},s\}_j$. The spin part remains unchanged. Asking for $\rho'(\vec{r}) = \rho(\vec{r})$ we see that condition (b) (ii) must be satisfied.

Because of the above changes of theorem 3, Eq. (13) must be replaced by

$$\tilde{F}(\rho) = \inf\{T(\rho) + U(\rho)\} \ ,$$

$$T(\rho) = \int (\vec{\nabla}\sqrt{\rho})^2 dr + \frac{1}{N} \int \rho(\vec{r}) \sum_i |\lambda_{\{\vec{k},s\}_i}|^2 \left[\sum_{\{\vec{k},s\}_i} [\vec{\nabla}\cdot(\vec{k}\cdot\vec{R})]^2 - \frac{1}{N} \left(\sum_{\{\vec{k},s\}_i} \vec{\nabla}\cdot(\vec{k}\cdot\vec{R}) \right)^2 \right] dr$$

$$+ \frac{1}{N} \sum_{i,j}{}' (-1)^{P_{i,j}} \lambda_{\{\vec{k},s\}_i} \lambda^*_{\{\vec{k},s\}_j} \int e^{i(\vec{q}-\vec{q}')\cdot\vec{R}} [\rho \vec{\nabla}(\vec{q}\cdot\vec{R}) \cdot \vec{\nabla}(\vec{q}'\cdot\vec{R}) + i\sqrt{\rho}(\vec{\nabla}\sqrt{\rho}) \cdot [\vec{\nabla}(\vec{q}\cdot\vec{R}) - \vec{\nabla}\cdot(\vec{q}'\cdot\vec{R})]] dr \ ,$$

$$U(\rho) = \tfrac{1}{2} \int\int dr\, dr' \frac{\rho(\vec{r})\rho(\vec{r}')}{|\vec{r}-\vec{r}'|} [1 - \epsilon_{xc}(\{\{\vec{k},s\}_i\}, \vec{r}, \vec{r}')] \ ,$$

$$\epsilon_{xc} = \sum_i |\lambda_{\{\vec{k},s\}_i}|^2 \frac{1}{N^2} \left(\left| \sum_{\{\vec{k},s=\mathrm{up}\}_i} e^{i\vec{k}\cdot\vec{\alpha}} \right|^2 + \left| \sum_{\{\vec{k},s=\mathrm{down}\}_i} e^{i\vec{k}\cdot\vec{\alpha}} \right|^2 \right)$$

$$+ \frac{1}{N^2} \sum_{i,j}{}' (-1)^{P_{i,j}} \lambda_{\{\vec{k},s\}_i} \lambda^*_{\{\vec{k},s\}_j} \left(\sum_{\substack{(\vec{k},s)\in\{\vec{k},s\}_i \\ \vec{k}\neq\vec{q}}} e^{i(\vec{q}\cdot\vec{R} + \vec{k}\cdot\vec{R}' - \vec{k}\cdot\vec{R} - \vec{q}'\cdot\vec{R}')} \right) \delta_{s_{\vec{q}} s_{\vec{k}}}$$

$$- \frac{1}{N^2} \sum_{i,j}{}'' (-1)^{P_{i,j}} \lambda_{\{\vec{k},s\}_i} \lambda^*_{\{\vec{k},s\}_j} \left(e^{i(\vec{q}_1\cdot\vec{R} + \vec{q}_2\cdot\vec{R}' - \vec{q}_1'\cdot\vec{R} - \vec{q}_2'\cdot\vec{R}')} - e^{i(\vec{q}_1\cdot\vec{R} + \vec{q}_2\cdot\vec{R}' - \vec{q}_2'\cdot\vec{R} - \vec{q}_1'\cdot\vec{R}')} \delta_{s_{\vec{q}_1} s_{\vec{q}_2}} \right) \ ,$$

$$\vec{R} = \vec{R}(\vec{r}), \quad \vec{R}' = \vec{R}(\vec{r}'), \quad \vec{\alpha} = \vec{R} - \vec{R}' \ .$$

The sum $\sum'$ runs over all i,j ($i \neq j$) for which the unordered sets $\{\vec{k},s\}_i$ and $\{\vec{k},s\}_j$ differ by exactly one $\vec{k}$ element, i.e., the element $(\vec{q},s_{\vec{q}})$ in $\{\vec{k},s\}_i$ is replaced by $(\vec{q}',s_{\vec{q}})$ in $\{\vec{k},s\}_j$. The sum $\sum''$ runs over all i,j ($i \neq j$) for which the unordered sets $\{\vec{k},s\}_i$ and $\{\vec{k},s\}_j$ differ by exactly two $\vec{k}$ elements, i.e., the elements $(\vec{q}_1,s_{\vec{q}_1})$, $(\vec{q}_2,s_{\vec{q}_2})$ in $\{\vec{k},s\}_i$ are replaced by $(\vec{q}_1',s_{\vec{q}_1})$, $(\vec{q}_2',s_{\vec{q}_2})$ in $\{\vec{k},s\}_j$. The spin parts remain unchanged. $P_{i,j}$ counts the numer of permutations which are necessary to obtain the ordered set $\{\vec{k},s\}_j$ after the replacement of the elements in $\{\vec{k},s\}_i$.

Furthermore, the following misprints must be corrected:

(1) Page 546, top of left column: Replace

$$\frac{2\pi}{N} \int_{-\infty}^{z} dz' \int_{-\infty}^{\infty} \int dy'\, dx' \rho(x',y',z)$$

by

$$\frac{2\pi}{N} \int_{-\infty}^{z} dz' \int_{-\infty}^{\infty} \int dy'\, dx'\, \rho(x',y',z') \ .$$

Replace $\langle \varphi \vec{k}' | \varphi^{\vec{k}} \rangle$ by $\langle \varphi^{\vec{k}'} | \varphi^{\vec{k}} \rangle$.

