Operator Identity and Applications to Models of Interacting Electrons

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By correct reduction of some quartic forms in fermion field operators, I eliminate all but a constant and some quadratic terms. I can use this to transform the Wolff model, of a magnetic impurity in a nonmagnetic metal, into a solvable quadratic form in fermions. Applying the same method (with less justification) to Hubbard's model in three dimensions, I obtain an oversimplified but nevertheless suggestive, and diagonal, Hamiltonian.

In this paper I present elements of a novel solution of a well-known model magnetic impurity in a nonmagnetic metal, first proposed by Wolff.[1] In an earlier study Tomonaga's method[2] was used to reduce this many-body problem to a solvable quadratic form in boson operators.[3] I have now transformed it further, into an exactly solvable quadratic form in fermion operators, by a method detailed below. Like the old, the new method indicates that there is a singularity at a value of the Coulomb parameter U_C of the order of the bandwidth, but unlike the old[4] it can provide detailed results in the critical region $U \approx U_C$ replete with symptoms of the Kondo effect: specific-heat anomaly, high magnetic susceptibility, low-frequency resonance which can translate into a resistance anomaly. Finally, an approximate extension of this method to Hubbard's model[5] of an interacting electron gas yields as the solution of that problem a simple, diagonal, yet physically plausible Hamiltonian.

I recapitulate parts of my earlier study.[3] The interaction between electrons of opposite spin σ at the impurity site $R_i = 0$ is given by

$$\begin{aligned}\mathcal{K}_2 &= U[n_\uparrow(0) - \tfrac{1}{2}][n_\downarrow(0) - \tfrac{1}{2}] \\ &= \tfrac{1}{4}U\{[n_\uparrow(0) + n_\downarrow(0) - 1]^2 - [n_\uparrow(0) - n_\downarrow(0)]^2\}. \quad (1)\end{aligned}$$

The dual representations of the local occupation-number operator are

$$n_\sigma(0) - \tfrac{1}{2} = N^{-1}\sum_k \sum_{k' \neq k} c_{k\sigma}^\dagger c_{k'\sigma}, \qquad (2a)$$

which is quadratic in the fermion field operators c_k, and

$$\begin{aligned} n_\sigma(0) - \tfrac{1}{2} &= N^{-1} \sum_{q>0} (\rho_{q\sigma} + \rho_{q\sigma}^\dagger), \\ \rho_{q\sigma} &= \rho_{-q\sigma}^\dagger = \sum_k c_{k\sigma}^\dagger c_{k+q,\sigma}, \end{aligned} \qquad (2b)$$

which is linear in the bosons. Momentary reflection suggests that $\mathcal{K}_2$, expressed in bosons, will become separable after a unitary transformation to new operators denoted $\rho_{q\tau} \equiv 2^{-1/2}(\rho_{q\uparrow} + \tau\rho_{q\downarrow})$, where $\tau = \pm 1$. The "kinetic energy" operator $\mathcal{K}_0$ of a half-filled band is invariant under such transformation. Originally there are two equivalent forms:

$$\mathcal{K}_0 = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma}, \quad \epsilon_k = v_F(k - k_F), \qquad (3a)$$

in the original fermions, or

$$\mathcal{K}_0 = 2\pi v_F N^{-1} \sum_{q>0,\sigma} \rho_{q\sigma}^\dagger \rho_{q\sigma}, \qquad (3b)$$

in the original bosons. After transformation to the new operators, $\rho_{q\tau}$, this last equation becomes

$$\mathcal{H}_0 \to 2\pi v_F N^{-1} \sum_{q>0,\tau} \rho_{q\tau}{}^\dagger \rho_{q\tau} \tag{4a}$$

which, in turn, possesses an equivalent form in a new set of fermion "quasiparticles" $c_{k\tau}$, viz.,

$$\mathcal{H}_0 \to \sum_{k,\tau} \epsilon_k c_{k\tau}{}^\dagger c_{k\tau}. \tag{4b}$$

We have now achieved a separation of variables, $\mathcal{H}_0 + \mathcal{H}_2 \to \mathcal{H}_+ + \mathcal{H}_-$,

$$\mathcal{H}_\tau = \sum_k \epsilon_k c_{k\tau}{}^\dagger c_{k\tau} + \tfrac{1}{2}\tau U[n_\tau(0) - \tfrac{1}{2}]^2,$$
$$\tau = \pm 1, \tag{5}$$

and $n_\tau(0) - \frac{1}{2}$ given in Eqs. (2) with τ replacing σ henceforth. The original work was based on representations (4a) above; the present goal is to make use of (4b). The new approach must overcome an obstacle that, according to the usual trivial identities, $[n_\tau(0) - \frac{1}{2}]^2 \equiv \frac{1}{4}$. This implies that the interaction Hamiltonian is a trivial constant, contrary to the results obtained by use of Tomonaga operators. The following section is devoted to a resolution of this paradox.

