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Correlation effects on the oscillator strength of optical absorption: Sum rule for the one-dimensional Hubbard model

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The optical sum rule which is related to the mean kinetic energy of band electrons is evaluated for the one-dimensional Hubbard Hamiltonian. The case of a half-filled band is treated exactly by use of the Bethe ansatz solution of Lieb and Wu. The kinetic energy decreases monotonically as a function of U and tends to zero like $1/U$ for $U \rightarrow \infty$. For other band fillings the Gutzwiller ansatz is used. Correlation effects increase quadratically with the density n of electrons (or holes) for $n << 1$ and exhibit a maximum at $n = 1$ (i.e., for the half-filled band).

Optical absorption experiments are efficient tools for determining the importance of electronic correlation in organic conductors.[1] It is found that the plasma frequency ω_p^0 as determined from the plasma edge is not sensitive to weak or intermediate correlation and therefore can be used to determine single-particle parameters like the hopping integral t. On the other hand, the plasma frequency ω_p as determined from the partial sum rule involving all intraband transitions turns out to depend rather sensitively on correlations. In fact, the ratio ω_p/ω_p^0 can be used as a measure for correlation effects.[1] In this note we evaluate the sum rule for a system of independent chains, each of which is described by the Hubbard Hamiltonian

$$H = T + V \, , \tag{1}$$

where

$$T = -t \sum_{ls} (c_{ls}^\dagger c_{l+1,s} + c_{l+1,s}^\dagger c_{ls}) \tag{2}$$

is the kinetic energy, and

$$V = U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{3}$$

is the on-site Coulomb interaction. (The operator c_{is} destroys an electron at site i with spin projection s, and $n_{is} = c_{is}^\dagger c_{is}$.) The f-sum rule for the conductivity is given by[2]

$$\int_0^\infty d\omega \, \sigma(\omega) = -\pi e^2 a \langle T \rangle / (2Nd^2\hbar^2) \, , \tag{4}$$

where a is the lattice constant, N is the number of sites per chain, and d is the interchain distance. Therefore, the sum rule provides the mean kinetic energy $\langle T \rangle$ per chain. Since the Hubbard term tends to localize the electrons, the absolute value of the kinetic energy is expected to decrease with increasing U. We evaluate $\langle T \rangle$ with respect to the ground state of the full Hamiltonian (1). It is related to the ground-state energy $E = \langle H \rangle$ by

$$\langle T \rangle = t \, \partial_t E \, . \tag{5}$$

This relation is easily derived by use of the Hellmann-Feynman theorem. For the particular case of a half-filled band (one electron per site), we use the exact result for E as obtained by Lieb and Wu[3] and obtain

$$-\langle T \rangle / (4Nt) = \int_0^\infty d\omega \, J_0(\omega) J_1(\omega) \{ [\omega(1+e^{2\omega u})]^{-1} + u/[1+\cosh(2\omega u)] \} \, , \tag{6}$$

where $u = U/(4t)$. The asymptotic behavior is found to be

$$-\langle T \rangle / (4Nt) \sim \begin{cases} (1 - 0.213\,58u^2)/\pi & \text{for } u << 1 \, , \\ [\frac{1}{2}\ln 2 - (\frac{3}{8})^2 \zeta(3) u^{-2}] u^{-1} & \text{for } u >> 1 \, . \end{cases} \tag{7}$$

For the limit $u \rightarrow 0$ we have used the asymptotic expansion of Economou and Poulopoulos.[4] The result of our numerical integration of Eq. (6) is shown in Fig. 1, together with the limiting behavior of Eq. (7). As expected the absolute value of the kinetic energy decreases monotonously

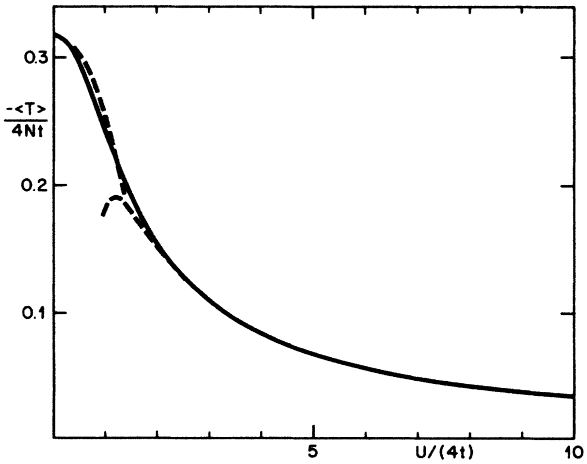

FIG. 1. Kinetic energy as a function of U. The solid line represents the exact solution, Eq. (6). The dashed lines correspond to the asymptotic expansions of Eq. (7).

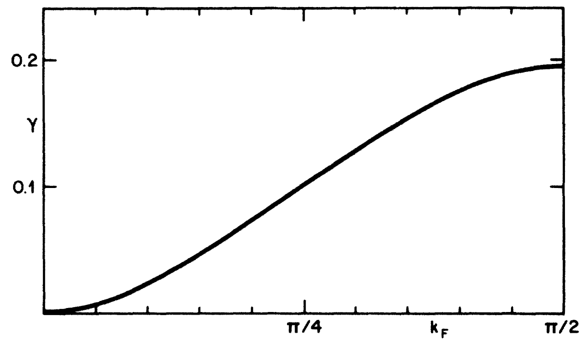

FIG. 2. Dependence of the correlation effect on band filling. Results for $k_F > \frac{1}{2}\pi$ are obtained from this figure by replacing k_F by $\pi - k_F$ (i.e., by substituting electrons by holes).

with U. The crossover between "small-U behavior" and "large-U behavior" occurs for $U \sim 4t$.

