Comments and Addenda

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Singularities in the X-Ray Absorption and Emission of Metals*

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It is shown that Nozières and de Dominicis's exact solution to Mahan's model x-ray problem may be obtained very simply using an equation-of-motion technique.

IN a recent series of papers, Nozières and co-workers[1–3] have thoroughly analyzed Mahan's[4] model x-ray problem using many-body techniques. In the final paper in the series, Nozières and de Dominicis[3] (ND) have shown that in reality one is dealing with a transient one-body problem, which in turn can be solved essentially exactly using a diagrammatic perturbation-theoretic expansion. Here we show that ND's one-body equations can be derived very simply using an equation-of-motion technique.

Except as noted below, we use the same notation as ND. In particular, the Hamiltonian is given by

$$H=\sum_q \epsilon_q a_q^\dagger a_q+E_0 b^\dagger b+\sum_{qq'} V_{qq'} a_q^\dagger a_{q'} bb^\dagger. \quad (1)$$

The Green's functions for the conduction electrons and the deep state are, respectively, defined by

$$G_{kk'}(\tau-\tau')=\langle Ta_k(\tau)a_{k'}^\dagger(\tau')\rangle, \quad (2a)$$

$$g(t-t')=\langle Tb(t)b^\dagger(t')\rangle. \quad (2b)$$

The x-ray absorption or emission is determined by the function[5]

$$F_{kk'}(\tau,\tau';t,t')=\langle Ta_k(\tau)a_{k'}^\dagger(\tau')b(t)b^\dagger(t')\rangle. \quad (3)$$

The notation $\langle\ \rangle$ represents the expectation value in the initial ground state which for absorption contains no deep (b-type) holes and for emission contains no deep electrons. It is this fact which causes the equation of motion for F to close on itself. To obtain this equation, we calculate the commutator of $a_k(\tau)$ with the Hamiltonian, set it equal to $i\partial_\tau a_k(\tau)$, and multiply both sides by $a_{k'}^\dagger(\tau')b(t)b^\dagger(t')$, so that

$$(\partial_\tau+i\epsilon_k)F_{kk'}(\tau,\tau';t,t')-\delta_{kk'}\delta(\tau-\tau')g(t-t')$$
$$=-i\sum_q V_{kq}\langle Ta_q(\tau)b(\tau)b^\dagger(\tau)a_{k'}^\dagger(\tau')b(t)b^\dagger(t')\rangle. \quad (4)$$

The last term on the left arises from commuting ∂_τ through the time-ordering operator.

Consider now the absorption case, where the initial ground state contains no deep holes. Then the right side of (4) vanishes except for the particular time ordering $t'>\tau>t$, that is, when the hole-number operator $b(\tau)b^\dagger(\tau)$ is sandwiched between $b^\dagger(t')$ on the left and $b(t)$ on the right; in this latter case $b(\tau)b^\dagger(\tau)$ is exactly equal to unity, so that the six-operator function on the right side of (4) reduces to the four-operator function F. Hence Eq. (4) becomes exactly

$$[\partial_\tau+i\epsilon_k]F_{kk'}(\tau,\tau';t,t')=\delta_{kk'}\delta(\tau-\tau')g(t-t')$$
$$-i\sum_q V_{kq}F_{qk'}(\tau,\tau';t,t')\chi(\tau;t,t') \quad \text{(absorption)}, \quad (5a)$$

where $\chi(\tau;t,t')$ is a two-sided unit step function which vanishes unless $t'>\tau>t$.