It is known that for boson and fermion representations to be unitarily equivalent, certain stability requirements must be imposed.[2] One of these requirements concerns the normal ordering of electron operators, with the filled Fermi sea as the vacuum, required in order to prove such important commutation relations as $[\rho_{q,\tau}, \rho_{-q',\tau'}] = (Nq/2\pi)\delta_{qq'}\delta_{\tau\tau'}$. In the present context, I have found that normal ordering of the boson operators is also required. Indicated by the conventional colon pairs, it is defined as follows:

$$:\rho_\alpha \rho_\beta{}^\dagger: = \rho_\beta{}^\dagger \rho_\alpha,$$
$$:\rho_\alpha \rho_\beta: = \rho_\alpha \rho_\beta, \quad \text{etc. all } q>0. \tag{6}$$

Normal-ordering eliminates from the expansion of $[n_\tau(0) - \frac{1}{2}]^2$ only those undesirable terms such as $\rho_{q\tau}\rho_{q\tau}{}^\dagger$ which can contribute large numbers to the vacuum energy, while, at the same time, preserving all the operator equations of motion upon which the earlier solution[3] was based. The effects of this procedure can only be gauged after the reintroduction of quasiparticle operators c_k into (5); e.g.,

$$:[n(0) - \tfrac{1}{2}]^2: = N^{-2} \sum_{q,q'>0} (\rho_q{}^\dagger \rho_{q'}{}^\dagger + \rho_q{}^\dagger \rho_{q'}) + \text{H.c.},$$

which, with the aid of (2b), becomes

$$:[n(0) - \tfrac{1}{2}]^2: = N^{-2} \sum_{3>2} \sum_{1>0} (c_3{}^\dagger c_2{}^\dagger c_1{}^\dagger c_0 + \text{H.c.}) + N^{-2} \sum_{3>2} \sum_{1>0} (c_3{}^\dagger c_2 c_1{}^\dagger c_0 + \text{H.c.}). \tag{7}$$

For brevity, k_i is simply denoted by i, $\epsilon_{ki} > \epsilon_{kj}$ by $i>j$, and the subscript τ is omitted. One now needs the integrated density-of-states function $S(\epsilon)$, defined as

$$S(\epsilon_k) = N^{-1} \sum_{\epsilon_{k'} < \epsilon_k}, \quad 1 = \int_{\epsilon_{\min}}^{\epsilon_k} d\epsilon' \mathfrak{N}(\epsilon'), \tag{8}$$

with $\mathfrak{N}(\epsilon)$ the density-of-states function, normalized to 1 per unit cell. After some additional algebraic drudgery, one obtains

$$:[n(0) - \tfrac{1}{2}]^2: = N^{-1} \sum_{3,0} [S(\epsilon_3) - S(\epsilon_F)][c_3{}^\dagger c_0 + \text{H.c.}] + N^{-1} S(\epsilon_F) \sum_{3,0} (c_3{}^\dagger c_0 + \text{H.c.})$$
$$+ 2N^{-2} \sum_{3,1,0} c_3{}^\dagger c_1{}^\dagger c_0 c_1 - N^{-2} \sum_{3,1} c_3{}^\dagger c_1{}^\dagger c_3 c_1 + N^{-2} \sum_{\substack{1\neq 0,2 \\ 3\neq 0,2}} c_3{}^\dagger c_1{}^\dagger c_0 c_2. \tag{9}$$

The last term, quartic in the c's, vanishes by antisymmetry. Because $S(\epsilon_F) = \frac{1}{2}$ in a half-filled band, the second and third terms cancel, with the fourth term precisely $\frac{1}{4}$. It is the first term, quadratic in the field operators, which is the principal consequence of the ordering procedure. Omitting the canceled terms and generalizing to an arbitrary point R_n, one obtains the new result,

$$:[n(R_n) - \tfrac{1}{2}]^2: = N^{-1} \sum_{k,k'} [S(\epsilon_k) - S(\epsilon_F)]\{c_k{}^\dagger c_{k'} \exp[i(k-k')R_n] + \text{H.c.}\} + \tfrac{1}{4}, \tag{10a}$$

as the alternative formulation of

$$:[n(R_n) - \tfrac{1}{2}]^2: = N^{-2} \sum_{q,q'>0} \{\exp[i(q+q')R_n]\rho_q{}^\dagger \rho_{q'}{}^\dagger + \exp[i(q-q')R_n]\rho_q{}^\dagger \rho_{q'}\} + \text{H.c.} \tag{10b}$$