(2) Page 547, Sec. III F: Replace $E'(\rho) \leq E_{\mathrm{HF}}(\rho)$ by $E'(\rho) \geq E_{\mathrm{HF}}(\rho)$.

(3) Page 550, fifth line: Replace $e^{i\vec{q}'\cdot(\vec{r}'-\vec{q}\cdot\vec{r})}$ by $e^{i(\vec{q}'\cdot\vec{r}'-\vec{q}\cdot\vec{r})}$.

(4) Page 550, ninth line: Replace

$$\sum_{\vec{r}_0} g(\vec{r}_0) \frac{1}{(D\vec{f}/D\vec{r})|_{\vec{r}=\vec{r}_0}} \vec{f}(\vec{r}_0) = 0$$

by

$$\sum_{\vec{r}_0} g(\vec{r}_0) \frac{1}{(D\vec{f}/D\vec{r})|_{\vec{r}=\vec{r}_0}} \ , \quad \text{with } \vec{f}(\vec{r}_0) = 0 \ .$$

(5) Page 551, Appendix D: Replace one of the expressions

$$N_\uparrow = N_\downarrow = \frac{N}{2}$$

by

$$N \to \infty, \quad V = L^3 \to \infty, \quad N/V = \text{const} \ .$$

(6) Page 552, fourth line: Replace

$$\frac{T(\rho)}{N} = \tfrac{3}{5} k_F^2 \{ \tfrac{9}{10} \alpha^2 + \tfrac{3}{4} \xi^2 [1 - (1-\alpha^2)^{1/2}] \}$$

by

$$\tfrac{1}{5} k_F^2 \int d^3 r \, \rho(\vec{r}) [(\vec{\nabla} R_1)^2 + (\vec{\nabla} R_2)^2 + (\vec{\nabla} R_3)^2] \ .$$

Erratum: NMR measurement of the nuclear shielding isotope shift in molecular hydrogen [Phys. Rev. A 24, 144 (1981)]

James R. Beckett and H. Y. Carr

In the abstract and in the second paragraph of Sec. II, the value for the isotope shift $\sigma(D_2) - \sigma(HD)$ at 296 K in the zero-density limit should be 0.0479 (not 0.0469) ± 0.0005 ppm. Correspondingly, in Sec. II, both in the text and in Fig. 5, the sign of the 0.0005-ppm density correction should be plus (not minus). The authors wish to thank Professor W. T. Raynes for finding this error.

Erratum: New *U*-matrix theory in quantum mechanics [Phys. Rev. A 27, 1760 (1983)]

C. C. Lam and P. C. W. Fung

We have gone through our paper and detected the following errors.

(1) After Eq. (3.1), $[\hat{P},\hat{Q}]_0 = \hat{Q}$. The error (a typing error, as the first line of (3.1) reads $e^{\hat{P}} \hat{Q} e^{-\hat{P}} = \hat{Q} + [\hat{P},\hat{Q}] + \cdots$; the first term $\hat{Q}$ represents $[\hat{P},\hat{Q}]_0$ obviously) appears in the definition of $[\hat{P},\hat{Q}]_0$ only and all the subsequent results of our deduction are based on (3.1), and *no error* is involved in all the crucial steps of our paper. On p. 1762, $[\hat{P},\hat{Q}]_0 = 1$ should read $[\hat{P},\hat{Q}]_0 = \hat{Q}$.

(2) In Fig. 1(b) the symbol attached to the horizontal dotted line before the time scale $t = -b$ should read $\hat{H}_0$ rather than $\hat{H}$.

(3) On p. 1770, (6.23) should read

$$\hat{P} = e^{-iG_t^\dagger e^{-i\omega t} \hat{a}^\dagger} , \qquad \hat{Q} = e^{-iG_t e^{i\omega t} \hat{a}} \ . \tag{6.23}$$

The statement before (6.27) should read $U_0(t,t_0) = 1$ (see Sec. III).

(4) On p. 1772, (7.6) should read

$$\hat{B}_r^{(s)}(t,t_0) = \sum_{j=0}^{r} (-i)^j \int_{t_0}^{t} du_1 \hat{H}(u_1) \int_{t_0}^{u_1} du_2 \hat{H}(u_2) \cdots \int_{t_0}^{u_j} du_{j+1} \hat{A}^{(s)}(u_{j+1},t_0) \hat{U}_{r-j}^{(s)}(u_{j+1},t_0) \ . \tag{7.6}$$

(5) On p. 1773, the seventh line of Appendix A should read as follows: ... then making the substitution $\hat{H}_1(u) = d\hat{F}/du$, $\hat{F} = \int du \hat{H}_1(u)$, $\hat{f}(u,t_0) = \hat{U}_{n-1}(u,t_0)$, and....

(6) On p. 1775, the last few lines should read

$$\begin{aligned} &+(-i)^{n-3} \int_{t_0}^{t} du_1 \hat{H}_1(u_1) \int_{t_0}^{u_1} du_2 \hat{H}_1(u_2) \cdots \int_{t_0}^{u_{n-3}} du_{n-2} \hat{A}(u_{n-2},t_0) \hat{U}_{n-(n-1)}(u_{n-2},t_0) \\ &+ \cdots \\ &+(-i) \int_{t_0}^{t} du_1 \hat{H}_1(u_1) \int_{t_0}^{u_1} du_2 \hat{A}(u_2,t_0) \hat{U}_{n-3}(u_2,t_0) \\ &+ \int_{t_0}^{t} du_1 \hat{A}(u_1,t_0) \hat{U}_{n-2}(u_1,t_0) \ . \end{aligned} \tag{B8}$$