The emission case is similar; here it is most convenient to commute $b(\tau)$ through $b^\dagger(\tau)$ on the right side of (4) and consider the electron-number operator $b^\dagger(\tau)b(\tau)$. This operator then vanishes in (4) unless $t>\tau>t'$, so that (4) becomes

$$\sum_q[(\partial_\tau+i\epsilon_k)\delta_{kq}+V_{kq}]F_{kk'}(\tau,\tau';t,t')$$
$$=\delta_{kk'}\delta(\tau-\tau')g(t-t')+i\sum_q V_{kq}F_{qk'}(\tau,\tau';t,t')$$
$$\times\chi(\tau;t',t) \quad \text{(emission)}. \quad (5b)$$

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[1] B. Roulet, J. Gavoret, and P. Nozières, Phys. Rev. **178**, 1072 (1969).
[2] P. Nozières, J. Gavoret, and B. Roulet, Phys. Rev. **178**, 1084 (1969).
[3] P. Nozières and C. T. de Dominicis, Phys. Rev. **178**, 1097 (1969).
[4] G. D. Mahan, Phys. Rev. **163**, 612 (1967).
[5] The function $F_{kk'}(t-t')$ of ND is equal to $-F_{k'k}(t',t;t,t')$.

Equations (5) may be easily converted to integral equations by noting that the operators in the square brackets on the left sides of (5a) and (5b) are simply the inverses of the conduction-electron Green's functions for absorption and emission, respectively. This should be obvious by inspection, but may be seen rigorously by constructing the equation of motion of G [Eq. (2a)] and noting that in the initial ground state $bb^\dagger$ ($b^\dagger b$) vanishes for absorption (emission). Hence Eqs. (5) become

$$F_{kk'}(\tau,\tau';t,t')=G_{kk'}(\tau-\tau')g(t-t')$$
$$+i\int_{t'}^{t}d\tau''\sum_{qq'}G_{kq}(\tau-\tau'')V_{qq'}F_{qk'}(\tau'',\tau';t,t') \quad (6)$$

for both emission and absorption (although G differs in the respective cases).

We may complete the set of equations by writing the equation of motion for $g(t-t')$. This is done in the usual way, by noting that $i\partial_t b(t)=[b,H]$, multiplying both sides by $b^\dagger(t')$, and taking the time-ordered expectation value

$$(\partial_t+iE_0)g(t-t')=\delta(t-t')-i\sum_{qq'}V_{qq'}F_{q'q}(t,t^+;t,t'), \quad (7)$$

where t^+ is infinitesimally greater than t (note that F is discontinuous at $\tau=\tau'$). Equations (6) and (7) are identical to Eqs. (17a), (17b), and (21) of ND; note that in ND's notation, $F_{kk'}(\tau,\tau';t,t')=\phi_{kk'}(\tau,\tau';t,t')\times g(t-t')$ and $g(t-t')=\exp[-iE_0(t-t')+C(t-t')]$.

It is also rather simple to derive ND's coupling-constant differentiation formulas for g. One defines the coupling constant λ in such a way that both the initial ground state and its energy eigenvalue are independent of λ. Thus for absorption we write

$$H_\lambda=\sum_q\epsilon_q a_q^\dagger a_q+E_0b^\dagger b+\lambda\sum_{qq'}V_{qq'}a_q^\dagger a_{q'}bb^\dagger, \quad (8a)$$

and for emission

$$H_\lambda=\sum_{qq'}(\epsilon_q\delta_{qq'}+V_{qq'})a_q^\dagger a_{q'}+E_0b^\dagger b$$
$$-\lambda\sum_{qq'}V_{qq'}a_q^\dagger a_{q'}b^\dagger b. \quad (8b)$$

Note that for $\lambda=1$, (8a) and (8b) are both identical to (1). Consider the case of absorption, where from inspection of (2b) and (8a) we see that

$$g_\lambda(t-t')=-e^{iE_0(t'-t)}\langle b^\dagger e^{-iH_\lambda(t'-t)}b\rangle\theta(t'-t). \quad (9)$$

The use of the mathematical identity

$$\frac{d}{d\lambda}e^{-iH_\lambda(t'-t)}=-i\int_t^{t'}e^{-iH_\lambda(t'-\tau)}\frac{dH}{d\lambda}e^{iH_\lambda(t-\tau)} \quad (10)$$

enables one to write

$$\frac{dg_\lambda(t-t')}{d\lambda}=i\sum_{qq'}V_{qq'}\int_t^{t'}F_{q'q}(\tau,\tau^+;t,t')d\tau, \quad (11)$$

which is the same as Eq. (22) of ND. A similar analysis shows that (11) holds for emission as well [using (8b) for H_λ].

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