Summing these over N equally spaced points R_n on a line and equating, one obtains the following relation:

$$\sum_k [S(\epsilon_k) - S(\epsilon_F)] c_k^\dagger c_k = N^{-1} \sum_{q>0} \rho_q^\dagger \rho_q . \tag{11}$$

For $\epsilon_k = v_F(k - k_F)$ and a constant density of states $\mathfrak{N} = (2\pi v_F)^{-1}$, this relation may be seen also to provide a new proof of the equivalence of the two forms of kinetic energy (3a) with (3b), and (4a) with (4b).

With (10a) substituted back into the $\mathcal{H}_T$, Eq. (5), this Hamiltonian is now quadratic in the c_k field operators and therefore exactly solvable. Whereas a study of $\mathcal{H}_-$ brings out an interesting singularity, $\mathcal{H}_+$, which can be studied in an analogous manner, demonstrates few noteworthy features for $U > 0$ and can be omitted in the present brief summary. Now, in a magnetic field $\mathcal{H}_-$ must be augmented by the Zeeman energy $-h[n_\uparrow(0) - n_\downarrow(0)] \to -h2^{1/2}[n_-(0) - \frac{1}{2}]$ and becomes

$$\mathcal{H}_- = \sum_k \epsilon_k c_{k-}^\dagger c_{k-} - \tfrac{1}{2} U N^{-1} \sum_{k,k'} [S(\epsilon_k) - S(\epsilon_F)][c_{k-}^\dagger c_{k'-} + \text{H.c.}] - h2^{1/2}[n_-(0) - \tfrac{1}{2}]. \tag{12}$$

Suppose one studies the Wannier operator at the $R_i = 0$ site, $a_0 \equiv N^{-1/2}\sum c_{k-}$, by means of its equation of motion:

$$[a_0, \mathcal{H}_-] = N^{-1/2} \sum_k \{\epsilon_k - \tfrac{1}{2} U [S(\epsilon_k) - S(\epsilon_F)] - h2^{1/2}\} c_{k-} . \tag{13}$$

One finds that, for a constant density of states $\mathfrak{N}$, a_0 becomes decoupled from the remaining fermion operators at a value of U to be denoted U_C, and given by $1 - \frac{1}{2} U_C \mathfrak{N} = 0$. For a calculation of the temperature-dependent susceptibility at $U \neq U_C$ it is more convenient to adopt a unit bandwidth and a semicircular density of states, $\epsilon_F = 0$. After some analysis one obtains

$$\chi(T) = (i\pi)^{-1} \oint dz\, f(\beta\epsilon)(1 - z^2)[L(U)z^2 + 1]^{-2}, \tag{14}$$

with $f(\beta\epsilon)$ the Fermi function at temperature $T = \beta^{-1}$, $\epsilon \equiv -\frac{1}{4}(z + z^{-1})$, $L(U) \equiv 2U/U_C - (U/U_C)^2$, and the indicated contour being the unit circle. At $T = 0$ this yields

$$\chi(0) = \pi^{-1}\{2(1 - U/U_C)^{-2} + L^{-1} - \tfrac{1}{2} L^{-3/2}(1 - U/U_C)^2 \ln[(1 + L^{1/2})(1 - L^{1/2})^{-1}]\} . \tag{15}$$

The zero-temperature susceptibility blows up at U_C. The high-temperature susceptibility approaches the free value $1/4T$ for all U.

For the study of thermodynamic functions such as entropy the most compact expressions involve the phase-shift function

$$\varphi(\epsilon, U) = \tan^{-1}[(1 - 4\epsilon^2)^{1/2}(1 - U/U_C)^2(-2\epsilon)^{-1}(1 + L)^{-1}], \tag{16}$$

or rather, the incremental phase-shifts $\Delta\varphi \equiv \varphi(\epsilon, U) - \varphi(\epsilon, 0)$. For the incremental entropy $\Delta S(T, U) \equiv S(T, U) - S(T, 0)$ one obtains

$$\Delta S(T, U) = -(\pi T)^{-1} \int d\epsilon [\partial f(\beta\epsilon)/\partial\epsilon] \epsilon\, \Delta\varphi(\epsilon, U) . \tag{17}$$

In zero magnetic field at $T = 0$, a partial integration reduces this to

$$\Delta S(0, U) = 2\Delta\varphi(0, U)\pi^{-1} \int_0^\infty dx\, f(x) = \begin{cases} 0 \text{ for } U \neq U_C \\ \ln 2 \text{ at } U = U_C \end{cases} . \tag{18}$$