For general band fillings an explicit expression like Eq. (6) is not available. Therefore we have evaluated the kinetic energy by use of the Gutzwiller ansatz for the ground state

$$|\psi\rangle = \exp\left[-\tfrac{1}{2}\eta \sum_i n_{i\uparrow} n_{i\downarrow}\right] |\phi\rangle \ , \tag{8}$$

where η is the correlation parameter and $|\phi\rangle$ the ground state of T. Following the procedure of Refs. 5 and 6 we expand the variational ground-state energy,

$$E(\eta) = \langle\psi|H|\psi\rangle / \langle\psi|\psi\rangle \ , \tag{9}$$

in powers of η. As shown in the Appendix, this corresponds to an expansion in powers of U. To second order in U we find for n electrons per site as a function of $k_F = \frac{1}{2}\pi n$,

$$-\langle T\rangle/(4Nt) = \pi^{-1}\sin k_F[1 - \gamma(k_F)u^2] \ , \tag{10}$$

where

$$\gamma(k_F) = \frac{k_F^4(1 - 4k_F/3\pi)^2}{\sin k_F[k_F(\pi - k_F) + \sin^2 k_F]} \ . \tag{11}$$

For the special case of a half-filled band where $k_F = \frac{1}{2}\pi$, Eqs. (10) and (11) lead to

$$-\langle T\rangle/(4Nt) = (1 - 0.1951u^2)/\pi \ , \tag{12}$$

in remarkable agreement with the exact result of Eq. (7). The function $\gamma(k_F)$ measures the effect of correlations as a function of band filling and is shown in Fig. 2 for $0 < k_F < \frac{1}{2}\pi$. It first increases quadratically and reaches a maximum for a half-filled band. The quadratic increase for small density can be easily understood since for a very dilute system the interaction effects are essentially due to two-particle scattering. This physically appealing behavior for $k_F \to 0$ and the good agreement with the exact result for $k_F = \frac{1}{2}\pi$ suggest that the Gutzwiller wave function represents a good approximation for the kinetic energy (and thus the f-sum rule) in the case of small U, $U \ll 4t$. For larger values of U, the exact diagonalization of the Hamiltonian (1) for short chains or rings[7] is expected to provide good answers for particular band fillings.

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APPENDIX

Using the linked-cluster theorem[5] we find the following expansion for the expectation value of the energy [Eq. (9)],

$$\begin{aligned} E = {} & \langle\phi|T|\phi\rangle - \tfrac{1}{2}\eta\langle\phi|\{W,T\}|\phi\rangle_c \\ & + \tfrac{1}{8}\eta^2\langle\phi|\{W,\{W,T\}\}|\phi\rangle_c \\ & + U(\langle\phi|W|\phi\rangle - \eta\langle\phi|W^2|\phi\rangle_c) \ , \end{aligned} \tag{A1}$$

where $\{W,T\} = WT + TW$ and

$$W = \sum_i n_{i\uparrow} n_{i\downarrow} \ . \tag{A2}$$

In Eq. (A1) we have omitted all terms which after minimalization turn out to be of higher order than U^2. Through the use of Wick's theorem, the various terms in Eq. (A1) are decomposed into products of correlation functions,

$$P_{ij} = \langle\phi|c_{is}^\dagger c_{js}|\phi\rangle . \tag{A3}$$

For a band filling up to k_F we find

$$P_{ij} = \begin{cases} k_F/\pi, & i = j \ , \\ \sin[k_F(i-j)]/[\pi(i-j)], & i \neq j \ . \end{cases} \tag{A4}$$

The different terms in Eq. (A1) are found to be

$$\langle\phi|T|\phi\rangle/(4Nt) = -P_{i,i+1} \ , \tag{A5}$$

$$\langle\phi|UW|\phi\rangle/(4Nt) = (k_F/\pi)^2 u \ , \tag{A6}$$

$$\langle\phi|\{W,T\}|\phi\rangle_c = 0 \ , \tag{A7}$$

$$\begin{aligned} & \langle\phi|\{W,\{W,T\}\}|\phi\rangle_c/(4Nt) \\ & \quad = -N^{-1}\sum_i P_{i,i+1}[P_{ii+1}^2 + k_F/\pi - (k_F/\pi)^2] \ , \end{aligned} \tag{A8}$$

$$\langle\phi|W^2|\phi\rangle/(4Nt) = (k_F/\pi)^2[1 - (4k_F)/(3\pi)] \ . \tag{A9}$$

Inserting Eqs. (A4) to (A9) into Eq. (A1) and minimalizing with respect to η we find,

$$\frac{E_{\min}}{(4Nt)} = -\pi^{-1}\sin k_F[1 - uk_F^2/(\pi\sin k_F) + u^2\gamma(k_F)] \ , \tag{A10}$$

where $\gamma(k_F)$ is defined by Eq. (11). From Eq. (A10), Eq. (10) is easily derived.

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