In the critical region $U \approx U_C$ the incremental entropy vanishes at $T = 0$ but rises rapidly to a magnitude approaching ln2 at a temperature T_m of the order of $(1 - U/U_C)^2$. The specific heat, given by

$$\Delta c(T, U) = -(\pi T)^{-1} \int d\epsilon\, \epsilon^2 [\partial f(\beta\epsilon)/\partial\epsilon] (\partial\Delta\varphi/\partial\epsilon), \tag{19}$$

also has a sharp, linear, initial rise when U is in the critical region, and displays a maximum at a temperature $O(T_m)$. This behavior is a consequence of the rapid variation of $\Delta\varphi$ in a region $\pm T_m$ of the Fermi energy. It is therefore reasonable to suppose that the electrical resistance will also drop for $T > T_m$, and that T_m is approximately the Kondo temperature. In the absence of the very complicated, detailed calculations required for the electrical resistance, there is not much more to add on this score. But it is amusing to compare, in the limit $U \to U_C$ when both $\Delta c(T)/T$ and $\chi(T)$ become infinite at low temperature, their ratio, which remains finite: $\lim(T \to 0, U \to U_C)\Delta c/\chi T = 2\pi^2/3$, in accord with Wilson's recent result[6] in the Kondo problem. The detailed comparison with other models exhibiting the Kondo effect, and detailed derivation of the results quoted above, will be published elsewhere.

The three-dimensional Hubbard model[5] incorporates interactions $U[n_\uparrow(R_i)-\frac{1}{2}][n_\downarrow(R_i)-\frac{1}{2}]$ at every site R_i of a three-dimensional lattice. Because the Tomonaga operators defined on the ith site do not commute with those on a jth site, the transformation to the $\pm$ operators is no longer exact. Ignoring the correction terms, we avail ourselves of (10a) and, after summing over sites, obtain

$$:\mathcal{H}_{\text{Hubbard}}: = \sum_{k,\tau}\{\epsilon_k + \tau U[S(\epsilon_k) - S(\epsilon_F)]\} c_{k\tau}{}^\dagger c_{k\tau}. \tag{20}$$

Note that the parameter $\frac{1}{2}U$ of Eqs. (12) *et seq.* is now replaced by U. As U is increased, the susceptibility rises until it diverges at U_0, given by

$$(\partial/\partial\epsilon_k)[\epsilon_k - U_0 S(\epsilon_k)]_{\epsilon_F} = 0, \text{ i.e., at } U_0\mathfrak{N}(\epsilon_F) = 1, \tag{21}$$

which is the usual ball-park figure for a phase transition. The bandwidth of the (+) quasiparticles has approximately doubled at U_0.

Unlike the reduction of the Wolff model, the result (20) is not exact. Nevertheless, it contains all the qualitative features one expects, except for the finite lifetime of quasiparticles away from the Fermi energy. Many such aspects of the problem appear to be of interest, and further details will be published in due course.

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[1]P. A. Wolff, Phys. Rev. 124, 1030 (1961), and solved by him in the Hartree-Fock approximation.

[2]S. Tomonaga, Prog. Theor. Phys. 5, 544 (1950). A review can be found in E. Lieb and D. Mattis, *Mathematical Physics in One Dimension* (Academic, New York, 1966), Chap. 2. More recent applications and extensions are given in K. Schotte and U. Schotte, Phys. Rev. 182, 479 (1969); D. Mattis, J. Math. Phys. (N. Y.) 15, 609 (1974); A. Luther and V. Emery, Phys. Rev. Lett. 33, 589 (1974), *inter alia.*

[3]D. Mattis, Ann. Phys. (N. Y.) 89, 45 (1975).

[4]At high temperature or with strong interactions, the number of degrees of freedom associated with bosons greatly surpasses that for fermions so that correct thermodynamic properties near U_c are difficult to extract from a pure Tomonaga model. Criteria for the validity of the Tomonaga operators have been given, e.g., by M. Aizenman and H. Gutfreund, J. Math. Phys. (N. Y.) 15, 643 (1974).

[5]See the review by C. Herring, in *Magnetism,* edited by G. Rado and H. Suhl (Academic, New York, 1966), where the model and several alternative solutions are compared.

[6]K. Wilson, in *Nobel Symposia, Proceedings of the 1973 Symposium,* edited by B. Lundqvist *et al.* (Academic, New York, 1974), p. 68; K. Wilson, Rev. Mod. Phys. 47, 773 (1975).